Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 08:07 PM EST

PDB ID	:	3EZQ
Title	:	Crystal Structure of the Fas/FADD Death Domain Complex
Authors	:	Schwarzenbacher, R.; Robinson, H.; Stec, B.; Riedl, S.J.
Deposited on	:	2008-10-23
Resolution	:	2.73 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:

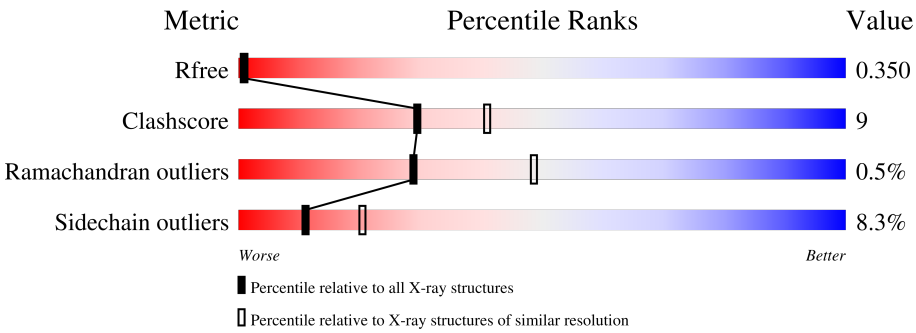
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)

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%

Mol	Chain	Length	Quality of chain
1	A	115	81% 18% •
1	C	115	80% 16% •
1	E	115	82% 17% •
1	G	115	87% 11% •
1	I	115	87% 10% •
1	K	115	77% 20% •
1	M	115	82% 16% •

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Mol	Chain	Length	Quality of chain
1	O	115	80% 17% •
2	B	122	49% 29% • 19%
2	D	122	58% 23% 19%
2	F	122	63% 16% • 19%
2	H	122	54% 25% • 19%
2	J	122	52% 25% • 19%
2	L	122	59% 21% • 19%
2	N	122	59% 20% • 19%
2	P	122	54% 23% • 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	K	13	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13933 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 Tumor necrosis factor receptor superfamily member 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	115	916	571	159	184	2	0	0	0
1	C	115	916	571	159	184	2	0	0	0
1	E	115	916	571	159	184	2	0	0	0
1	G	115	916	571	159	184	2	0	0	0
1	I	115	916	571	159	184	2	0	0	0
1	K	115	916	571	159	184	2	0	0	0
1	M	115	916	571	159	184	2	0	0	0
1	O	115	916	571	159	184	2	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	336	LEU	-	expression tag	UNP P25445
A	337	GLU	-	expression tag	UNP P25445
C	336	LEU	-	expression tag	UNP P25445
C	337	GLU	-	expression tag	UNP P25445
E	336	LEU	-	expression tag	UNP P25445
E	337	GLU	-	expression tag	UNP P25445
G	336	LEU	-	expression tag	UNP P25445
G	337	GLU	-	expression tag	UNP P25445
I	336	LEU	-	expression tag	UNP P25445
I	337	GLU	-	expression tag	UNP P25445
K	336	LEU	-	expression tag	UNP P25445
K	337	GLU	-	expression tag	UNP P25445
M	336	LEU	-	expression tag	UNP P25445

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Chain	Residue	Modelled	Actual	Comment	Reference
M	337	GLU	-	expression tag	UNP P25445
O	336	LEU	-	expression tag	UNP P25445
O	337	GLU	-	expression tag	UNP P25445

- Molecule 2 is a protein called Protein FADD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	795	483	154	154	4	0	0	0
2	D	99	795	483	154	154	4	0	0	0
2	F	99	795	483	154	154	4	0	0	0
2	H	99	795	483	154	154	4	0	0	0
2	J	99	795	483	154	154	4	0	0	0
2	L	99	795	483	154	154	4	0	0	0
2	N	99	795	483	154	154	4	0	0	0
2	P	99	795	483	154	154	4	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	209	HIS	-	expression tag	UNP Q13158
B	210	HIS	-	expression tag	UNP Q13158
B	211	HIS	-	expression tag	UNP Q13158
B	212	HIS	-	expression tag	UNP Q13158
B	213	HIS	-	expression tag	UNP Q13158
B	214	HIS	-	expression tag	UNP Q13158
D	209	HIS	-	expression tag	UNP Q13158
D	210	HIS	-	expression tag	UNP Q13158
D	211	HIS	-	expression tag	UNP Q13158
D	212	HIS	-	expression tag	UNP Q13158
D	213	HIS	-	expression tag	UNP Q13158
D	214	HIS	-	expression tag	UNP Q13158
F	209	HIS	-	expression tag	UNP Q13158
F	210	HIS	-	expression tag	UNP Q13158
F	211	HIS	-	expression tag	UNP Q13158

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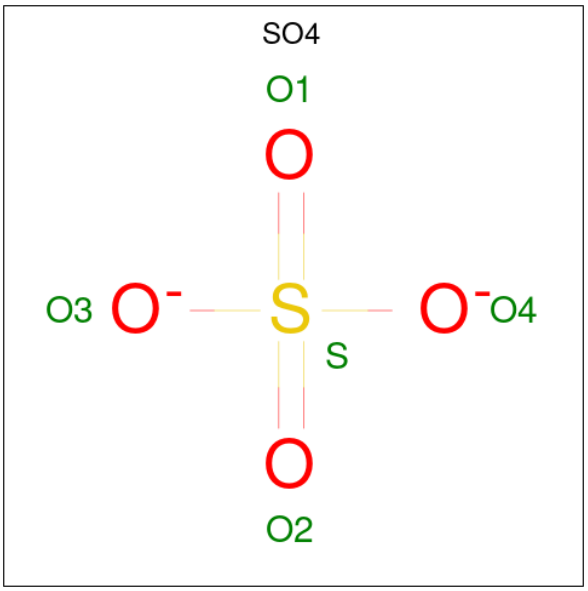
Chain	Residue	Modelled	Actual	Comment	Reference
F	212	HIS	-	expression tag	UNP Q13158
F	213	HIS	-	expression tag	UNP Q13158
F	214	HIS	-	expression tag	UNP Q13158
H	209	HIS	-	expression tag	UNP Q13158
H	210	HIS	-	expression tag	UNP Q13158
H	211	HIS	-	expression tag	UNP Q13158
H	212	HIS	-	expression tag	UNP Q13158
H	213	HIS	-	expression tag	UNP Q13158
H	214	HIS	-	expression tag	UNP Q13158
J	209	HIS	-	expression tag	UNP Q13158
J	210	HIS	-	expression tag	UNP Q13158
J	211	HIS	-	expression tag	UNP Q13158
J	212	HIS	-	expression tag	UNP Q13158
J	213	HIS	-	expression tag	UNP Q13158
J	214	HIS	-	expression tag	UNP Q13158
L	209	HIS	-	expression tag	UNP Q13158
L	210	HIS	-	expression tag	UNP Q13158
L	211	HIS	-	expression tag	UNP Q13158
L	212	HIS	-	expression tag	UNP Q13158
L	213	HIS	-	expression tag	UNP Q13158
L	214	HIS	-	expression tag	UNP Q13158
N	209	HIS	-	expression tag	UNP Q13158
N	210	HIS	-	expression tag	UNP Q13158
N	211	HIS	-	expression tag	UNP Q13158
N	212	HIS	-	expression tag	UNP Q13158
N	213	HIS	-	expression tag	UNP Q13158
N	214	HIS	-	expression tag	UNP Q13158
P	209	HIS	-	expression tag	UNP Q13158
P	210	HIS	-	expression tag	UNP Q13158
P	211	HIS	-	expression tag	UNP Q13158
P	212	HIS	-	expression tag	UNP Q13158
P	213	HIS	-	expression tag	UNP Q13158
P	214	HIS	-	expression tag	UNP Q13158

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
3	C	1	5	4	1	0	0
3	E	1	5	4	1	0	0
3	E	1	5	4	1	0	0
3	G	1	5	4	1	0	0
3	I	1	5	4	1	0	0
3	J	1	5	4	1	0	0
3	K	1	5	4	1	0	0
3	K	1	5	4	1	0	0
3	M	1	5	4	1	0	0
3	M	1	5	4	1	0	0
3	O	1	5	4	1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	E	1	1	1	0	0
4	H	1	1	1	0	0
4	J	1	1	1	0	0
4	K	1	1	1	0	0
4	M	1	1	1	0	0
4	P	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	7	7	7	0	0
5	B	2	2	2	0	0
5	C	8	8	8	0	0
5	D	4	4	4	0	0
5	E	9	9	9	0	0
5	F	4	4	4	0	0
5	G	11	11	11	0	0
5	H	8	8	8	0	0
5	I	84	84	84	0	0
5	J	8	8	8	0	0
5	K	6	6	6	0	0
5	L	7	7	7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	M	9	9	9	0	0
			Total	O		
5	N	3	3	3	0	0
			Total	O		
5	O	5	5	5	0	0
			Total	O		
5	P	2	2	2	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. 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. 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: Tumor necrosis factor receptor superfamily member 6

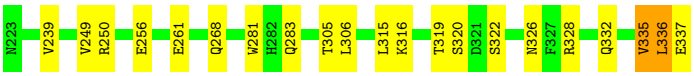
Chain A:

• Molecule 1: Tumor necrosis factor receptor superfamily member 6

Chain C:

• Molecule 1: Tumor necrosis factor receptor superfamily member 6

Chain E:



• Molecule 1: Tumor necrosis factor receptor superfamily member 6

Chain G:

• Molecule 1: Tumor necrosis factor receptor superfamily member 6

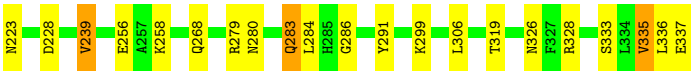
Chain I:

• Molecule 1: Tumor necrosis factor receptor superfamily member 6

Chain K:

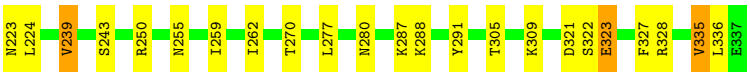
• Molecule 1: Tumor necrosis factor receptor superfamily member 6

Chain M:



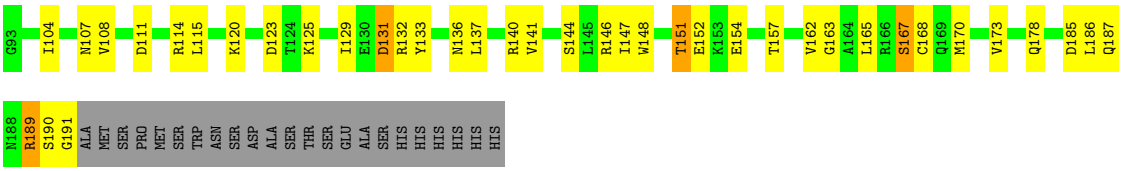
• Molecule 1: Tumor necrosis factor receptor superfamily member 6

Chain O:



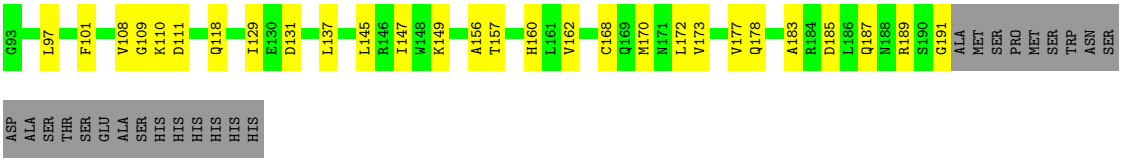
• Molecule 2: Protein FADD

Chain B:



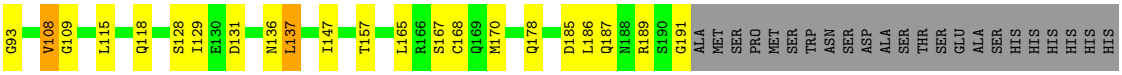
• Molecule 2: Protein FADD

Chain D:



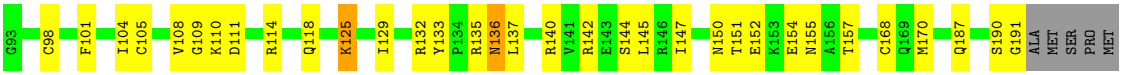
• Molecule 2: Protein FADD

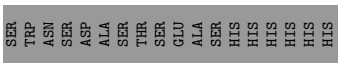
Chain F:



• Molecule 2: Protein FADD

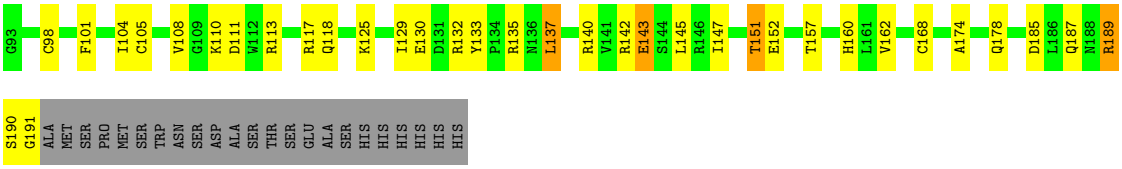
Chain H:





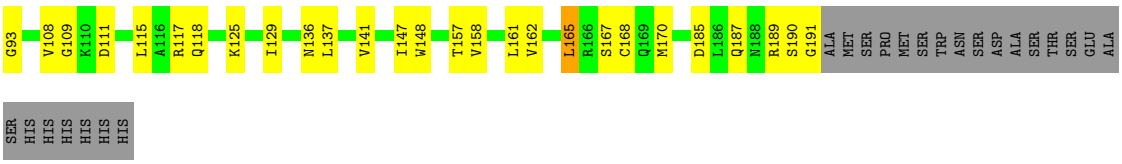
- Molecule 2: Protein FADD

Chain J:



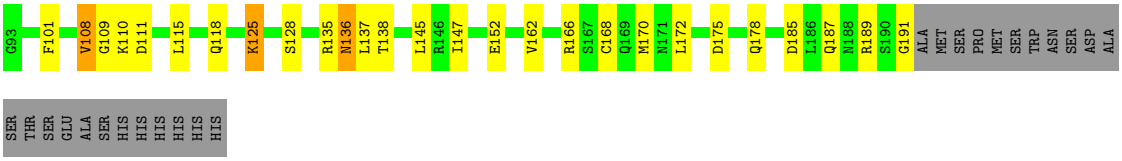
- Molecule 2: Protein FADD

Chain L:



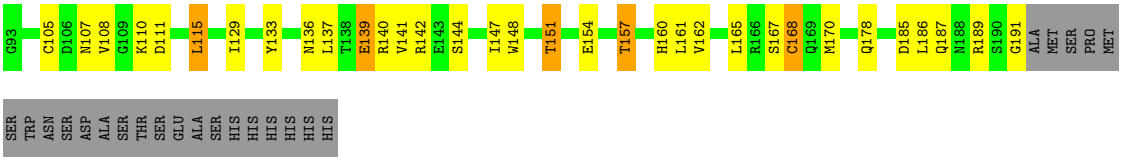
- Molecule 2: Protein FADD

Chain N:



- Molecule 2: Protein FADD

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	126.22Å 126.22Å 299.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.73 29.71 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-2.73) 98.8 (29.71-2.73)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.278 0.336 , 0.350	Depositor DCC
R_{free} test set	3556 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	73.2	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.499 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13933	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2821e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: NA, SO4

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	0.61	0/923	0.68	0/1241
1	C	0.71	1/923 (0.1%)	0.70	0/1241
1	E	0.67	0/923	0.67	0/1241
1	G	0.73	0/923	0.74	0/1241
1	I	0.70	0/923	0.74	0/1241
1	K	0.64	0/923	0.71	0/1241
1	M	0.72	1/923 (0.1%)	0.72	0/1241
1	O	0.61	0/923	0.66	0/1241
2	B	0.57	0/802	0.61	0/1080
2	D	0.54	1/802 (0.1%)	0.61	0/1080
2	F	0.49	0/802	0.62	0/1080
2	H	0.57	1/802 (0.1%)	0.66	0/1080
2	J	0.55	1/802 (0.1%)	0.65	0/1080
2	L	0.51	0/802	0.59	0/1080
2	N	0.50	0/802	0.63	0/1080
2	P	0.58	2/802 (0.2%)	0.58	0/1080
All	All	0.62	7/13800 (0.1%)	0.66	0/18568

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	279	ARG	NE-CZ	5.70	1.40	1.33
1	M	228	ASP	CG-OD1	5.59	1.38	1.25
2	J	98	CYS	CB-SG	-5.55	1.72	1.81
2	H	98	CYS	CB-SG	-5.33	1.73	1.81
2	D	131	ASP	CG-OD2	5.29	1.37	1.25
2	P	154	GLU	CD-OE1	5.28	1.31	1.25
2	P	154	GLU	CD-OE2	5.02	1.31	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	916	0	939	16	0
1	C	916	0	939	17	0
1	E	916	0	939	14	0
1	G	916	0	939	13	0
1	I	916	0	939	17	0
1	K	916	0	939	21	0
1	M	916	0	939	15	0
1	O	916	0	939	26	0
2	B	795	0	793	24	0
2	D	795	0	793	17	0
2	F	795	0	793	20	0
2	H	795	0	793	20	0
2	J	795	0	793	26	0
2	L	795	0	793	23	0
2	N	795	0	793	19	0
2	P	795	0	793	29	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
3	E	10	0	0	0	0
3	G	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	10	0	0	2	0
3	M	10	0	0	1	0
3	O	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	7	0	0	1	0
5	B	2	0	0	0	0
5	C	8	0	0	1	0
5	D	4	0	0	0	0
5	E	9	0	0	0	0
5	F	4	0	0	0	0
5	G	11	0	0	0	0
5	H	8	0	0	1	0
5	I	84	0	0	4	0
5	J	8	0	0	0	0
5	K	6	0	0	0	0
5	L	7	0	0	1	0
5	M	9	0	0	1	0
5	N	3	0	0	0	0
5	O	5	0	0	0	0
5	P	2	0	0	3	0
All	All	13933	0	13856	261	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 9.

All (261) 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)
2:L:109:GLY:HA2	2:L:137:LEU:HD21	1.37	1.04
2:B:115:LEU:HD11	2:B:165:LEU:HD23	1.42	1.01
1:K:328:ARG:HE	1:K:332:GLN:HE22	1.13	0.95
2:F:109:GLY:HA2	2:F:137:LEU:HD21	1.47	0.91
1:A:289:GLU:O	1:A:293:THR:HG22	1.73	0.89
1:K:258:LYS:HG2	1:K:280:ASN:ND2	1.86	0.89
2:F:108:VAL:HG13	2:F:170:MET:HE1	1.59	0.84
1:A:328:ARG:HG3	1:C:335:VAL:HG13	1.60	0.83
1:K:258:LYS:HG2	1:K:280:ASN:HD21	1.44	0.80
2:H:108:VAL:HG22	2:H:170:MET:HE1	1.64	0.80
1:K:328:ARG:NE	1:K:332:GLN:HE22	1.78	0.79
2:P:162:VAL:HG11	2:P:178:GLN:HE21	1.47	0.79
1:K:328:ARG:HE	1:K:332:GLN:NE2	1.79	0.79
2:D:162:VAL:HG11	2:D:178:GLN:HE21	1.51	0.75
1:I:223:ASN:HB2	2:J:135:ARG:CZ	2.17	0.74
2:L:129:ILE:HD11	2:L:147:ILE:HD12	1.69	0.74
1:K:250:ARG:CZ	1:K:256:GLU:OE2	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:328:ARG:HG3	1:O:335:VAL:HG13	1.70	0.73
1:G:223:ASN:HB2	2:H:135:ARG:CZ	2.18	0.73
2:F:115:LEU:HD11	2:F:165:LEU:HD12	1.70	0.73
2:J:137:LEU:HG	2:J:140:ARG:NH2	2.04	0.72
2:H:151:THR:HG22	2:H:152:GLU:OE1	1.90	0.72
2:L:108:VAL:HG23	2:L:109:GLY:H	1.55	0.71
2:H:136:ASN:HB2	5:H:19:HOH:O	1.90	0.71
2:B:115:LEU:CD1	2:B:165:LEU:HD23	2.20	0.71
1:M:291:TYR:HB3	2:N:172:LEU:HD12	1.74	0.70
2:F:93:GLY:N	5:I:175:HOH:O	2.24	0.70
1:O:309:LYS:NZ	2:P:189:ARG:HB3	2.07	0.69
1:G:248:PHE:CZ	1:G:293:THR:HG22	2.27	0.68
5:I:106:HOH:O	2:N:136:ASN:ND2	2.27	0.68
2:F:129:ILE:HD11	2:F:147:ILE:HD12	1.77	0.67
2:H:108:VAL:HG13	2:H:170:MET:CE	2.25	0.67
1:G:248:PHE:CE1	1:G:293:THR:HG22	2.30	0.66
2:P:115:LEU:HD11	2:P:165:LEU:HD23	1.78	0.65
1:A:322:SER:O	1:C:299:LYS:NZ	2.29	0.65
2:B:129:ILE:HD11	2:B:147:ILE:HD12	1.78	0.65
2:N:101:PHE:CD1	2:N:145:LEU:HD13	2.32	0.65
1:I:309:LYS:HZ2	2:J:189:ARG:HB3	1.62	0.65
1:O:323:GLU:OE2	1:O:323:GLU:HA	1.96	0.64
2:J:151:THR:HG23	2:J:152:GLU:OE2	1.97	0.64
2:D:157:THR:HG23	2:D:160:HIS:H	1.62	0.63
1:C:291:TYR:HB3	2:D:172:LEU:HD12	1.79	0.63
2:B:162:VAL:HG11	2:B:178:GLN:HE21	1.61	0.63
2:B:115:LEU:HD11	2:B:165:LEU:CD2	2.26	0.63
2:P:148:TRP:O	2:P:151:THR:HG22	1.99	0.62
1:G:223:ASN:HB2	2:H:135:ARG:NE	2.14	0.62
2:B:178:GLN:NE2	5:I:97:HOH:O	2.31	0.62
1:G:239:VAL:O	1:G:239:VAL:HG13	2.00	0.62
2:N:175:ASP:CG	1:O:323:GLU:HG2	2.20	0.62
2:N:162:VAL:HG11	2:N:178:GLN:HE21	1.64	0.62
2:H:132:ARG:HD3	2:H:133:TYR:CE1	2.35	0.61
2:P:129:ILE:HD11	2:P:147:ILE:HD12	1.80	0.61
1:A:291:TYR:OH	2:B:107:ASN:HB3	2.01	0.61
1:E:239:VAL:HA	2:F:187:GLN:HE22	1.64	0.61
1:A:255:ASN:OD1	1:A:258:LYS:HG3	2.00	0.61
2:L:115:LEU:HD11	2:L:165:LEU:HD12	1.83	0.60
2:J:151:THR:CG2	2:J:152:GLU:OE2	2.49	0.60
2:D:108:VAL:HG22	2:D:170:MET:HE1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:VAL:HG13	2:B:170:MET:CE	2.31	0.60
2:B:148:TRP:O	2:B:151:THR:HG22	2.02	0.60
2:D:118:GLN:HG3	2:D:168:CYS:SG	2.42	0.60
2:L:109:GLY:HA2	2:L:137:LEU:CD2	2.24	0.60
2:J:118:GLN:HG3	2:J:168:CYS:SG	2.42	0.59
2:L:108:VAL:HG21	2:L:141:VAL:HG11	1.84	0.59
1:M:279:ARG:O	1:M:283:GLN:HG3	2.02	0.59
1:C:270:THR:HG23	5:C:199:HOH:O	2.02	0.59
1:O:239:VAL:HG13	1:O:239:VAL:O	2.01	0.59
1:I:336:LEU:O	2:J:185:ASP:OD2	2.21	0.59
2:P:115:LEU:HD12	2:P:168:CYS:SG	2.44	0.58
2:H:118:GLN:HG3	2:H:168:CYS:SG	2.43	0.58
2:L:108:VAL:HG23	2:L:141:VAL:HG21	1.85	0.58
1:O:309:LYS:NZ	2:P:189:ARG:CD	2.67	0.57
2:F:118:GLN:HG3	2:F:168:CYS:SG	2.44	0.57
2:N:118:GLN:HG3	2:N:168:CYS:SG	2.44	0.57
2:P:189:ARG:HB2	5:P:217:HOH:O	2.04	0.57
2:D:108:VAL:HG13	2:D:170:MET:HE3	1.85	0.57
2:L:129:ILE:HD11	2:L:147:ILE:CD1	2.35	0.57
2:L:115:LEU:CD1	2:L:165:LEU:HD12	2.35	0.57
1:O:323:GLU:OE2	1:O:323:GLU:CA	2.53	0.57
2:H:108:VAL:HG13	2:H:170:MET:HE3	1.88	0.56
1:I:250:ARG:NE	1:I:256:GLU:OE1	2.38	0.56
1:M:306:LEU:HD13	1:O:327:PHE:CE2	2.41	0.56
2:F:109:GLY:C	2:F:137:LEU:HD11	2.26	0.55
1:O:309:LYS:NZ	2:P:189:ARG:HD2	2.22	0.55
1:A:327:PHE:CE2	1:C:306:LEU:HD13	2.42	0.55
2:J:187:GLN:O	2:J:191:GLY:N	2.38	0.55
2:N:125:LYS:HG2	2:N:147:ILE:HD13	1.88	0.55
2:N:137:LEU:HD12	2:N:137:LEU:H	1.71	0.55
2:P:189:ARG:CB	5:P:217:HOH:O	2.54	0.55
2:L:109:GLY:C	2:L:137:LEU:HD11	2.27	0.55
2:B:108:VAL:HG13	2:B:170:MET:HE3	1.88	0.55
1:I:239:VAL:O	1:I:239:VAL:HG13	2.06	0.55
1:O:305:THR:HB	2:P:186:LEU:HD13	1.88	0.54
2:D:187:GLN:O	2:D:191:GLY:N	2.39	0.54
1:O:291:TYR:OH	2:P:107:ASN:HB3	2.07	0.54
2:F:129:ILE:HD11	2:F:147:ILE:CD1	2.37	0.54
1:O:335:VAL:HG13	1:O:335:VAL:O	2.06	0.54
1:A:317:ASP:OD1	1:A:324:ASN:ND2	2.40	0.53
1:O:309:LYS:HZ2	2:P:189:ARG:HB3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:309:LYS:HZ2	2:P:189:ARG:HD2	1.72	0.53
2:H:187:GLN:O	2:H:191:GLY:N	2.39	0.53
1:K:239:VAL:HG13	1:K:239:VAL:O	2.09	0.53
2:F:109:GLY:HA2	2:F:137:LEU:CD2	2.32	0.53
1:A:250:ARG:HG3	1:A:259:ILE:HD11	1.91	0.53
1:A:223:ASN:HB3	2:B:136:ASN:HD21	1.74	0.53
1:M:326:ASN:HB2	3:M:12:SO4:S	2.49	0.53
1:E:239:VAL:HA	2:F:187:GLN:NE2	2.24	0.52
1:O:250:ARG:HG3	1:O:259:ILE:HD11	1.92	0.52
2:H:108:VAL:HG13	2:H:170:MET:HE1	1.90	0.52
2:L:187:GLN:O	2:L:191:GLY:N	2.42	0.52
2:N:108:VAL:HG13	2:N:170:MET:HE3	1.91	0.52
2:L:108:VAL:CG2	2:L:141:VAL:HG11	2.39	0.52
2:B:125:LYS:HG2	2:B:147:ILE:HD13	1.92	0.52
2:B:187:GLN:O	2:B:191:GLY:N	2.40	0.52
2:D:97:LEU:HD11	2:D:156:ALA:O	2.10	0.52
1:K:336:LEU:O	2:L:185:ASP:OD2	2.28	0.52
1:M:336:LEU:O	2:N:185:ASP:OD2	2.28	0.52
2:F:115:LEU:CD1	2:F:165:LEU:HD12	2.39	0.51
1:I:327:PHE:CE2	1:K:306:LEU:HD13	2.45	0.51
1:O:336:LEU:O	2:P:185:ASP:OD2	2.29	0.51
2:P:129:ILE:HD11	2:P:147:ILE:CD1	2.40	0.51
1:C:250:ARG:HE	1:C:256:GLU:HG3	1.75	0.51
1:K:249:VAL:HG12	1:K:281:TRP:HB2	1.93	0.51
1:K:326:ASN:HB2	3:K:13:SO4:S	2.51	0.51
1:G:239:VAL:O	1:G:239:VAL:CG1	2.59	0.51
2:H:101:PHE:CD1	2:H:145:LEU:HD13	2.46	0.51
2:P:187:GLN:O	2:P:191:GLY:N	2.41	0.51
1:O:262:ILE:HD12	1:O:277:LEU:HD23	1.92	0.51
2:P:115:LEU:HD11	2:P:165:LEU:CD2	2.41	0.51
2:F:187:GLN:O	2:F:191:GLY:N	2.42	0.51
2:N:175:ASP:OD2	1:O:323:GLU:HG2	2.10	0.50
1:I:223:ASN:HB2	2:J:135:ARG:NE	2.26	0.50
2:H:137:LEU:HD12	2:H:140:ARG:HH22	1.75	0.50
2:N:125:LYS:CG	2:N:147:ILE:HD13	2.42	0.50
2:P:133:TYR:O	2:P:140:ARG:HD3	2.11	0.50
2:J:113:ARG:NH1	2:J:130:GLU:OE1	2.45	0.50
1:A:305:THR:HB	2:B:186:LEU:HD13	1.92	0.50
2:B:129:ILE:HD11	2:B:147:ILE:CD1	2.41	0.50
2:F:108:VAL:HG22	2:F:170:MET:CE	2.42	0.50
2:L:118:GLN:HG3	2:L:168:CYS:SG	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:239:VAL:O	1:O:239:VAL:CG1	2.59	0.50
1:M:239:VAL:HG13	1:M:239:VAL:O	2.12	0.49
1:A:326:ASN:HA	1:A:329:ASN:HD22	1.76	0.49
1:C:242:LEU:HD12	1:C:274:LYS:HG3	1.94	0.49
1:C:337:GLU:OE1	2:D:178:GLN:HG2	2.11	0.49
1:K:337:GLU:HG3	2:L:158:VAL:HG23	1.94	0.49
2:N:108:VAL:HG12	2:N:109:GLY:N	2.28	0.49
2:N:187:GLN:O	2:N:191:GLY:N	2.41	0.49
1:A:336:LEU:O	2:B:185:ASP:OD2	2.30	0.49
2:B:132:ARG:HG2	2:B:133:TYR:CE2	2.47	0.49
2:D:101:PHE:CD1	2:D:145:LEU:HD13	2.46	0.49
2:H:132:ARG:HD3	2:H:133:TYR:CZ	2.48	0.49
1:I:256:GLU:OE2	1:I:256:GLU:HA	2.12	0.49
1:I:335:VAL:HG13	1:K:328:ARG:HG3	1.93	0.49
2:J:125:LYS:HG2	2:J:147:ILE:HD13	1.95	0.49
1:I:328:ARG:HG3	1:K:335:VAL:HG13	1.95	0.49
1:O:309:LYS:HZ1	2:P:189:ARG:HB3	1.76	0.49
2:J:137:LEU:CG	2:J:140:ARG:NH2	2.76	0.48
1:A:246:LYS:NZ	5:A:64:HOH:O	2.45	0.48
1:I:309:LYS:HZ2	2:J:189:ARG:CD	2.27	0.48
1:E:305:THR:HB	2:F:186:LEU:HD13	1.96	0.48
1:E:328:ARG:HG3	1:G:335:VAL:HG13	1.95	0.48
1:M:335:VAL:HG13	1:O:328:ARG:HG3	1.96	0.48
1:E:336:LEU:O	2:F:185:ASP:OD2	2.31	0.47
1:C:272:GLU:HA	1:C:275:VAL:HG22	1.94	0.47
2:J:101:PHE:CD1	2:J:145:LEU:HD13	2.50	0.47
2:J:105:CYS:SG	2:J:142:ARG:HB2	2.54	0.47
2:L:158:VAL:O	2:L:162:VAL:HG23	2.14	0.47
1:C:280:ASN:O	1:C:284:LEU:HG	2.14	0.47
2:D:129:ILE:HD11	2:D:147:ILE:HD12	1.97	0.47
1:K:239:VAL:O	1:K:239:VAL:CG1	2.62	0.47
2:L:108:VAL:CG2	2:L:141:VAL:HG21	2.44	0.47
2:H:105:CYS:SG	2:H:142:ARG:HB2	2.55	0.47
1:K:272:GLU:HA	1:K:272:GLU:OE1	2.14	0.47
1:C:336:LEU:O	2:D:185:ASP:OD2	2.33	0.47
2:J:104:ILE:HG23	2:J:108:VAL:CG2	2.44	0.47
1:M:223:ASN:HB2	2:N:135:ARG:HE	1.80	0.47
2:F:108:VAL:HG22	2:F:170:MET:HE1	1.97	0.47
1:I:239:VAL:O	1:I:239:VAL:CG1	2.62	0.47
1:A:242:LEU:HD11	1:A:273:GLN:HE21	1.79	0.46
2:L:108:VAL:HG12	2:L:170:MET:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:LEU:HD21	1:C:273:GLN:OE1	2.16	0.46
1:I:309:LYS:NZ	2:J:189:ARG:HB3	2.29	0.46
2:H:109:GLY:HA2	2:H:137:LEU:HD23	1.97	0.46
2:P:157:THR:CG2	2:P:160:HIS:ND1	2.79	0.46
1:E:306:LEU:HD13	1:G:327:PHE:CE2	2.51	0.46
1:M:337:GLU:OE1	2:N:178:GLN:HG2	2.15	0.46
1:E:315:LEU:O	1:E:319:THR:HG22	2.16	0.46
2:B:165:LEU:HD13	2:B:173:VAL:HG12	1.98	0.46
2:D:137:LEU:HD12	2:D:137:LEU:H	1.81	0.46
1:G:250:ARG:HG3	1:G:259:ILE:HD11	1.98	0.45
2:J:104:ILE:HG23	2:J:108:VAL:HG21	1.98	0.45
2:H:125:LYS:HG2	2:H:147:ILE:HD13	1.98	0.45
2:L:115:LEU:HD11	2:L:165:LEU:CD1	2.46	0.45
2:H:152:GLU:HB3	2:H:155:ASN:HB2	1.99	0.45
1:C:255:ASN:OD1	1:C:258:LYS:HG3	2.16	0.45
1:M:299:LYS:NZ	1:O:322:SER:O	2.47	0.45
1:E:316:LYS:O	1:E:319:THR:HG22	2.17	0.44
1:E:328:ARG:HH21	1:E:332:GLN:HE22	1.65	0.44
5:I:106:HOH:O	2:N:138:THR:HG23	2.18	0.44
2:P:133:TYR:CG	2:P:139:GLU:HG3	2.53	0.44
1:E:335:VAL:HG13	1:G:328:ARG:HG3	1.98	0.44
1:E:337:GLU:OE1	2:F:178:GLN:HG2	2.18	0.44
2:B:131:ASP:OD2	2:B:132:ARG:N	2.51	0.44
2:J:162:VAL:HG11	2:J:178:GLN:HE21	1.83	0.44
1:O:223:ASN:HB3	5:P:61:HOH:O	2.18	0.44
2:B:137:LEU:O	2:B:141:VAL:HG23	2.17	0.44
2:F:128:SER:O	2:F:131:ASP:OD2	2.36	0.43
2:H:104:ILE:HG23	2:H:108:VAL:CG2	2.48	0.43
1:A:328:ARG:HG3	1:C:335:VAL:CG1	2.42	0.43
1:I:335:VAL:HG13	1:I:335:VAL:O	2.18	0.43
1:G:242:LEU:HD21	1:G:273:GLN:NE2	2.34	0.43
2:D:108:VAL:HG13	2:D:170:MET:CE	2.47	0.43
2:J:129:ILE:HD11	2:J:147:ILE:HD12	2.00	0.43
1:M:258:LYS:CD	1:M:280:ASN:HD21	2.32	0.43
1:C:242:LEU:CD1	1:C:274:LYS:HG3	2.49	0.43
1:O:224:LEU:HB2	2:P:136:ASN:HD22	1.84	0.43
1:I:258:LYS:HA	1:I:258:LYS:HD3	1.89	0.42
2:J:137:LEU:HG	2:J:140:ARG:HH22	1.81	0.42
1:E:249:VAL:HG12	1:E:281:TRP:HB2	2.02	0.42
2:L:108:VAL:HG21	2:L:141:VAL:CG1	2.48	0.42
1:E:328:ARG:HE	1:E:332:GLN:NE2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:328:ARG:NE	1:K:332:GLN:NE2	2.52	0.42
2:D:108:VAL:HG12	2:D:109:GLY:N	2.35	0.42
2:H:129:ILE:HD11	2:H:147:ILE:HD12	2.01	0.42
2:P:133:TYR:HB3	2:P:139:GLU:CG	2.50	0.42
2:J:132:ARG:HG2	2:J:133:TYR:CE2	2.55	0.42
2:J:133:TYR:HE1	2:J:143:GLU:HG3	1.85	0.42
1:O:309:LYS:HZ2	2:P:189:ARG:CD	2.31	0.42
2:F:108:VAL:HG12	2:F:109:GLY:N	2.35	0.41
1:K:275:VAL:O	1:K:279:ARG:HG3	2.20	0.41
1:G:335:VAL:HG13	1:G:335:VAL:O	2.20	0.41
1:A:289:GLU:O	1:A:293:THR:CG2	2.56	0.41
1:K:249:VAL:HG12	1:K:281:TRP:CB	2.50	0.41
1:K:324:ASN:ND2	3:K:13:SO4:O3	2.45	0.41
2:P:129:ILE:HG22	2:P:140:ARG:HG2	2.01	0.41
2:P:157:THR:HG23	2:P:160:HIS:ND1	2.34	0.41
1:C:239:VAL:HB	2:D:183:ALA:HB1	2.01	0.41
1:O:309:LYS:HZ3	2:P:189:ARG:CD	2.33	0.41
2:B:189:ARG:C	2:B:189:ARG:HD3	2.41	0.41
1:M:280:ASN:O	1:M:284:LEU:HG	2.21	0.41
2:D:173:VAL:O	2:D:177:VAL:HG23	2.21	0.41
1:I:309:LYS:HZ2	2:J:189:ARG:HD2	1.86	0.41
1:G:248:PHE:CE1	1:G:293:THR:CG2	3.00	0.41
1:M:239:VAL:O	1:M:239:VAL:CG1	2.67	0.41
2:N:162:VAL:HG11	2:N:178:GLN:NE2	2.33	0.41
2:L:93:GLY:N	5:L:90:HOH:O	2.54	0.40
2:J:162:VAL:HG13	2:J:174:ALA:HB1	2.03	0.40
2:B:137:LEU:HG	2:B:140:ARG:NH2	2.37	0.40
1:C:335:VAL:HG13	1:C:335:VAL:O	2.21	0.40
1:E:250:ARG:HD2	1:E:256:GLU:OE2	2.21	0.40
1:K:331:ILE:HD13	1:K:331:ILE:HA	1.93	0.40
2:L:148:TRP:CH2	2:L:161:LEU:HG	2.56	0.40
1:M:286:GLY:N	5:M:222:HOH:O	2.29	0.40
2:N:162:VAL:O	2:N:166:ARG:HG3	2.21	0.40
2:B:104:ILE:HG23	2:B:108:VAL:CG2	2.51	0.40
2:J:189:ARG:C	2:J:189:ARG:HD3	2.42	0.40
2:L:108:VAL:HG23	2:L:109:GLY:N	2.28	0.40
2:B:163:GLY:O	2:B:167:SER:OG	2.38	0.40
1:I:316:LYS:O	1:I:319:THR:HG22	2.20	0.40
2:P:137:LEU:O	2:P:141:VAL:HG23	2.21	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	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	17	32
1	C	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	17	32
1	E	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
1	G	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
1	I	113/115 (98%)	108 (96%)	4 (4%)	1 (1%)	17	32
1	K	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	17	32
1	M	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	17	32
1	O	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
2	B	97/122 (80%)	92 (95%)	5 (5%)	0	100	100
2	D	97/122 (80%)	92 (95%)	5 (5%)	0	100	100
2	F	97/122 (80%)	93 (96%)	3 (3%)	1 (1%)	15	28
2	H	97/122 (80%)	92 (95%)	5 (5%)	0	100	100
2	J	97/122 (80%)	93 (96%)	4 (4%)	0	100	100
2	L	97/122 (80%)	92 (95%)	5 (5%)	0	100	100
2	N	97/122 (80%)	93 (96%)	3 (3%)	1 (1%)	15	28
2	P	97/122 (80%)	93 (96%)	3 (3%)	1 (1%)	15	28
All	All	1680/1896 (89%)	1592 (95%)	80 (5%)	8 (0%)	29	48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	GLU
1	C	256	GLU
1	K	256	GLU
1	M	256	GLU
1	I	256	GLU
2	F	108	VAL

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Mol	Chain	Res	Type
2	N	108	VAL
2	P	108	VAL

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	105/105 (100%)	103 (98%)	2 (2%)	57	74
1	C	105/105 (100%)	98 (93%)	7 (7%)	16	29
1	E	105/105 (100%)	97 (92%)	8 (8%)	13	23
1	G	105/105 (100%)	99 (94%)	6 (6%)	20	36
1	I	105/105 (100%)	99 (94%)	6 (6%)	20	36
1	K	105/105 (100%)	96 (91%)	9 (9%)	10	19
1	M	105/105 (100%)	99 (94%)	6 (6%)	20	36
1	O	105/105 (100%)	95 (90%)	10 (10%)	8	15
2	B	87/107 (81%)	72 (83%)	15 (17%)	2	3
2	D	87/107 (81%)	83 (95%)	4 (5%)	27	46
2	F	87/107 (81%)	82 (94%)	5 (6%)	20	36
2	H	87/107 (81%)	77 (88%)	10 (12%)	5	9
2	J	87/107 (81%)	77 (88%)	10 (12%)	5	9
2	L	87/107 (81%)	78 (90%)	9 (10%)	7	13
2	N	87/107 (81%)	79 (91%)	8 (9%)	9	17
2	P	87/107 (81%)	74 (85%)	13 (15%)	3	3
All	All	1536/1696 (91%)	1408 (92%)	128 (8%)	11	20

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	ASP
1	A	322	SER

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Mol	Chain	Res	Type
2	B	111	ASP
2	B	114	ARG
2	B	120	LYS
2	B	123	ASP
2	B	131	ASP
2	B	144	SER
2	B	146	ARG
2	B	151	THR
2	B	152	GLU
2	B	154	GLU
2	B	157	THR
2	B	167	SER
2	B	168	CYS
2	B	189	ARG
2	B	190	SER
1	C	270	THR
1	C	272	GLU
1	C	319	THR
1	C	322	SER
1	C	333	SER
1	C	335	VAL
1	C	336	LEU
2	D	110	LYS
2	D	111	ASP
2	D	149	LYS
2	D	189	ARG
1	E	261	GLU
1	E	268	GLN
1	E	283	GLN
1	E	320	SER
1	E	322	SER
1	E	326	ASN
1	E	335	VAL
1	E	336	LEU
2	F	136	ASN
2	F	137	LEU
2	F	157	THR
2	F	167	SER
2	F	189	ARG
1	G	225	SER
1	G	239	VAL
1	G	243	SER

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Mol	Chain	Res	Type
1	G	270	THR
1	G	287	LYS
1	G	335	VAL
2	H	110	LYS
2	H	111	ASP
2	H	114	ARG
2	H	125	LYS
2	H	136	ASN
2	H	144	SER
2	H	150	ASN
2	H	154	GLU
2	H	157	THR
2	H	190	SER
1	I	239	VAL
1	I	243	SER
1	I	270	THR
1	I	283	GLN
1	I	319	THR
1	I	335	VAL
2	J	110	LYS
2	J	111	ASP
2	J	117	ARG
2	J	137	LEU
2	J	143	GLU
2	J	151	THR
2	J	157	THR
2	J	160	HIS
2	J	189	ARG
2	J	190	SER
1	K	223	ASN
1	K	239	VAL
1	K	243	SER
1	K	276	GLN
1	K	287	LYS
1	K	319	THR
1	K	320	SER
1	K	333	SER
1	K	335	VAL
2	L	111	ASP
2	L	117	ARG
2	L	125	LYS
2	L	136	ASN

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Mol	Chain	Res	Type
2	L	157	THR
2	L	165	LEU
2	L	167	SER
2	L	189	ARG
2	L	190	SER
1	M	239	VAL
1	M	268	GLN
1	M	283	GLN
1	M	319	THR
1	M	333	SER
1	M	335	VAL
2	N	110	LYS
2	N	111	ASP
2	N	115	LEU
2	N	125	LYS
2	N	128	SER
2	N	136	ASN
2	N	152	GLU
2	N	189	ARG
1	O	239	VAL
1	O	243	SER
1	O	255	ASN
1	O	270	THR
1	O	280	ASN
1	O	287	LYS
1	O	288	LYS
1	O	321	ASP
1	O	323	GLU
1	O	335	VAL
2	P	105	CYS
2	P	110	LYS
2	P	111	ASP
2	P	115	LEU
2	P	139	GLU
2	P	142	ARG
2	P	144	SER
2	P	151	THR
2	P	157	THR
2	P	161	LEU
2	P	167	SER
2	P	168	CYS
2	P	170	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	A	324	ASN
1	A	329	ASN
1	A	332	GLN
2	B	136	ASN
2	B	178	GLN
1	C	252	ASN
1	C	280	ASN
2	D	160	HIS
2	D	178	GLN
1	E	280	ASN
1	E	332	GLN
1	G	273	GLN
1	K	252	ASN
1	K	280	ASN
1	K	332	GLN
2	L	155	ASN
1	M	252	ASN
1	M	280	ASN
1	M	311	GLN
2	N	107	ASN
2	N	178	GLN
1	O	280	ASN
1	O	332	GLN
2	P	136	ASN
2	P	178	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 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
3	SO4	C	7	-	4,4,4	0.15	0	6,6,6	0.50	0
3	SO4	K	3	-	4,4,4	0.17	0	6,6,6	0.69	0
3	SO4	I	6	-	4,4,4	0.11	0	6,6,6	0.42	0
3	SO4	A	10	-	4,4,4	0.18	0	6,6,6	0.23	0
3	SO4	J	8	-	4,4,4	0.14	0	6,6,6	0.20	0
3	SO4	K	13	-	4,4,4	0.15	0	6,6,6	0.36	0
3	SO4	O	4	-	4,4,4	0.11	0	6,6,6	0.30	0
3	SO4	G	2	-	4,4,4	0.14	0	6,6,6	0.50	0
3	SO4	M	12	-	4,4,4	0.18	0	6,6,6	0.13	0
3	SO4	E	1	-	4,4,4	0.19	0	6,6,6	0.50	0
3	SO4	M	9	-	4,4,4	0.13	0	6,6,6	0.35	0
3	SO4	E	11	-	4,4,4	0.15	0	6,6,6	0.12	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	13	SO4	2	0
3	M	12	SO4	1	0

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.