Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 12:00 AM EST

PDB ID	:	3OEV
Title	:	Structure of yeast 20S open-gate proteasome with Compound 25
Authors	:	Sintchak, M.D.
Deposited on	:	2010-08-13
Resolution	:	2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

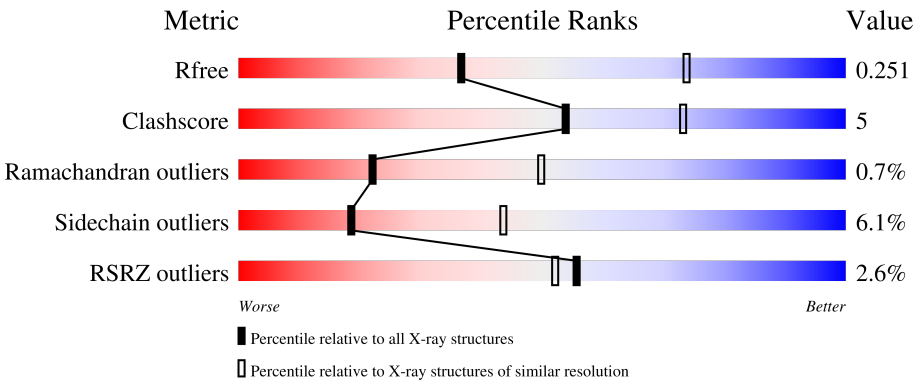
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	2%, 87%, 11%, •
1	O	250	2%, 84%, 14%, •
2	B	235	3%, 81%, 18%, •
2	P	235	2%, 80%, 17%, •
3	C	241	10%, 85%, 13%, •

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Mol	Chain	Length	Quality of chain
3	Q	241	15% 81% 17%
4	D	260	5% 79% 13% 7%
4	R	260	4% 75% 17% 7%
5	E	233	2% 82% 17%
5	S	233	8% 78% 18%
6	F	242	2% 84% 10%
6	T	242	2% 80% 17%
7	G	243	% 81% 16%
7	U	243	% 84% 16%
8	H	222	87% 13%
8	V	222	85% 14%
9	I	204	88% 11%
9	W	204	% 87% 11%
10	J	198	3% 81% 16%
10	X	198	4% 81% 16%
11	K	212	% 86% 11%
11	Y	212	% 85% 13%
12	L	222	88% 10%
12	Z	222	84% 14%
13	1	233	% 84% 14%
13	M	233	85% 12%
14	2	196	85% 14%
14	N	196	85% 14%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 49398 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	1915	1219	315	377	4	0	0	0
1	O	250	1915	1219	315	377	4	0	0	0

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	235	1829	1158	303	365	3	0	0	0
2	P	235	1829	1158	303	365	3	0	0	0

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	241	1891	1181	331	375	4	0	0	0
3	Q	241	1891	1181	331	375	4	0	0	0

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	242	1861	1162	314	378	7	0	0	0
4	R	242	1861	1162	314	378	7	0	0	0

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	233	1795	1129	312	350	4	0	0	0
5	S	233	1788	1123	312	349	4	0	0	0

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	237	1848	1175	323	346	4	0	0	0
6	T	237	1848	1175	323	346	4	0	0	0

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	243	1921	1221	322	370	8	0	0	0
7	U	243	1921	1221	322	370	8	0	0	0

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	222	1685	1061	293	324	7	0	0	0
8	V	222	1685	1061	293	324	7	0	0	0

- Molecule 9 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	204	1581	1010	258	305	8	0	0	0
9	W	204	1581	1010	258	305	8	0	0	0

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	198	1582	1003	269	305	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	X	197	1577	1000	268	304	5	0	0	0

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	212	1644	1045	280	312	7	0	0	0
11	Y	212	1644	1045	280	312	7	0	0	0

- Molecule 12 is a protein called Proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	222	1757	1115	303	335	4	0	0	0
12	Z	222	1757	1115	303	335	4	0	0	0

- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	233	1824	1154	312	351	7	0	0	0
13	1	233	1824	1154	312	351	7	0	0	0

- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	196	1512	955	250	300	7	0	0	0
14	2	196	1512	955	250	300	7	0	0	0

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
15	F	2	2	2	0	0
15	G	1	1	1	0	0

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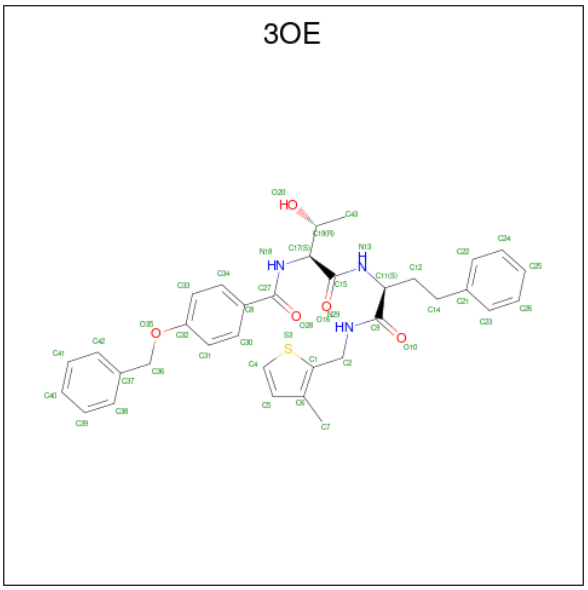
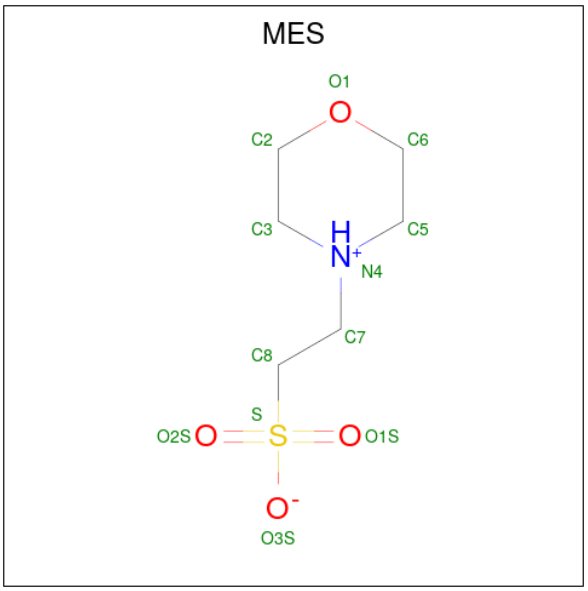
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
15	H	1	1	1	0	0
			Total	Mg		
15	I	2	2	2	0	0
			Total	Mg		
15	K	1	1	1	0	0
			Total	Mg		
15	L	2	2	2	0	0
			Total	Mg		
15	N	1	1	1	0	0

- Molecule 16 is 4-(benzyloxy)-N-[(2S,3R)-3-hydroxy-1-{[(2S)-1-{[(3-methylthiophen-2-yl)methyl]amino}-1-oxo-4-phenylbutan-2-yl]amino}-1-oxobutan-2-yl]benzamide (three-letter code: 3OE) (formula: $C_{34}H_{37}N_3O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
16	K	1	43	34	3	5	1	0	0
			Total	C	N	O	S		
16	Y	1	43	34	3	5	1	0	0

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



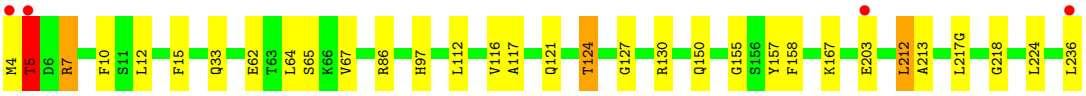
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
17	K	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
17	Y	1	12	6	1	4	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

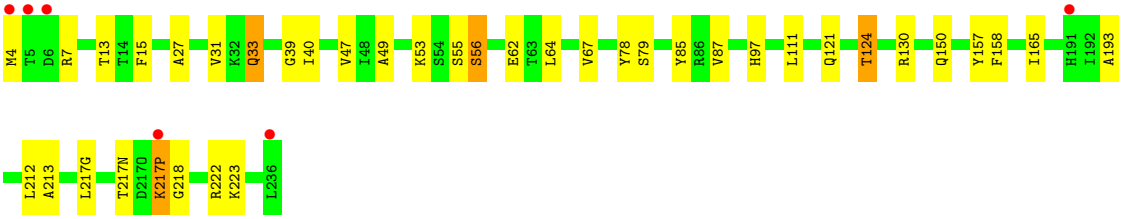
• Molecule 1: Proteasome component Y7

Chain A:



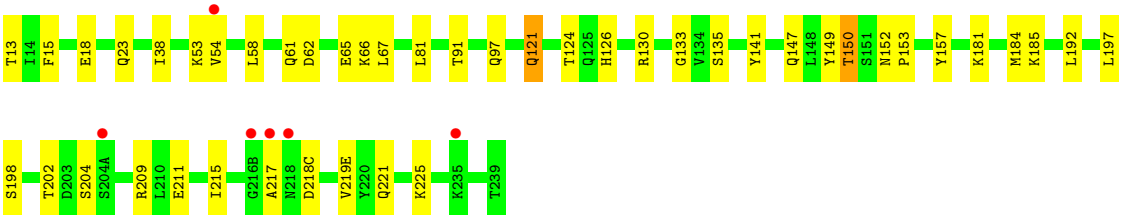
• Molecule 1: Proteasome component Y7

Chain O:



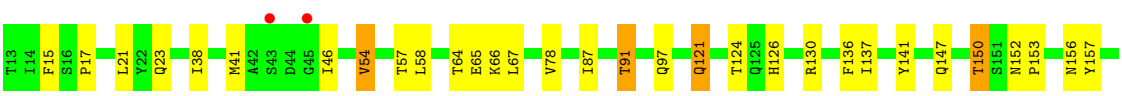
• Molecule 2: Proteasome component Y13

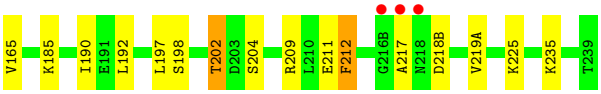
Chain B:



• Molecule 2: Proteasome component Y13

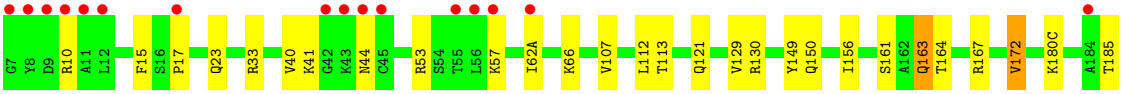
Chain P:

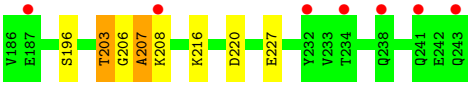




- Molecule 3: Proteasome component PRE6

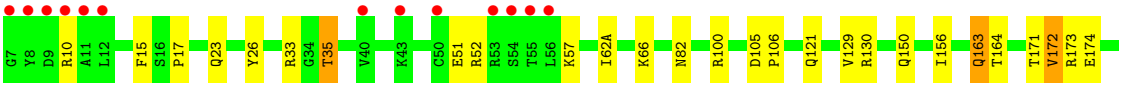
Chain C:

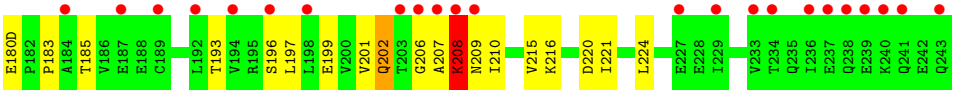




- Molecule 3: Proteasome component PRE6

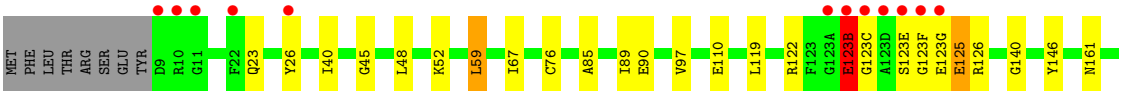
Chain Q:

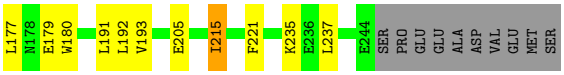




- Molecule 4: Proteasome component PUP2

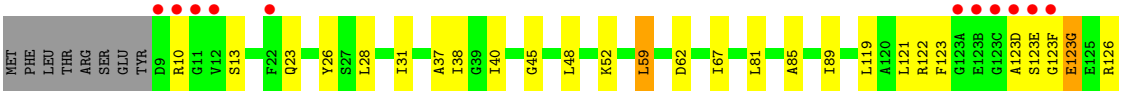
Chain D:

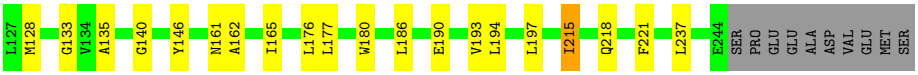




- Molecule 4: Proteasome component PUP2

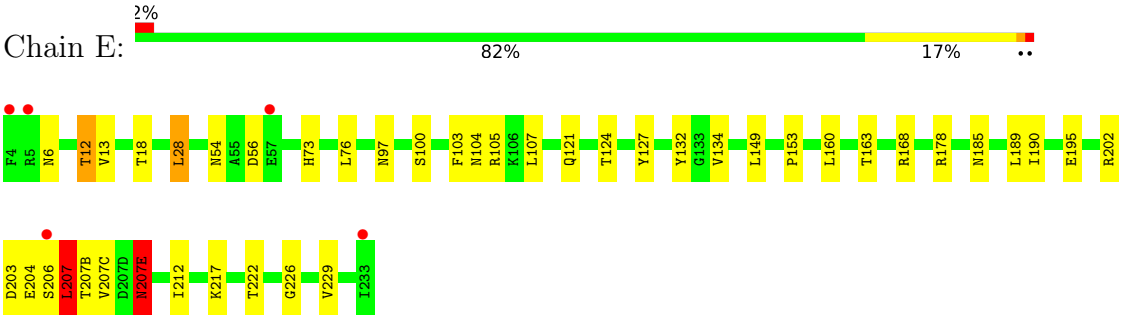
Chain R:





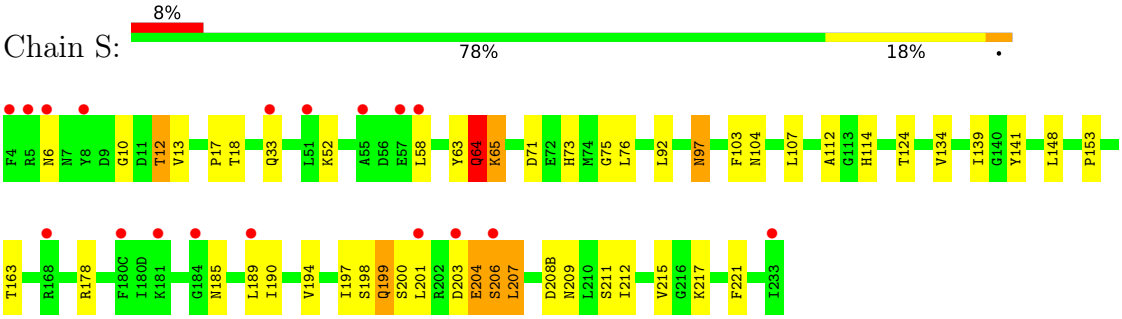
- Molecule 5: Proteasome component PRE5

Chain E:



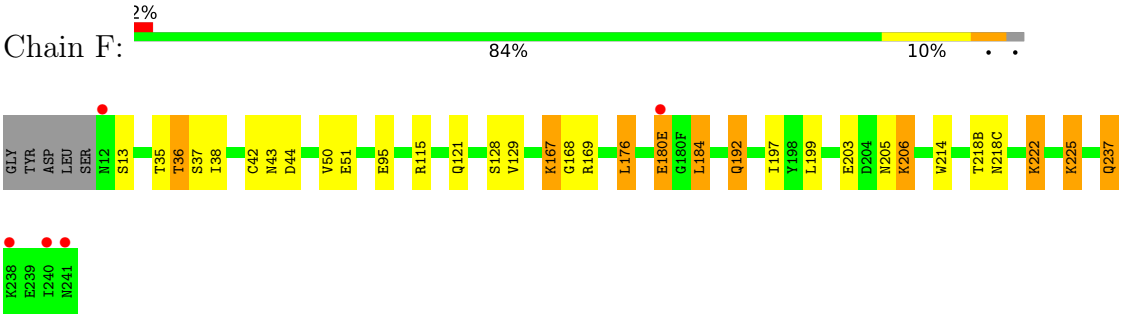
- Molecule 5: Proteasome component PRE5

Chain S:



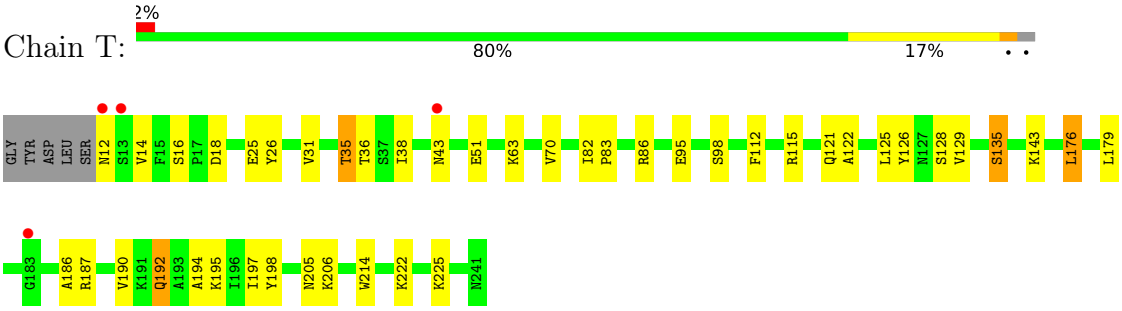
- Molecule 6: Proteasome component C1

Chain F:



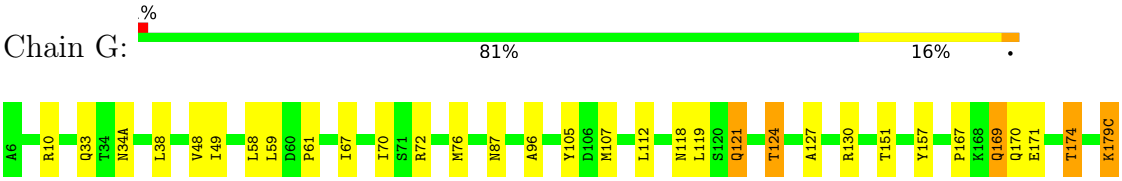
- Molecule 6: Proteasome component C1

Chain T:



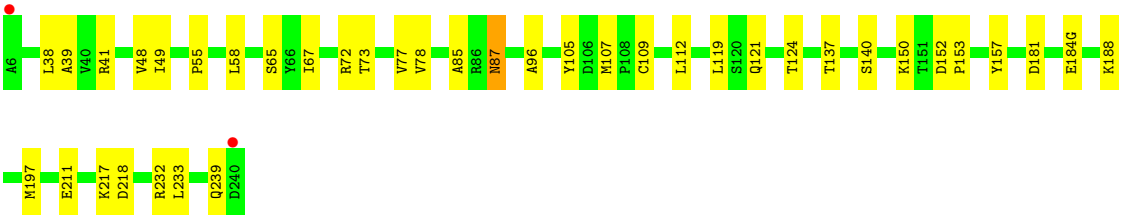
- Molecule 7: Proteasome component C7-alpha

Chain G:



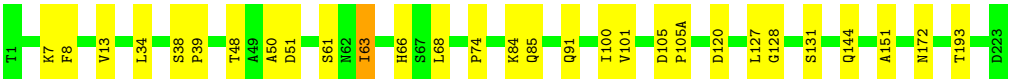
• Molecule 7: Proteasome component C7-alpha

Chain U:



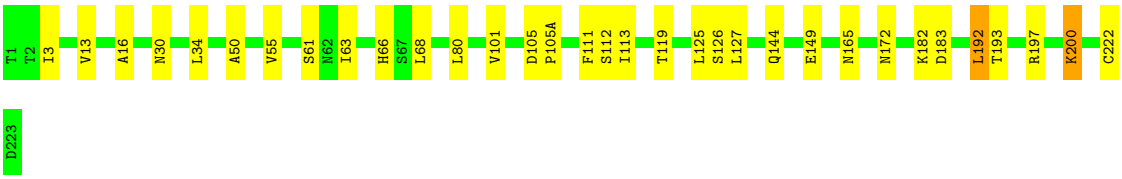
• Molecule 8: Proteasome component PUP1

Chain H:



• Molecule 8: Proteasome component PUP1

Chain V:



• Molecule 9: Proteasome component PUP3

Chain I:

• Molecule 9: Proteasome component PUP3

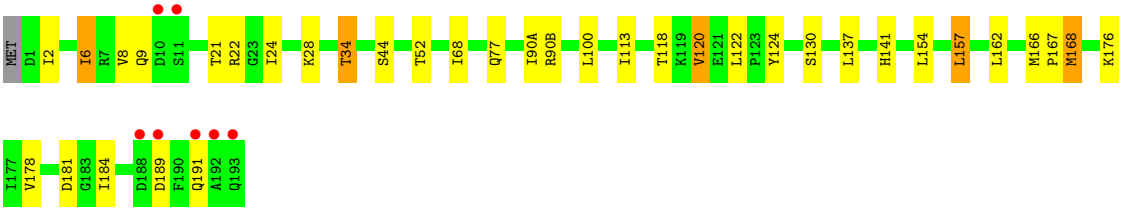
Chain W:

• Molecule 10: Proteasome component C11

Chain J:

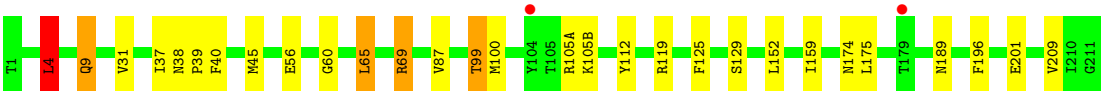
- Molecule 10: Proteasome component C11

Chain X:



- Molecule 11: Proteasome component PRE2

Chain K:

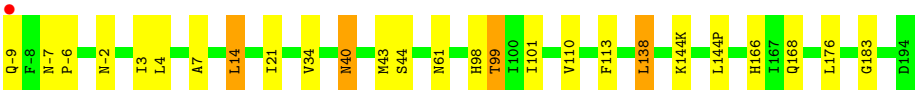


- Molecule 11: Proteasome component PRE2

Chain Y:

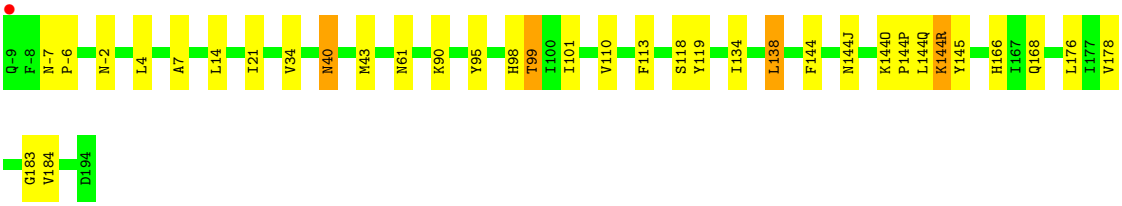
- Molecule 12: Proteasome component C5

Chain L:



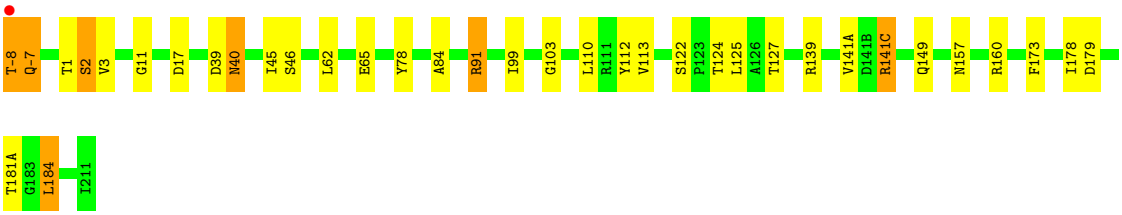
- Molecule 12: Proteasome component C5

Chain Z:



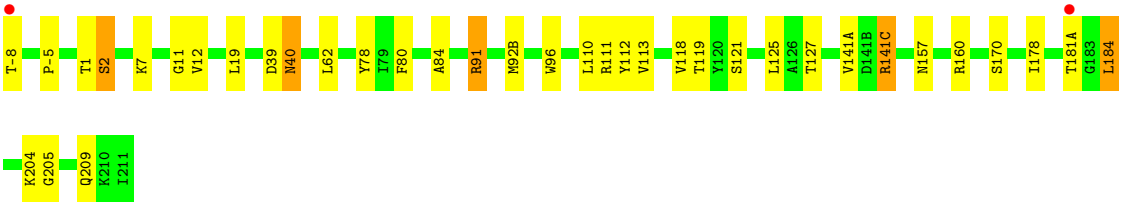
• Molecule 13: Proteasome component PRE4

Chain M:



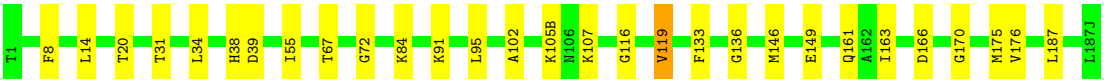
• Molecule 13: Proteasome component PRE4

Chain 1:



• Molecule 14: Proteasome component PRE3

Chain N:



• Molecule 14: Proteasome component PRE3

Chain 2:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.07Å 299.95Å 145.62Å 90.00° 113.17° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 49.00 – 2.84	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.85) 98.3 (49.00-2.84)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.257 0.215 , 0.251	Depositor DCC
R_{free} test set	4967 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	55.9	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 22.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	49398	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MES, 3OE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.39	0/1952	0.55	0/2642
1	O	0.42	0/1952	0.56	0/2642
2	B	0.38	0/1858	0.55	0/2516
2	P	0.39	0/1858	0.55	0/2516
3	C	0.39	0/1920	0.55	0/2598
3	Q	0.45	1/1920 (0.1%)	0.56	0/2598
4	D	0.39	0/1886	0.57	1/2541 (0.0%)
4	R	0.43	0/1886	0.88	4/2541 (0.2%)
5	E	0.50	1/1823 (0.1%)	0.77	3/2463 (0.1%)
5	S	0.44	1/1815 (0.1%)	0.55	0/2452
6	F	0.40	0/1887	0.53	0/2546
6	T	0.41	0/1887	0.55	0/2546
7	G	0.41	0/1959	0.55	0/2652
7	U	0.41	0/1959	0.55	0/2652
8	H	0.41	0/1716	0.55	0/2326
8	V	0.46	0/1716	0.55	0/2326
9	I	0.50	0/1611	0.56	0/2174
9	W	0.49	0/1611	0.56	0/2174
10	J	0.41	0/1610	0.57	0/2170
10	X	0.39	0/1605	0.56	0/2163
11	K	0.40	0/1681	0.56	1/2274 (0.0%)
11	Y	0.39	0/1681	0.57	1/2274 (0.0%)
12	L	0.44	0/1795	0.56	0/2420
12	Z	0.44	0/1795	0.57	0/2420
13	1	0.45	0/1855	0.61	0/2514
13	M	0.44	0/1855	0.61	0/2514
14	2	0.51	0/1541	0.55	0/2087
14	N	0.50	0/1541	0.54	0/2087
All	All	0.43	3/50175 (0.0%)	0.58	10/67828 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	1
4	R	0	1
5	E	0	2
5	S	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	207	LEU	CA-C	-10.54	1.25	1.52
3	Q	180(D)	GLU	C-O	6.35	1.35	1.23
5	S	206	SER	CA-CB	5.61	1.61	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	123(G)	GLU	CA-C-N	-21.19	70.59	117.20
4	R	123(G)	GLU	O-C-N	-18.41	93.24	122.70
4	R	123(G)	GLU	CA-C-O	17.94	157.78	120.10
5	E	207(E)	ASN	CA-C-N	-16.08	81.83	117.20
5	E	207(E)	ASN	O-C-N	-15.68	97.62	122.70
5	E	207(E)	ASN	CA-C-O	13.45	148.34	120.10
4	R	59	LEU	CA-CB-CG	5.65	128.29	115.30
11	Y	4	LEU	CA-CB-CG	5.62	128.21	115.30
4	D	59	LEU	CA-CB-CG	5.38	127.67	115.30
11	K	4	LEU	CA-CB-CG	5.17	127.19	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	204	GLU	Peptide
5	E	207(E)	ASN	Mainchain
1	O	217(N)	THR	Peptide
4	R	123(G)	GLU	Mainchain
5	S	204	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	23	0
1	O	1915	0	1926	25	0
2	B	1829	0	1829	23	0
2	P	1829	0	1829	28	0
3	C	1891	0	1900	28	0
3	Q	1891	0	1900	29	0
4	D	1861	0	1836	15	0
4	R	1861	0	1835	21	0
5	E	1795	0	1797	24	0
5	S	1788	0	1790	27	0
6	F	1848	0	1844	20	0
6	T	1848	0	1844	27	0
7	G	1921	0	1910	28	0
7	U	1921	0	1910	28	0
8	H	1685	0	1688	12	0
8	V	1685	0	1688	17	0
9	I	1581	0	1574	17	0
9	W	1581	0	1574	14	0
10	J	1582	0	1583	18	0
10	X	1577	0	1581	18	0
11	K	1644	0	1595	16	0
11	Y	1644	0	1595	14	0
12	L	1757	0	1711	16	0
12	Z	1757	0	1711	27	0
13	1	1824	0	1832	24	0
13	M	1824	0	1832	25	0
14	2	1512	0	1481	14	0
14	N	1512	0	1481	18	0
15	F	2	0	0	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	2	0	0	0	0
15	N	1	0	0	0	0
16	K	43	0	37	2	0
16	Y	43	0	37	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	K	12	0	13	1	0
17	Y	12	0	13	0	0
All	All	49398	0	49102	519	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (519) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:52:LYS:HB3	5:S:63:TYR:O	1.35	1.24
3:C:203:THR:HG22	3:C:206:GLY:N	1.65	1.06
12:Z:144(P):PRO:O	12:Z:144(R):LYS:HG2	1.53	1.05
1:O:7:ARG:HG3	6:T:128:SER:HB3	1.38	1.03
7:U:96:ALA:HA	7:U:107:MET:HE2	1.42	1.01
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.24	1.00
5:E:207:LEU:HD23	5:E:207:LEU:H	1.30	0.96
3:C:203:THR:HG22	3:C:206:GLY:H	1.24	0.94
3:C:163:GLN:HE21	3:C:164:THR:H	1.11	0.94
4:D:123(C):GLY:HA2	4:D:125:GLU:HA	1.49	0.93
12:Z:144(O):LYS:HG3	12:Z:144(R):LYS:HZ3	1.34	0.90
13:1:1:THR:HG23	13:1:2:SER:N	1.83	0.90
5:S:52:LYS:CB	5:S:63:TYR:O	2.22	0.88
13:1:1:THR:HG23	13:1:2:SER:H	1.40	0.87
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.87	0.86
3:C:163:GLN:NE2	3:C:164:THR:H	1.72	0.86
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.40	0.86
3:C:203:THR:HG22	3:C:207:ALA:H	1.39	0.85
6:F:167:LYS:HD3	6:F:205:ASN:HD21	1.41	0.85
12:Z:144(O):LYS:HG3	12:Z:144(R):LYS:NZ	1.91	0.84
6:F:35:THR:HG21	6:F:51:GLU:O	1.79	0.83
5:E:207:LEU:HA	5:E:207(E):ASN:HD22	1.44	0.83
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.61	0.82
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.60	0.81
13:M:40:ASN:H	13:M:40:ASN:HD22	1.24	0.81
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.26	0.80
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.95	0.80
9:I:181:LYS:H	9:I:181:LYS:HD2	1.47	0.79
3:C:15:PHE:H	4:D:23:GLN:HE22	1.29	0.79
5:E:207(B):THR:H	5:E:207(E):ASN:HD22	1.30	0.77
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:96:ALA:HA	7:G:107:MET:HE2	1.65	0.77
14:N:34:LEU:HD13	14:N:176:VAL:HG23	1.67	0.77
3:C:163:GLN:HE21	3:C:164:THR:N	1.83	0.76
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.32	0.76
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.51	0.76
2:B:15:PHE:H	3:C:23:GLN:HE22	1.32	0.76
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.67	0.75
13:M:141(C):ARG:HG3	13:M:141(C):ARG:HH11	1.51	0.75
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.68	0.74
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.69	0.74
3:C:206:GLY:O	3:C:207:ALA:O	2.05	0.74
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.54	0.72
5:E:73:HIS:HE1	5:E:107:LEU:O	1.72	0.71
5:E:207:LEU:HD23	5:E:207:LEU:N	2.05	0.71
12:L:166:HIS:HD2	12:L:168:GLN:H	1.37	0.70
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.55	0.70
7:G:238:GLU:O	7:G:239:GLN:HB3	1.91	0.69
11:K:31:VAL:HG11	16:K:213:3OE:S3	2.32	0.69
3:C:203:THR:CG2	3:C:206:GLY:N	2.40	0.69
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.57	0.69
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.57	0.68
9:I:10:ASP:HB3	9:I:181:LYS:HE2	1.74	0.68
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.06	0.68
5:E:132:TYR:O	5:E:153:PRO:HB3	1.94	0.67
5:S:73:HIS:HE1	5:S:107:LEU:O	1.77	0.67
14:N:67:THR:HA	14:N:72:GLY:O	1.93	0.67
5:E:207:LEU:HA	5:E:207(E):ASN:ND2	2.10	0.67
12:Z:144(O):LYS:HE3	12:Z:144(R):LYS:HD2	1.76	0.67
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.77	0.67
1:O:217(G):LEU:HD13	1:O:218:GLY:HA2	1.77	0.67
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.60	0.67
10:J:2:ILE:HB	10:J:17:SER:HB3	1.77	0.66
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.77	0.66
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.44	0.66
1:A:15:PHE:H	2:B:23:GLN:HE22	1.44	0.65
11:Y:196:PHE:HZ	11:Y:209:VAL:HG21	1.61	0.65
3:C:203:THR:CG2	3:C:206:GLY:H	1.94	0.65
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.61	0.65
9:W:110:ILE:HD12	9:W:125:ILE:HG12	1.79	0.64
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.45	0.64
2:B:181:LYS:O	2:B:184:MET:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:40:ASN:HD22	13:M:40:ASN:N	1.93	0.64
13:1:111:ARG:HH11	13:1:121:SER:HB2	1.62	0.64
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.62	0.64
3:Q:163:GLN:HE21	3:Q:163:GLN:HA	1.63	0.64
3:Q:52:ARG:HB2	3:Q:209:ASN:HD22	1.62	0.64
3:Q:171:THR:O	3:Q:174:GLU:HB3	1.98	0.63
2:P:156:ASN:OD1	3:Q:82:ASN:HB2	1.99	0.63
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.81	0.63
5:S:134:VAL:O	5:S:153:PRO:HG3	1.99	0.63
14:2:88:TYR:O	14:2:91:LYS:HG2	1.99	0.62
2:P:121:GLN:O	2:P:124:THR:HB	1.99	0.62
10:J:12:VAL:HG23	10:J:108:PRO:HB2	1.81	0.62
13:M:1:THR:HG23	13:M:2:SER:N	2.13	0.62
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.80	0.62
6:T:179:LEU:HD11	6:T:192:GLN:HG2	1.81	0.62
3:Q:100:ARG:NH1	3:Q:106:PRO:HG3	2.14	0.61
12:Z:144(P):PRO:CD	12:Z:144(R):LYS:HZ1	2.13	0.61
1:O:121:GLN:O	1:O:124:THR:HB	2.00	0.61
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.83	0.61
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.31	0.61
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.66	0.61
1:O:15:PHE:H	2:P:23:GLN:HE22	1.48	0.60
8:H:128:GLY:O	8:H:131:SER:HB2	2.01	0.60
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.14	0.60
4:R:123(D):ALA:HB3	4:R:126:ARG:HG3	1.83	0.60
1:A:7:ARG:HD2	5:E:127:TYR:HD2	1.67	0.60
1:O:7:ARG:HG3	6:T:128:SER:CB	2.23	0.60
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.65	0.60
7:U:121:GLN:O	7:U:124:THR:HB	2.02	0.60
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.84	0.59
7:U:184(G):GLU:HG2	7:U:188:LYS:CB	2.32	0.59
12:Z:144(P):PRO:HD2	12:Z:144(R):LYS:HZ1	1.67	0.59
7:U:96:ALA:CA	7:U:107:MET:HE2	2.25	0.59
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.84	0.59
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.15	0.59
6:T:192:GLN:HE21	6:T:192:GLN:HA	1.68	0.59
7:U:184(G):GLU:HG2	7:U:188:LYS:HB2	1.85	0.59
4:R:10:ARG:HD2	5:S:10:GLY:HA2	1.84	0.59
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.67	0.59
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.03	0.59
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:121:GLN:O	7:G:124:THR:HB	2.03	0.58
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.50	0.58
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.85	0.58
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.85	0.58
12:L:43:MET:HG3	12:L:101:ILE:HG22	1.85	0.58
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.08	0.58
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.85	0.58
2:B:13:THR:O	3:C:130:ARG:HD3	2.03	0.58
4:R:215:ILE:HG22	4:R:221:PHE:HD2	1.69	0.57
6:T:12:ASN:C	6:T:14:VAL:H	2.07	0.57
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.35	0.57
6:F:35:THR:CG2	6:F:51:GLU:O	2.52	0.57
6:T:176:LEU:HB3	7:U:58:LEU:HD21	1.87	0.57
3:C:53:ARG:HG3	3:C:167:ARG:HH12	1.70	0.56
1:O:55:SER:O	1:O:56:SER:HB3	2.04	0.56
4:R:38:ILE:HD12	4:R:197:LEU:HG	1.86	0.56
8:H:50:ALA:HB2	9:I:118:CYS:HB2	1.86	0.56
13:M:39:ASP:HA	13:M:184:LEU:HD12	1.87	0.56
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.87	0.56
6:F:218(B):THR:HB	6:F:222:LYS:HE3	1.88	0.56
3:Q:100:ARG:HH11	3:Q:106:PRO:HG3	1.70	0.56
8:V:3:ILE:HG22	8:V:16:ALA:HB2	1.87	0.56
10:X:28:LYS:HE3	11:Y:121:LYS:O	2.06	0.55
5:E:207:LEU:N	5:E:207:LEU:CD2	2.69	0.55
6:T:186:ALA:O	6:T:190:VAL:HG23	2.06	0.55
1:A:97:HIS:HD2	8:H:61:SER:OG	1.90	0.55
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.89	0.55
5:S:12:THR:HG21	5:S:124:THR:HA	1.89	0.55
5:E:12:THR:HG21	5:E:124:THR:HA	1.89	0.55
8:H:105:ASP:HB2	8:H:105(A):PRO:HD2	1.90	0.54
3:C:203:THR:CG2	3:C:207:ALA:H	2.16	0.54
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.90	0.54
2:P:141:TYR:CD1	2:P:219(A):VAL:HG21	2.43	0.54
2:P:38:ILE:HD12	2:P:197:LEU:HG	1.89	0.54
13:1:40:ASN:H	13:1:40:ASN:HD22	1.55	0.54
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.90	0.53
4:D:123(B):GLU:N	4:D:126:ARG:HB2	2.23	0.53
2:P:54:VAL:HA	2:P:209:ARG:HH12	1.73	0.53
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.90	0.53
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.90	0.53
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.23	0.53
1:O:49:ALA:HB2	1:O:212:LEU:HG	1.91	0.53
13:1:7:LYS:HB3	13:1:12:VAL:HG12	1.91	0.53
6:F:203:GLU:O	6:F:206:LYS:HG3	2.08	0.53
10:X:2:ILE:HG12	10:X:130:SER:HB3	1.91	0.53
14:2:34:LEU:HD13	14:2:176:VAL:HG23	1.90	0.53
6:T:16:SER:OG	6:T:18:ASP:OD1	2.23	0.53
8:V:197:ARG:NH1	8:V:200:LYS:HD3	2.23	0.53
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.57	0.52
12:L:-2:ASN:HA	12:L:21:ILE:O	2.09	0.52
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.90	0.52
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.92	0.52
10:J:2:ILE:HD12	10:J:162:LEU:HD13	1.91	0.52
9:W:12:VAL:HG13	9:W:108:PRO:HB3	1.91	0.52
10:X:6:ILE:HD12	10:X:124:TYR:HB3	1.92	0.52
4:D:90:GLU:OE2	11:K:69:ARG:NH1	2.42	0.52
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.92	0.52
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.40	0.52
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.92	0.52
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.92	0.52
10:X:113:ILE:HA	10:X:118:THR:O	2.10	0.52
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.45	0.51
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.75	0.51
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.75	0.51
2:B:121:GLN:O	2:B:124:THR:HB	2.11	0.51
13:M:40:ASN:H	13:M:40:ASN:ND2	2.02	0.51
5:S:190:ILE:HG23	5:S:212:ILE:HG21	1.93	0.51
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.26	0.51
4:R:140:GLY:HA2	4:R:215:ILE:HG12	1.93	0.51
7:U:107:MET:CE	7:U:112:LEU:HD13	2.40	0.51
12:Z:178:VAL:HG22	12:Z:184:VAL:HG22	1.92	0.51
13:1:141(C):ARG:HG3	13:1:141(C):ARG:HH11	1.76	0.51
7:G:215:ALA:HB2	7:G:221:PHE:HD2	1.76	0.51
3:C:203:THR:HG22	3:C:207:ALA:N	2.18	0.51
5:E:168:ARG:HD3	5:E:202:ARG:HE	1.76	0.51
6:T:122:ALA:HA	6:T:125:LEU:HD12	1.92	0.51
14:2:13:ILE:HG12	14:2:177:VAL:HG13	1.92	0.51
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.93	0.50
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.46	0.50
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.26	0.50
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.38	0.50
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.10	0.50
6:F:237:GLN:HE21	6:F:237:GLN:HA	1.76	0.50
7:G:238:GLU:O	7:G:239:GLN:CB	2.59	0.50
3:C:15:PHE:N	4:D:23:GLN:HE22	2.04	0.50
3:Q:215:VAL:HG12	3:Q:221:ILE:HG12	1.93	0.50
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.40	0.50
8:V:126:SER:O	8:V:127:LEU:HD23	2.11	0.50
11:Y:104:TYR:CD1	11:Y:180:GLU:HA	2.46	0.50
8:V:172:ASN:HB3	8:V:192:LEU:O	2.10	0.50
1:A:7:ARG:HG2	6:F:128:SER:HB3	1.94	0.50
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.93	0.50
11:Y:174:ASN:ND2	11:Y:186:TYR:OH	2.44	0.50
14:N:133:PHE:HE2	14:N:166:ASP:HB2	1.76	0.50
11:K:196:PHE:HZ	11:K:209:VAL:HG21	1.76	0.49
11:Y:31:VAL:HG11	16:Y:212:3OE:S3	2.52	0.49
2:P:78:VAL:HG22	2:P:136:PHE:CE2	2.47	0.49
13:M:45:ILE:HG12	13:M:99:ILE:HG12	1.93	0.49
14:N:149:GLU:CD	14:N:149:GLU:H	2.15	0.49
6:T:38:ILE:HG12	6:T:197:ILE:HD11	1.94	0.49
6:T:126:TYR:HB2	6:T:129:VAL:HG22	1.93	0.49
4:R:123(D):ALA:C	4:R:123(F):GLY:H	2.16	0.49
5:S:63:TYR:O	5:S:64:GLN:O	2.30	0.49
5:E:226:GLY:O	5:E:229:VAL:HG22	2.13	0.49
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.95	0.49
13:M:40:ASN:N	13:M:40:ASN:ND2	2.61	0.49
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.60	0.49
4:D:85:ALA:O	4:D:89:ILE:HG12	2.13	0.49
9:W:51:ASP:OD2	10:X:90(B):ARG:NH2	2.46	0.49
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.13	0.49
10:J:36:GLN:HG3	10:J:184:ILE:CD1	2.43	0.49
11:K:38:ASN:O	11:K:40:PHE:N	2.46	0.49
4:R:81:LEU:HD12	4:R:133:GLY:HA3	1.94	0.49
5:S:198:SER:HA	5:S:201:LEU:HD12	1.95	0.49
1:O:13:THR:O	2:P:130:ARG:HD3	2.13	0.48
7:U:87:ASN:C	7:U:87:ASN:HD22	2.16	0.48
13:1:11:GLY:HA3	13:1:178:ILE:O	2.13	0.48
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	2.11	0.48
12:Z:40:ASN:ND2	12:Z:183:GLY:HA2	2.27	0.48
6:T:35:THR:HG21	6:T:51:GLU:O	2.13	0.48
8:V:105:ASP:HB2	8:V:105(A):PRO:CD	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:4:LEU:HD13	11:K:159:ILE:HD11	1.96	0.48
1:A:12:LEU:HD11	7:G:127:ALA:HB2	1.94	0.48
14:2:156:LYS:HG2	14:2:187(J):LEU:HD11	1.94	0.48
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.96	0.48
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.96	0.48
5:E:100:SER:O	5:E:104:ASN:HA	2.14	0.48
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.96	0.48
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.42	0.47
2:B:204:SER:OG	2:B:209:ARG:NH2	2.48	0.47
5:S:139:ILE:HD12	5:S:215:VAL:HG12	1.94	0.47
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.49	0.47
2:P:97:GLN:HB3	9:W:61:TYR:CD2	2.49	0.47
4:R:121:LEU:O	4:R:123:PHE:N	2.43	0.47
5:S:194:VAL:O	5:S:197:ILE:HG22	2.14	0.47
5:S:198:SER:C	5:S:200:SER:H	2.17	0.47
1:A:217(G):LEU:HD13	1:A:218:GLY:HA2	1.95	0.47
6:T:179:LEU:HD21	6:T:192:GLN:HG2	1.96	0.47
8:H:100:ILE:HG13	8:H:127:LEU:HD12	1.97	0.47
6:F:42:CYS:HB2	6:F:184:LEU:O	2.14	0.47
5:S:148:LEU:HD21	5:S:163:THR:HG22	1.96	0.47
6:F:36:THR:HB	6:F:168:GLY:H	1.80	0.47
10:J:167:PRO:HB3	10:X:21:THR:HG21	1.96	0.47
11:K:129:SER:HB3	17:K:214:MES:H72	1.95	0.47
2:P:78:VAL:HG22	2:P:136:PHE:HE2	1.79	0.47
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.15	0.47
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.30	0.47
3:Q:33:ARG:NH1	3:Q:33:ARG:HB2	2.30	0.47
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.96	0.47
7:U:73:THR:HG22	7:U:218:ASP:HA	1.96	0.47
14:N:91:LYS:HE2	14:N:116:GLY:O	2.15	0.47
1:A:7:ARG:CG	6:F:128:SER:HB3	2.46	0.46
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.13	0.46
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.96	0.46
13:1:112:TYR:HE1	13:1:127:THR:HG22	1.80	0.46
7:G:96:ALA:CA	7:G:107:MET:HE2	2.39	0.46
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.44	0.46
1:O:150:GLN:O	1:O:157:TYR:HA	2.15	0.46
2:P:147:GLN:HG2	3:Q:62(A):ILE:HG21	1.97	0.46
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.98	0.46
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.63	0.46
7:U:184(G):GLU:HG2	7:U:188:LYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:45:MET:C	16:K:213:3OE:H7B	2.36	0.46
1:A:121:GLN:O	1:A:124:THR:HB	2.15	0.46
12:L:34:VAL:HG12	12:L:176:LEU:HD22	1.96	0.46
1:O:87:VAL:HG11	7:U:121:GLN:NE2	2.31	0.46
7:U:107:MET:HE1	7:U:112:LEU:HD13	1.97	0.46
4:D:179:GLU:HB3	4:D:192:LEU:HD21	1.98	0.46
5:E:160:LEU:HD13	5:E:163:THR:HB	1.98	0.46
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.97	0.46
4:D:140:GLY:HA2	4:D:215:ILE:HG12	1.97	0.46
6:F:13:SER:HB2	7:G:130:ARG:HB3	1.97	0.46
7:G:59:LEU:O	7:G:61:PRO:HD3	2.15	0.46
9:W:62:LYS:HD3	9:W:82:LEU:HD11	1.97	0.46
9:I:110:ILE:HD12	9:I:125:ILE:HG12	1.98	0.46
12:L:3:ILE:HG21	12:L:44:SER:OG	2.15	0.46
13:M:157:ASN:HD22	13:M:160:ARG:NH1	2.04	0.46
5:E:134:VAL:O	5:E:153:PRO:HG3	2.16	0.46
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.81	0.46
12:L:144(K):LYS:HD3	12:L:144(K):LYS:C	2.36	0.46
4:R:215:ILE:HG13	4:R:215:ILE:O	2.15	0.46
14:2:91:LYS:HE2	14:2:116:GLY:O	2.15	0.46
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.97	0.46
13:1:80:PHE:CZ	13:1:111:ARG:HG2	2.51	0.46
1:A:7:ARG:HD2	5:E:127:TYR:CD2	2.47	0.45
9:W:121:GLU:HA	9:W:121:GLU:OE2	2.16	0.45
6:F:38:ILE:HG12	6:F:197:ILE:HD11	1.98	0.45
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.98	0.45
11:Y:97:MET:HG2	11:Y:115:SER:HB3	1.97	0.45
10:J:113:ILE:HA	10:J:118:THR:O	2.15	0.45
3:Q:208:LYS:HD2	3:Q:208:LYS:O	2.15	0.45
9:I:33:LYS:O	9:I:44:GLY:HA2	2.17	0.45
9:W:33:LYS:O	9:W:44:GLY:HA2	2.17	0.45
10:X:141:HIS:CB	10:X:154:LEU:HD11	2.46	0.45
13:M:179:ASP:HB3	13:M:181(A):THR:HB	1.99	0.45
14:N:8:PHE:HB2	14:N:146:MET:O	2.16	0.45
14:N:38:HIS:O	14:N:39:ASP:C	2.55	0.45
1:O:97:HIS:HD2	8:V:61:SER:OG	1.99	0.45
2:P:67:LEU:HD22	2:P:211:GLU:HB3	1.98	0.45
11:Y:49:ALA:O	11:Y:53:GLN:HB2	2.17	0.45
12:Z:113:PHE:HA	12:Z:118:SER:O	2.17	0.45
1:A:112:LEU:O	1:A:116:VAL:HG23	2.16	0.45
1:A:150:GLN:O	1:A:157:TYR:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:192:GLN:HE21	6:F:192:GLN:HA	1.82	0.45
7:G:179(C):LYS:HE3	7:G:179(C):LYS:HA	1.98	0.45
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.82	0.45
13:M:-8:THR:O	13:M:-7:GLN:HB3	2.15	0.45
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.99	0.45
5:S:103:PHE:O	13:1:78:TYR:HA	2.16	0.45
4:R:162:ALA:HB1	4:R:176:LEU:HD22	1.99	0.45
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.99	0.45
10:X:2:ILE:HD13	10:X:162:LEU:HD13	1.98	0.45
13:1:113:VAL:HA	13:1:118:VAL:O	2.17	0.45
5:E:207(B):THR:H	5:E:207(E):ASN:ND2	2.06	0.45
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.99	0.45
2:P:41:MET:HG2	2:P:46:ILE:HG12	1.98	0.45
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.99	0.45
12:Z:144(P):PRO:O	12:Z:144(R):LYS:N	2.50	0.45
8:H:38:SER:HB2	8:H:39:PRO:HD2	1.98	0.45
11:K:152:LEU:HD22	11:K:175:LEU:HD13	1.99	0.45
7:U:77:VAL:CG1	7:U:137:THR:HB	2.47	0.45
13:1:39:ASP:HA	13:1:184:LEU:HD12	1.99	0.44
1:A:5:THR:HB	1:A:7:ARG:HH21	1.82	0.44
9:I:182:ASP:OD1	9:I:182:ASP:N	2.50	0.44
1:O:33:GLN:H	1:O:33:GLN:HG2	1.59	0.44
4:R:31:ILE:HD13	4:R:135:ALA:HB2	2.00	0.44
9:I:20:LEU:HB3	9:I:28:SER:HB3	1.99	0.44
10:J:24:ILE:HG12	10:J:24:ILE:O	2.17	0.44
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.99	0.44
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.99	0.44
3:C:113:THR:HG21	3:C:149:TYR:HB3	1.99	0.44
7:G:184(G):GLU:HG2	7:G:188:LYS:CB	2.48	0.44
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.98	0.44
5:S:207:LEU:HA	5:S:209:ASN:HD22	1.83	0.44
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.99	0.44
3:Q:206:GLY:HA2	3:Q:210:ILE:HD12	2.00	0.44
2:P:202:THR:HG22	2:P:204:SER:H	1.81	0.44
5:S:65:LYS:H	5:S:65:LYS:HG2	1.43	0.44
1:A:117:ALA:HB1	1:A:155:GLY:O	2.18	0.44
10:J:141:HIS:HB2	10:J:154:LEU:HD11	1.99	0.44
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.64	0.44
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.53	0.44
13:1:141(A):VAL:HG23	13:1:141(A):VAL:O	2.17	0.44
2:P:65:GLU:HG3	2:P:66:LYS:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:87:ASN:C	7:U:87:ASN:ND2	2.70	0.44
2:P:87:ILE:O	2:P:91:THR:HG23	2.18	0.43
3:Q:51:GLU:HA	3:Q:209:ASN:O	2.18	0.43
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.53	0.43
7:U:41:ARG:NH2	7:U:181:ASP:O	2.46	0.43
10:X:44:SER:OG	10:X:100:LEU:HB2	2.18	0.43
2:B:126:HIS:HB3	3:C:129:VAL:HG12	2.00	0.43
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.99	0.43
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.19	0.43
4:R:186:LEU:O	4:R:190:GLU:HG3	2.18	0.43
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.54	0.43
4:D:40:ILE:HD12	4:D:193:VAL:HG23	2.01	0.43
5:E:28:LEU:HD12	5:E:153:PRO:HD2	2.00	0.43
8:H:84:LYS:HG3	8:H:85:GLN:N	2.33	0.43
2:P:21:LEU:HD13	2:P:124:THR:HG23	2.01	0.43
13:1:112:TYR:O	13:1:119:THR:HA	2.19	0.43
5:S:17:PRO:HA	6:T:26:TYR:CD1	2.53	0.43
5:E:190:ILE:HG23	5:E:212:ILE:HG21	2.00	0.43
11:K:112:TYR:O	11:K:119:ARG:HA	2.19	0.43
13:M:122:SER:HB3	13:M:124:THR:O	2.18	0.43
1:O:39:GLY:HA2	1:O:47:VAL:O	2.19	0.43
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.66	0.43
7:U:150:LYS:O	7:U:157:TYR:HA	2.18	0.43
11:Y:87:VAL:CG1	11:Y:115:SER:HA	2.49	0.43
10:J:36:GLN:HG3	10:J:184:ILE:HD13	2.00	0.43
13:M:3:VAL:HG23	13:M:46:SER:HB3	2.01	0.43
1:O:40:ILE:HD12	1:O:193:ALA:HB2	2.01	0.43
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.54	0.43
8:V:182:LYS:HB3	8:V:183:ASP:H	1.70	0.43
13:1:157:ASN:HD22	13:1:160:ARG:NH1	2.15	0.43
5:S:71:ASP:HB3	5:S:73:HIS:CD2	2.54	0.43
9:I:87:LEU:HD11	9:I:99:PRO:HG2	2.01	0.43
3:Q:57:LYS:HD2	3:Q:57:LYS:HA	1.73	0.43
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.53	0.43
11:Y:152:LEU:HD23	11:Y:175:LEU:HD22	1.99	0.43
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	2.01	0.43
11:K:196:PHE:CZ	11:K:209:VAL:HG21	2.53	0.43
3:Q:163:GLN:NE2	3:Q:164:THR:H	2.16	0.43
6:T:192:GLN:HA	6:T:192:GLN:NE2	2.34	0.43
7:U:109:CYS:HB2	7:U:140:SER:OG	2.19	0.43
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:217(P):LYS:N	1:O:217(P):LYS:HE3	2.33	0.42
6:T:194:ALA:O	6:T:198:TYR:HD1	2.02	0.42
8:V:172:ASN:HD22	8:V:193:THR:HA	1.84	0.42
10:J:17:SER:HB2	10:J:170:PHE:HB2	2.00	0.42
2:P:17:PRO:HA	3:Q:26:TYR:CD1	2.53	0.42
8:V:113:ILE:HG12	8:V:119:THR:HG22	2.01	0.42
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.83	0.42
7:G:107:MET:CE	7:G:112:LEU:HD13	2.49	0.42
9:I:181:LYS:HD2	9:I:181:LYS:N	2.25	0.42
14:N:14:LEU:O	14:N:175:MET:HA	2.19	0.42
9:W:113:PHE:HA	9:W:118:CYS:O	2.19	0.42
13:1:205:GLY:HA3	13:1:209:GLN:HB3	2.01	0.42
9:I:51:ASP:OD2	10:J:90(B):ARG:NH2	2.53	0.42
1:O:27:ALA:O	1:O:31:VAL:HG23	2.18	0.42
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.30	0.42
7:U:78:VAL:HG11	7:U:85:ALA:HB2	2.02	0.42
10:X:90(A):ILE:HD12	10:X:90(A):ILE:HA	1.89	0.42
7:G:179(D):SER:C	7:G:180(A):ILE:H	2.23	0.42
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.00	0.42
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.54	0.42
8:H:172:ASN:HD22	8:H:193:THR:HA	1.83	0.42
13:M:11:GLY:HA3	13:M:178:ILE:O	2.19	0.42
9:W:87:LEU:HD11	9:W:99:PRO:HG2	2.00	0.42
11:Y:196:PHE:CZ	11:Y:209:VAL:HG21	2.49	0.42
12:Z:99:THR:HG23	12:Z:113:PHE:HB2	2.02	0.42
13:1:-8:THR:N	13:1:92(B):MET:O	2.53	0.42
1:A:10:PHE:O	1:A:127:GLY:HA2	2.19	0.42
7:G:151:THR:HG22	7:G:157:TYR:HB3	2.01	0.42
10:J:6:ILE:HD11	10:J:8:VAL:HG13	2.02	0.42
10:J:178:VAL:HG22	10:J:184:ILE:HG12	2.02	0.42
14:2:38:HIS:O	14:2:39:ASP:C	2.58	0.42
2:B:141:TYR:CD1	2:B:219(E):VAL:HG21	2.55	0.42
10:X:166:MET:HA	10:X:167:PRO:HD3	1.90	0.42
7:G:184(G):GLU:HG2	7:G:188:LYS:HB2	2.02	0.42
10:J:2:ILE:HD13	10:J:130:SER:HB3	2.02	0.42
10:J:9:GLN:HE21	10:J:9:GLN:HB3	1.67	0.42
6:T:35:THR:CG2	6:T:51:GLU:O	2.67	0.42
11:Y:22:ALA:O	11:Y:25:TRP:HB3	2.20	0.42
2:B:67:LEU:HD22	2:B:211:GLU:HB3	2.02	0.41
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.55	0.41
9:I:48:LEU:HG	9:I:50:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.15	0.41
1:O:67:VAL:HG11	1:O:213:ALA:HB3	2.01	0.41
5:S:52:LYS:HD2	5:S:63:TYR:O	2.20	0.41
6:T:12:ASN:C	6:T:14:VAL:N	2.73	0.41
4:D:122:ARG:HA	4:D:126:ARG:HD3	2.01	0.41
6:F:180(E):GLU:H	6:F:180(E):GLU:CD	2.23	0.41
9:I:101:VAL:O	9:I:110:ILE:HA	2.20	0.41
1:O:79:SER:HB2	1:O:165:ILE:HD12	2.01	0.41
8:V:101:VAL:HG13	8:V:111:PHE:HB2	2.02	0.41
10:X:178:VAL:HG22	10:X:184:ILE:HG12	2.02	0.41
3:C:163:GLN:HE21	3:C:163:GLN:HA	1.85	0.41
6:F:225:LYS:HD3	6:F:225:LYS:H	1.84	0.41
2:P:137:ILE:HD11	2:P:165:VAL:HG22	2.01	0.41
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.50	0.41
7:G:70:ILE:HD11	7:G:76:MET:HE2	2.01	0.41
11:K:100:MET:SD	11:K:125:PHE:HB2	2.60	0.41
13:M:103:GLY:HA2	13:M:178:ILE:HD13	2.02	0.41
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.20	0.41
14:N:84:LYS:HG3	14:N:119:VAL:HG22	2.01	0.41
8:V:172:ASN:ND2	8:V:193:THR:HA	2.35	0.41
9:W:181:LYS:H	9:W:181:LYS:HD2	1.86	0.41
1:A:212:LEU:HD22	1:A:224:LEU:HD12	2.02	0.41
2:B:81:LEU:HD23	2:B:133:GLY:HA3	2.02	0.41
5:E:103:PHE:O	13:M:78:TYR:HA	2.21	0.41
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.02	0.41
7:U:65:SER:HA	7:U:211:GLU:OE2	2.21	0.41
10:X:24:ILE:O	10:X:24:ILE:HG12	2.21	0.41
10:X:141:HIS:HB2	10:X:154:LEU:HD11	2.02	0.41
2:B:215:ILE:HG12	2:B:221:GLN:HG2	2.01	0.41
5:E:54:ASN:ND2	5:E:56:ASP:O	2.53	0.41
1:O:78:TYR:HB3	1:O:85:TYR:CD1	2.55	0.41
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.56	0.41
12:Z:144:PHE:CE2	12:Z:144(R):LYS:HG3	2.55	0.41
13:1:1:THR:CG2	13:1:2:SER:H	2.16	0.41
7:G:169:GLN:HE21	7:G:169:GLN:HB3	1.73	0.41
13:M:17:ASP:HA	13:M:173:PHE:CB	2.50	0.41
14:N:133:PHE:CE2	14:N:166:ASP:HB2	2.55	0.41
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.28	0.41
4:R:85:ALA:O	4:R:89:ILE:HG12	2.21	0.41
5:S:65:LYS:HB3	5:S:65:LYS:HE2	1.53	0.41
7:U:105:TYR:OH	8:V:66:HIS:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:20:LEU:HB3	9:W:28:SER:HB3	2.03	0.41
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.51	0.41
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.56	0.41
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.68	0.41
6:F:192:GLN:HA	6:F:192:GLN:NE2	2.36	0.41
10:J:168:MET:HA	10:X:168:MET:HA	2.03	0.41
13:M:141(A):VAL:HG23	13:M:141(A):VAL:O	2.20	0.41
4:R:37:ALA:HB3	4:R:165:ILE:HG13	2.03	0.41
5:S:114:HIS:HB3	6:T:86:ARG:NH2	2.36	0.41
6:T:31:VAL:HG11	6:T:135:SER:HB2	2.02	0.41
2:P:150:THR:O	2:P:157:TYR:HA	2.20	0.41
6:T:95:GLU:HG2	6:T:115:ARG:CB	2.44	0.41
9:W:48:LEU:HG	9:W:50:THR:HG22	2.03	0.41
2:B:150:THR:O	2:B:157:TYR:HA	2.21	0.40
12:Z:134:ILE:HG22	12:Z:138:LEU:HD22	2.02	0.40
3:C:41:LYS:HG2	3:C:161:SER:O	2.22	0.40
5:E:97:ASN:ND2	12:L:61:ASN:HD21	2.16	0.40
5:E:105:ARG:HG3	13:M:78:TYR:CZ	2.56	0.40
4:R:123:PHE:O	4:R:123:PHE:CD2	2.75	0.40
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.56	0.40
7:U:152:ASP:HB2	7:U:153:PRO:HD2	2.02	0.40
11:Y:104:TYR:CE1	11:Y:180:GLU:HA	2.57	0.40
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.31	0.40
3:C:53:ARG:HG3	3:C:167:ARG:NH1	2.36	0.40
6:F:176:LEU:HB3	7:G:58:LEU:HD21	2.02	0.40
9:I:99:PRO:HB2	9:I:113:PHE:HD2	1.87	0.40
11:K:56:GLU:OE2	11:K:99:THR:OG1	2.36	0.40
2:P:190:ILE:HG23	2:P:212:PHE:CE2	2.57	0.40
6:T:206:LYS:HB2	6:T:206:LYS:HE3	1.83	0.40
7:U:78:VAL:HG11	7:U:85:ALA:CB	2.52	0.40
10:X:137:LEU:HD21	10:X:157:LEU:HB3	2.04	0.40
7:G:67:ILE:HD12	7:G:211:GLU:HG2	2.03	0.40
8:H:48:THR:HB	8:H:51:ASP:HB2	2.02	0.40
9:I:55:LEU:HA	9:I:55:LEU:HD23	1.85	0.40
13:M:112:TYR:HE1	13:M:127:THR:HG22	1.87	0.40
10:X:120:VAL:HG13	10:X:122:LEU:HG	2.03	0.40
12:Z:43:MET:HG3	12:Z:101:ILE:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	238 (96%)	8 (3%)	2 (1%)	19	46
1	O	248/250 (99%)	236 (95%)	10 (4%)	2 (1%)	19	46
2	B	233/235 (99%)	223 (96%)	7 (3%)	3 (1%)	12	33
2	P	233/235 (99%)	219 (94%)	11 (5%)	3 (1%)	12	33
3	C	239/241 (99%)	231 (97%)	6 (2%)	2 (1%)	19	46
3	Q	239/241 (99%)	226 (95%)	9 (4%)	4 (2%)	9	27
4	D	240/260 (92%)	222 (92%)	14 (6%)	4 (2%)	9	27
4	R	240/260 (92%)	227 (95%)	11 (5%)	2 (1%)	19	46
5	E	231/233 (99%)	217 (94%)	10 (4%)	4 (2%)	9	27
5	S	231/233 (99%)	212 (92%)	14 (6%)	5 (2%)	6	21
6	F	235/242 (97%)	224 (95%)	10 (4%)	1 (0%)	34	62
6	T	235/242 (97%)	225 (96%)	10 (4%)	0	100	100
7	G	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	34	62
7	U	241/243 (99%)	234 (97%)	5 (2%)	2 (1%)	19	46
8	H	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	29	57
8	V	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
9	I	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
9	W	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
10	J	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	29	57
10	X	195/198 (98%)	184 (94%)	9 (5%)	2 (1%)	15	40
11	K	210/212 (99%)	204 (97%)	4 (2%)	2 (1%)	15	40
11	Y	210/212 (99%)	201 (96%)	7 (3%)	2 (1%)	15	40
12	L	220/222 (99%)	208 (94%)	12 (6%)	0	100	100
12	Z	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	29	57
13	1	231/233 (99%)	220 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	231/233 (99%)	220 (95%)	10 (4%)	1 (0%)	34	62
14	2	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	N	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
All	All	6279/6382 (98%)	5988 (95%)	246 (4%)	45 (1%)	22	50

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	217	ALA
3	C	203	THR
3	C	207	ALA
4	D	123(E)	SER
5	E	203	ASP
6	F	184	LEU
7	G	239	GLN
11	K	39	PRO
1	O	53	LYS
2	P	54	VAL
2	P	217	ALA
3	Q	202	GLN
5	S	64	GLN
5	S	203	ASP
5	S	206	SER
2	B	54	VAL
5	E	6	ASN
8	H	91	GLN
3	Q	207	ALA
5	S	199	GLN
1	A	5	THR
2	B	218(C)	ASP
4	D	123(B)	GLU
5	E	217	LYS
2	P	218(B)	ASP
4	R	123(E)	SER
4	R	128	MET
5	S	6	ASN
7	U	239	GLN
10	X	189	ASP
11	Y	39	PRO
12	Z	144(Q)	LEU
5	E	206	SER

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Mol	Chain	Res	Type
1	O	56	SER
3	Q	183	PRO
1	A	167	LYS
4	D	123(G)	GLU
11	K	9	GLN
3	Q	208	LYS
7	U	55	PRO
13	M	-7	GLN
11	Y	146	LEU
10	X	8	VAL
10	J	8	VAL
4	D	123(F)	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	197 (94%)	12 (6%)	20	47
1	O	209/209 (100%)	199 (95%)	10 (5%)	25	55
2	B	195/195 (100%)	181 (93%)	14 (7%)	14	35
2	P	195/195 (100%)	182 (93%)	13 (7%)	16	39
3	C	213/213 (100%)	196 (92%)	17 (8%)	12	31
3	Q	213/213 (100%)	200 (94%)	13 (6%)	18	43
4	D	198/215 (92%)	184 (93%)	14 (7%)	14	36
4	R	198/215 (92%)	185 (93%)	13 (7%)	16	40
5	E	192/192 (100%)	178 (93%)	14 (7%)	14	35
5	S	191/192 (100%)	173 (91%)	18 (9%)	8	23
6	F	196/200 (98%)	179 (91%)	17 (9%)	10	27
6	T	196/200 (98%)	180 (92%)	16 (8%)	11	29
7	G	207/207 (100%)	190 (92%)	17 (8%)	11	29
7	U	207/207 (100%)	198 (96%)	9 (4%)	29	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	181/181 (100%)	173 (96%)	8 (4%)	28	58
8	V	181/181 (100%)	170 (94%)	11 (6%)	18	43
9	I	172/172 (100%)	168 (98%)	4 (2%)	50	78
9	W	172/172 (100%)	165 (96%)	7 (4%)	30	61
10	J	174/175 (99%)	158 (91%)	16 (9%)	9	24
10	X	174/175 (99%)	162 (93%)	12 (7%)	15	38
11	K	169/169 (100%)	160 (95%)	9 (5%)	22	50
11	Y	169/169 (100%)	159 (94%)	10 (6%)	19	45
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	64
12	Z	185/185 (100%)	177 (96%)	8 (4%)	29	59
13	1	199/199 (100%)	191 (96%)	8 (4%)	31	62
13	M	199/199 (100%)	190 (96%)	9 (4%)	27	57
14	2	162/162 (100%)	150 (93%)	12 (7%)	13	35
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	71
All	All	5303/5348 (99%)	4980 (94%)	323 (6%)	18	43

All (323) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	5	THR
1	A	7	ARG
1	A	33	GLN
1	A	62	GLU
1	A	64	LEU
1	A	65	SER
1	A	124	THR
1	A	158	PHE
1	A	203	GLU
1	A	212	LEU
1	A	236	LEU
2	B	18	GLU
2	B	53	LYS
2	B	58	LEU
2	B	61	GLN
2	B	62	ASP
2	B	91	THR

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Mol	Chain	Res	Type
2	B	121	GLN
2	B	135	SER
2	B	150	THR
2	B	185	LYS
2	B	192	LEU
2	B	198	SER
2	B	202	THR
2	B	225	LYS
3	C	10	ARG
3	C	33	ARG
3	C	40	VAL
3	C	44	ASN
3	C	57	LYS
3	C	66	LYS
3	C	107	VAL
3	C	112	LEU
3	C	121	GLN
3	C	150	GLN
3	C	156	ILE
3	C	163	GLN
3	C	172	VAL
3	C	180(C)	LYS
3	C	185	THR
3	C	208	LYS
3	C	227	GLU
4	D	48	LEU
4	D	52	LYS
4	D	59	LEU
4	D	76	CYS
4	D	110	GLU
4	D	119	LEU
4	D	123(B)	GLU
4	D	125	GLU
4	D	177	LEU
4	D	191	LEU
4	D	205	GLU
4	D	215	ILE
4	D	235	LYS
4	D	237	LEU
5	E	12	THR
5	E	13	VAL
5	E	18	THR

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Mol	Chain	Res	Type
5	E	28	LEU
5	E	76	LEU
5	E	121	GLN
5	E	149	LEU
5	E	178	ARG
5	E	185	ASN
5	E	189	LEU
5	E	195	GLU
5	E	207	LEU
5	E	207(C)	VAL
5	E	222	THR
6	F	36	THR
6	F	43	ASN
6	F	44	ASP
6	F	121	GLN
6	F	129	VAL
6	F	167	LYS
6	F	169	ARG
6	F	176	LEU
6	F	180(E)	GLU
6	F	192	GLN
6	F	199	LEU
6	F	206	LYS
6	F	214	TRP
6	F	218(C)	ASN
6	F	222	LYS
6	F	225	LYS
6	F	237	GLN
7	G	10	ARG
7	G	33	GLN
7	G	38	LEU
7	G	48	VAL
7	G	49	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	124	THR
7	G	169	GLN
7	G	171	GLU
7	G	174	THR
7	G	179(C)	LYS

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Mol	Chain	Res	Type
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	7	LYS
8	H	13	VAL
8	H	34	LEU
8	H	63	ILE
8	H	68	LEU
8	H	101	VAL
8	H	120	ASP
8	H	144	GLN
9	I	121	GLU
9	I	160	LEU
9	I	171	TRP
9	I	181	LYS
10	J	6	ILE
10	J	9	GLN
10	J	10	ASP
10	J	34	THR
10	J	35	ARG
10	J	51	ASP
10	J	52	THR
10	J	68	ILE
10	J	70	GLU
10	J	77	GLN
10	J	90	SER
10	J	137	LEU
10	J	155	LEU
10	J	160	GLN
10	J	168	MET
10	J	191	GLN
11	K	4	LEU
11	K	9	GLN
11	K	65	LEU
11	K	69	ARG
11	K	87	VAL
11	K	99	THR
11	K	105(A)	ARG
11	K	105(B)	LYS
11	K	201	GLU
12	L	-9	GLN
12	L	14	LEU

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Mol	Chain	Res	Type
12	L	40	ASN
12	L	98	HIS
12	L	99	THR
12	L	138	LEU
12	L	144(P)	LEU
13	M	-8	THR
13	M	2	SER
13	M	40	ASN
13	M	62	LEU
13	M	65	GLU
13	M	91	ARG
13	M	141(C)	ARG
13	M	149	GLN
13	M	184	LEU
14	N	20	THR
14	N	31	THR
14	N	105(B)	LYS
14	N	107	LYS
14	N	119	VAL
1	O	4	MET
1	O	33	GLN
1	O	62	GLU
1	O	64	LEU
1	O	111	LEU
1	O	124	THR
1	O	158	PHE
1	O	217(P)	LYS
1	O	222	ARG
1	O	223	LYS
2	P	57	THR
2	P	58	LEU
2	P	64	THR
2	P	91	THR
2	P	121	GLN
2	P	150	THR
2	P	185	LYS
2	P	192	LEU
2	P	198	SER
2	P	202	THR
2	P	212	PHE
2	P	225	LYS
2	P	235	LYS

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Mol	Chain	Res	Type
3	Q	10	ARG
3	Q	35	THR
3	Q	66	LYS
3	Q	121	GLN
3	Q	150	GLN
3	Q	156	ILE
3	Q	163	GLN
3	Q	172	VAL
3	Q	185	THR
3	Q	193	THR
3	Q	199	GLU
3	Q	208	LYS
3	Q	224	LEU
4	R	13	SER
4	R	28	LEU
4	R	48	LEU
4	R	52	LYS
4	R	59	LEU
4	R	62	ASP
4	R	119	LEU
4	R	122	ARG
4	R	177	LEU
4	R	194	LEU
4	R	215	ILE
4	R	218	GLN
4	R	237	LEU
5	S	12	THR
5	S	13	VAL
5	S	18	THR
5	S	33	GLN
5	S	58	LEU
5	S	64	GLN
5	S	65	LYS
5	S	76	LEU
5	S	97	ASN
5	S	104	ASN
5	S	178	ARG
5	S	185	ASN
5	S	189	LEU
5	S	199	GLN
5	S	204	GLU
5	S	207	LEU

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Mol	Chain	Res	Type
5	S	208(B)	ASP
5	S	211	SER
6	T	25	GLU
6	T	35	THR
6	T	36	THR
6	T	43	ASN
6	T	63	LYS
6	T	98	SER
6	T	121	GLN
6	T	135	SER
6	T	143	LYS
6	T	176	LEU
6	T	187	ARG
6	T	192	GLN
6	T	205	ASN
6	T	214	TRP
6	T	222	LYS
6	T	225	LYS
7	U	38	LEU
7	U	49	ILE
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	13	VAL
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	63	ILE
8	V	68	LEU
8	V	144	GLN
8	V	149	GLU
8	V	192	LEU
8	V	200	LYS
8	V	222	CYS
9	W	-8	SER
9	W	12	VAL
9	W	107	LYS
9	W	121	GLU

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Mol	Chain	Res	Type
9	W	160	LEU
9	W	171	TRP
9	W	181	LYS
10	X	6	ILE
10	X	9	GLN
10	X	22	ARG
10	X	34	THR
10	X	52	THR
10	X	68	ILE
10	X	77	GLN
10	X	120	VAL
10	X	157	LEU
10	X	168	MET
10	X	181	ASP
10	X	191	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	31	VAL
11	Y	65	LEU
11	Y	69	ARG
11	Y	84	SER
11	Y	105(B)	LYS
11	Y	146	LEU
11	Y	181	ASP
11	Y	208	ASN
12	Z	14	LEU
12	Z	40	ASN
12	Z	98	HIS
12	Z	99	THR
12	Z	138	LEU
12	Z	144(J)	ASN
12	Z	144(R)	LYS
12	Z	145	TYR
13	1	2	SER
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	141(C)	ARG
13	1	181(A)	THR
13	1	184	LEU
13	1	204	LYS
14	2	20	THR

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Mol	Chain	Res	Type
14	2	36	ARG
14	2	48	SER
14	2	105	ASP
14	2	105(B)	LYS
14	2	112	THR
14	2	119	VAL
14	2	132	THR
14	2	149	GLU
14	2	178	LEU
14	2	186	ARG
14	2	187(F)	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (147) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
2	B	23	GLN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	44	ASN
3	C	82	ASN
3	C	150	GLN
3	C	163	GLN
3	C	209	ASN
4	D	23	GLN
4	D	108	ASN
4	D	147	GLN
4	D	211	GLN
4	D	226	ASN
5	E	73	HIS
5	E	104	ASN
5	E	121	GLN
5	E	125	GLN
5	E	185	ASN
5	E	207(E)	ASN
6	F	43	ASN
6	F	90	ASN

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Mol	Chain	Res	Type
6	F	121	GLN
6	F	192	GLN
6	F	205	ASN
6	F	237	GLN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	170	GLN
7	G	178	ASN
8	H	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	86	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
10	J	9	GLN
10	J	54	GLN
10	J	85	GLN
10	J	112	GLN
10	J	186	GLN
11	K	85	ASN
11	K	174	ASN
12	L	-7	ASN
12	L	40	ASN
12	L	61	ASN
12	L	70(A)	ASN
12	L	123	GLN
12	L	166	HIS
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	149	GLN
13	M	157	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS

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Mol	Chain	Res	Type
2	P	23	GLN
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	177	GLN
3	Q	82	ASN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
4	R	23	GLN
4	R	108	ASN
4	R	141	HIS
4	R	147	GLN
4	R	199	GLN
4	R	211	GLN
4	R	226	ASN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	125	GLN
5	S	185	ASN
5	S	209	ASN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	147	HIS
6	T	192	GLN
6	T	205	ASN
6	T	241	ASN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	178	ASN
7	U	182	HIS
7	U	184	ASN
8	V	30	ASN
8	V	66	HIS
8	V	86	HIS

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Mol	Chain	Res	Type
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	64	ASN
9	W	81	GLN
10	X	36	GLN
10	X	54	GLN
10	X	77	GLN
10	X	96	GLN
10	X	112	GLN
10	X	140	HIS
10	X	186	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	174	ASN
11	Y	189	ASN
11	Y	208	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	61	ASN
12	Z	70(A)	ASN
12	Z	144(B)	ASN
12	Z	144(J)	ASN
12	Z	166	HIS
13	1	10	ASN
13	1	40	ASN
13	1	89	GLN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	191	GLN
14	2	38	HIS
14	2	106	ASN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	MES	Y	213	-	12,12,12	2.14	1 (8%)	14,16,16	1.40	1 (7%)
16	3OE	Y	212	-	43,46,46	1.00	1 (2%)	53,61,61	0.86	2 (3%)
16	3OE	K	213	-	43,46,46	1.05	2 (4%)	53,61,61	0.76	2 (3%)
17	MES	K	214	-	12,12,12	2.15	1 (8%)	14,16,16	1.38	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MES	Y	213	-	-	3/6/14/14	0/1/1/1
16	3OE	Y	212	-	-	6/37/39/39	0/4/4/4
16	3OE	K	213	-	-	2/37/39/39	0/4/4/4
17	MES	K	214	-	-	5/6/14/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	214	MES	C8-S	-7.14	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	213	MES	C8-S	-7.10	1.67	1.77
16	K	213	3OE	C36-C37	-4.77	1.39	1.50
16	Y	212	3OE	C36-C37	-4.43	1.40	1.50
16	K	213	3OE	C2-C1	2.48	1.54	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	212	3OE	O35-C36-C37	4.04	121.27	109.16
17	Y	213	MES	O3S-S-C8	3.83	111.97	105.77
17	K	214	MES	O3S-S-C8	3.57	111.54	105.77
16	K	213	3OE	O35-C36-C37	2.51	116.68	109.16
16	K	213	3OE	C7-C6-C5	-2.20	122.16	125.59
16	Y	212	3OE	C7-C6-C5	-2.12	122.29	125.59

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	214	MES	C7-C8-S-O1S
17	K	214	MES	C7-C8-S-O3S
17	Y	213	MES	C7-C8-S-O1S
17	Y	213	MES	C7-C8-S-O2S
16	Y	212	3OE	O28-C27-C8-C34
16	Y	212	3OE	O28-C27-C8-C30
16	Y	212	3OE	N18-C27-C8-C34
16	Y	212	3OE	N18-C27-C8-C30
16	Y	212	3OE	C33-C32-O35-C36
16	Y	212	3OE	C31-C32-O35-C36
17	Y	213	MES	C7-C8-S-O3S
17	K	214	MES	C8-C7-N4-C3
16	K	213	3OE	C33-C32-O35-C36
16	K	213	3OE	C31-C32-O35-C36
17	K	214	MES	C7-C8-S-O2S
17	K	214	MES	C8-C7-N4-C5

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Y	212	3OE	1	0

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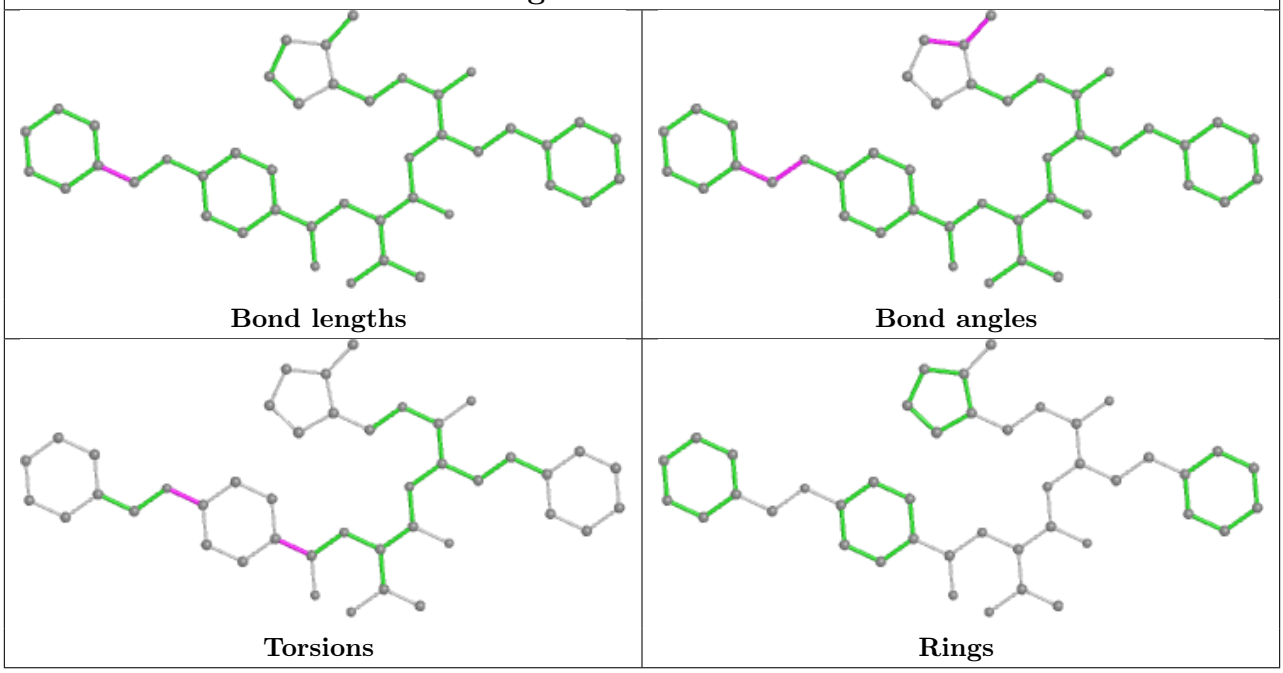
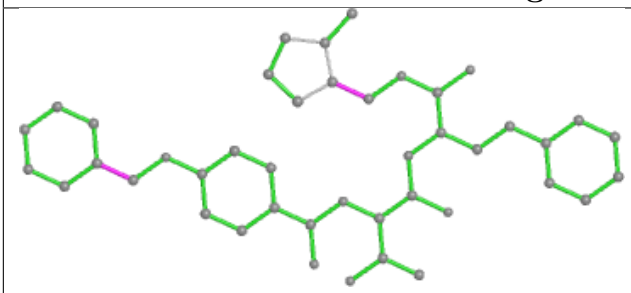
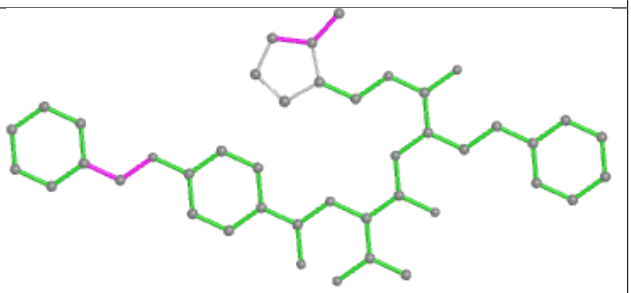
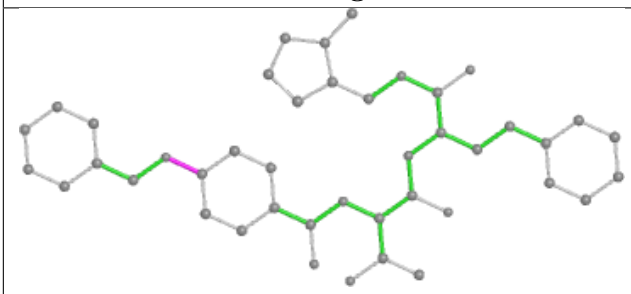
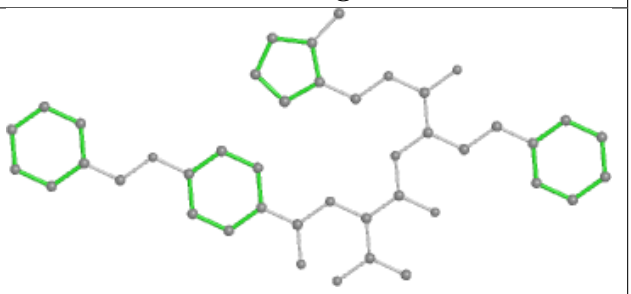
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	213	3OE	2	0
17	K	214	MES	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 3OE Y 212



Ligand 3OE K 213	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.10	4 (1%)	72	70	35, 51, 76, 102	0
1	O	250/250 (100%)	-0.12	6 (2%)	59	56	35, 52, 78, 104	0
2	B	235/235 (100%)	-0.02	6 (2%)	56	52	33, 56, 86, 101	0
2	P	235/235 (100%)	-0.00	5 (2%)	63	60	32, 56, 89, 101	0
3	C	241/241 (100%)	0.37	23 (9%)	8	5	39, 67, 108, 124	0
3	Q	241/241 (100%)	0.50	36 (14%)	2	1	39, 68, 109, 129	0
4	D	242/260 (93%)	0.03	12 (4%)	28	24	36, 59, 95, 111	0
4	R	242/260 (93%)	0.09	11 (4%)	33	28	37, 59, 98, 116	0
5	E	233/233 (100%)	0.06	5 (2%)	63	60	39, 59, 88, 110	0
5	S	233/233 (100%)	0.24	18 (7%)	13	10	39, 59, 92, 115	0
6	F	237/242 (97%)	-0.14	5 (2%)	63	60	34, 51, 83, 95	0
6	T	237/242 (97%)	-0.07	4 (1%)	70	68	34, 52, 81, 98	0
7	G	243/243 (100%)	-0.17	3 (1%)	79	78	31, 45, 72, 102	0
7	U	243/243 (100%)	-0.29	2 (0%)	86	85	31, 46, 70, 99	0
8	H	222/222 (100%)	-0.27	0	100	100	33, 43, 63, 92	0
8	V	222/222 (100%)	-0.33	0	100	100	33, 44, 64, 94	0
9	I	204/204 (100%)	-0.37	1 (0%)	91	90	31, 43, 60, 74	0
9	W	204/204 (100%)	-0.33	2 (0%)	82	81	31, 43, 60, 75	0
10	J	198/198 (100%)	-0.13	5 (2%)	57	54	32, 46, 61, 113	0
10	X	197/198 (99%)	-0.12	7 (3%)	42	37	33, 46, 61, 111	0
11	K	212/212 (100%)	-0.16	2 (0%)	84	84	31, 46, 72, 81	0
11	Y	212/212 (100%)	-0.25	3 (1%)	75	74	31, 46, 73, 80	0
12	L	222/222 (100%)	-0.33	1 (0%)	91	90	31, 44, 72, 80	0
12	Z	222/222 (100%)	-0.28	1 (0%)	91	90	31, 44, 70, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1	233/233 (100%)	-0.29	2 (0%) 84 84	29, 43, 56, 63	0
13	M	233/233 (100%)	-0.34	1 (0%) 92 92	29, 42, 56, 63	0
14	2	196/196 (100%)	-0.37	0 100 100	30, 40, 57, 66	0
14	N	196/196 (100%)	-0.36	0 100 100	31, 40, 57, 66	0
All	All	6335/6382 (99%)	-0.12	165 (2%) 56 52	29, 49, 85, 129	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	7	GLY	9.4
4	R	123(C)	GLY	8.7
4	D	123(E)	SER	8.1
5	S	4	PHE	7.7
3	Q	55	THR	7.4
10	J	192	ALA	7.4
4	R	123(E)	SER	7.2
2	P	218	ASN	6.5
3	C	8	TYR	6.4
10	J	193	GLN	6.3
6	F	12	ASN	6.3
3	Q	54	SER	6.2
13	1	-8	THR	6.2
5	E	4	PHE	6.1
2	B	218	ASN	6.0
3	C	9	ASP	5.9
4	D	123(B)	GLU	5.9
5	S	206	SER	5.8
3	C	11	ALA	5.7
2	B	217	ALA	5.7
7	U	6	ALA	5.5
4	R	123(B)	GLU	5.5
1	A	4	MET	5.5
10	J	191	GLN	5.5
1	A	5	THR	5.4
1	O	4	MET	5.4
10	J	-1	MET	5.4
3	Q	56	LEU	5.3
4	R	123(F)	GLY	5.3
2	P	217	ALA	5.3
4	D	123(C)	GLY	5.2
4	R	123(D)	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
4	R	10	ARG	5.1
7	U	240	ASP	4.9
3	C	55	THR	4.7
3	Q	238	GLN	4.7
5	S	6	ASN	4.6
10	X	191	GLN	4.6
7	G	240	ASP	4.6
13	M	-8	THR	4.6
6	T	12	ASN	4.5
5	S	5	ARG	4.5
4	D	10	ARG	4.5
10	X	192	ALA	4.5
4	D	9	ASP	4.4
3	Q	7	GLY	4.4
4	D	123(F)	GLY	4.4
1	O	217(P)	LYS	4.4
3	C	243	GLN	4.3
1	O	5	THR	4.2
4	R	9	ASP	4.1
2	B	54	VAL	3.9
1	O	6	ASP	3.8
3	Q	8	TYR	3.8
3	Q	241	GLN	3.8
3	C	208	LYS	3.7
3	C	12	LEU	3.7
4	R	11	GLY	3.6
3	Q	236	ILE	3.5
3	Q	240	LYS	3.5
4	D	123(A)	GLY	3.5
3	C	43	LYS	3.4
3	Q	234	THR	3.4
3	Q	233	VAL	3.4
3	C	10	ARG	3.3
4	D	123(D)	ALA	3.2
4	D	11	GLY	3.2
1	O	236	LEU	3.2
2	P	216(B)	GLY	3.2
3	Q	207	ALA	3.1
1	A	203	GLU	3.1
3	Q	10	ARG	3.1
3	Q	237	GLU	3.1
3	Q	184	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	241	GLN	3.0
4	D	123(G)	GLU	3.0
3	Q	189	CYS	3.0
5	E	5	ARG	2.9
5	S	233	ILE	2.9
3	Q	239	GLU	2.9
7	G	184(H)	GLU	2.9
3	Q	208	LYS	2.9
11	K	179	THR	2.9
5	E	206	SER	2.8
3	Q	243	GLN	2.8
3	C	56	LEU	2.8
5	S	57	GLU	2.8
2	B	216(B)	GLY	2.8
3	Q	192	LEU	2.8
3	Q	187	GLU	2.8
5	S	203	ASP	2.8
5	S	8	TYR	2.8
6	F	241	ASN	2.7
10	X	10	ASP	2.7
5	S	181	LYS	2.7
5	S	180(C)	PHE	2.7
6	F	240	ILE	2.7
5	S	58	LEU	2.6
11	Y	180	GLU	2.6
3	Q	11	ALA	2.6
7	G	239	GLN	2.6
5	E	233	ILE	2.5
10	X	188	ASP	2.5
3	Q	198	LEU	2.5
3	Q	40	VAL	2.5
1	O	191	HIS	2.5
10	X	11	SER	2.4
9	W	182	ASP	2.4
3	C	57	LYS	2.4
3	Q	206	GLY	2.4
3	Q	203	THR	2.4
9	W	181	LYS	2.4
4	D	26	TYR	2.4
3	Q	209	ASN	2.4
4	R	123(A)	GLY	2.4
12	L	-9	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
5	S	201	LEU	2.4
5	S	51	LEU	2.3
2	P	45	GLY	2.3
11	Y	179	THR	2.3
9	I	-8	SER	2.3
4	R	12	VAL	2.3
10	X	193	GLN	2.3
5	E	57	GLU	2.3
10	J	92	ARG	2.3
3	Q	9	ASP	2.3
3	Q	12	LEU	2.3
3	C	44	ASN	2.3
3	C	234	THR	2.3
10	X	189	ASP	2.3
3	Q	53	ARG	2.2
3	C	42	GLY	2.2
4	R	22	PHE	2.2
6	F	180(E)	GLU	2.2
12	Z	-9	GLN	2.2
3	Q	196	SER	2.2
6	T	43	ASN	2.2
11	Y	181	ASP	2.2
5	S	168	ARG	2.2
11	K	104	TYR	2.2
3	Q	50	CYS	2.2
3	Q	227	GLU	2.2
5	S	189	LEU	2.2
2	P	43	SER	2.2
13	1	181(A)	THR	2.2
3	Q	229	ILE	2.2
3	C	45	CYS	2.1
3	Q	43	LYS	2.1
3	C	187	GLU	2.1
6	T	183	GLY	2.1
2	B	204(A)	SER	2.1
3	C	238	GLN	2.1
3	C	17	PRO	2.1
3	Q	194	VAL	2.1
2	B	235	LYS	2.1
3	C	62(A)	ILE	2.0
5	S	184	GLY	2.0
3	C	184	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
6	F	238	LYS	2.0
5	S	55	ALA	2.0
6	T	13	SER	2.0
3	C	232	TYR	2.0
4	D	22	PHE	2.0
1	A	236	LEU	2.0
5	S	33	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

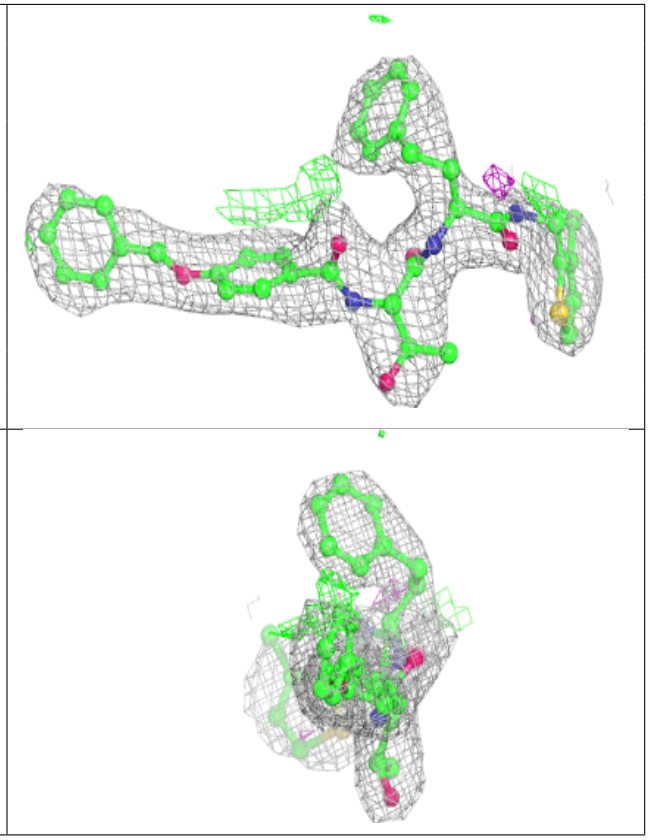
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	L	195	1/1	0.69	0.13	56,56,56,56	0
15	MG	I	195	1/1	0.73	0.33	57,57,57,57	0
15	MG	F	243	1/1	0.83	0.68	105,105,105,105	0
15	MG	F	242	1/1	0.89	0.40	67,67,67,67	0
16	3OE	Y	212	43/43	0.90	0.24	71,72,74,75	0
16	3OE	K	213	43/43	0.91	0.23	55,60,68,68	0
15	MG	H	224	1/1	0.91	0.20	68,68,68,68	0
17	MES	Y	213	12/12	0.91	0.25	101,102,102,102	0
17	MES	K	214	12/12	0.92	0.23	92,93,93,93	0
15	MG	G	1	1/1	0.96	0.05	41,41,41,41	0
15	MG	L	196	1/1	0.96	0.15	50,50,50,50	0
15	MG	I	196	1/1	0.96	0.25	46,46,46,46	0
15	MG	K	212	1/1	0.98	0.25	47,47,47,47	0
15	MG	N	188	1/1	0.98	0.15	36,36,36,36	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

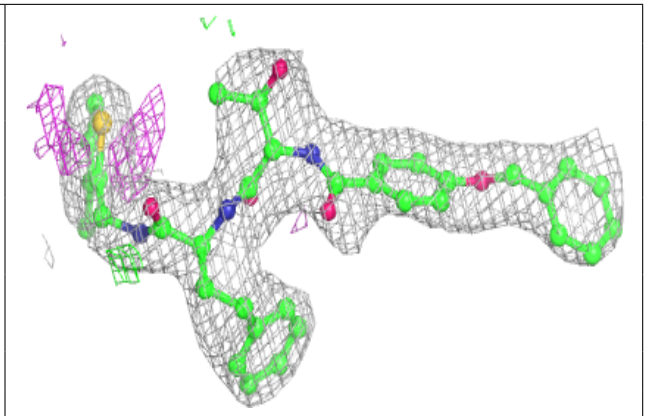
Electron density around 3OE Y 212:

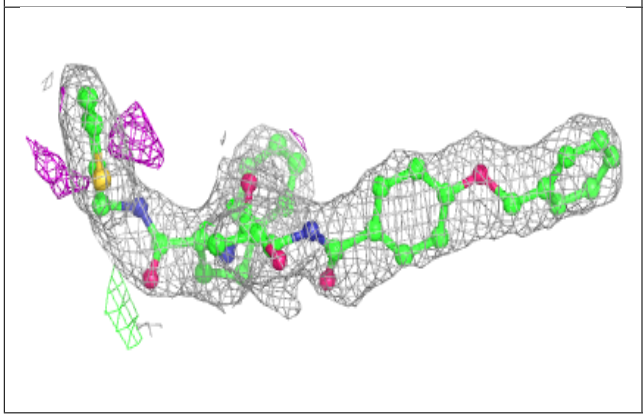
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

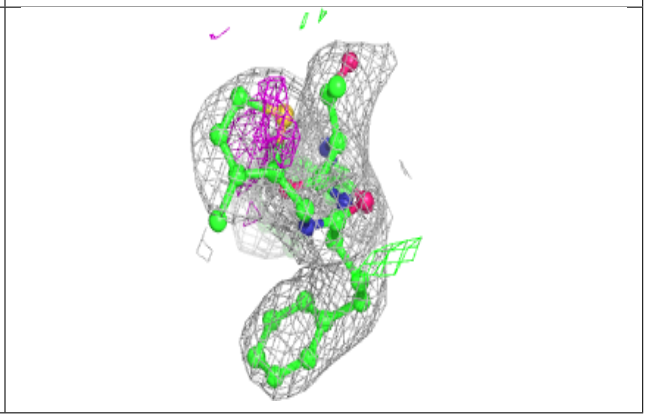


Electron density around 3OE K 213:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.