Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 10:18 PM EDT

PDB ID	:	2FUM
Title	:	Catalytic domain of protein kinase PknB from Mycobacterium tuberculosis in complex with mitoxantrone
Authors	:	Wehenkel, A.; Alzari, P.M.
Deposited on	:	2006-01-27
Resolution	:	2.89 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:

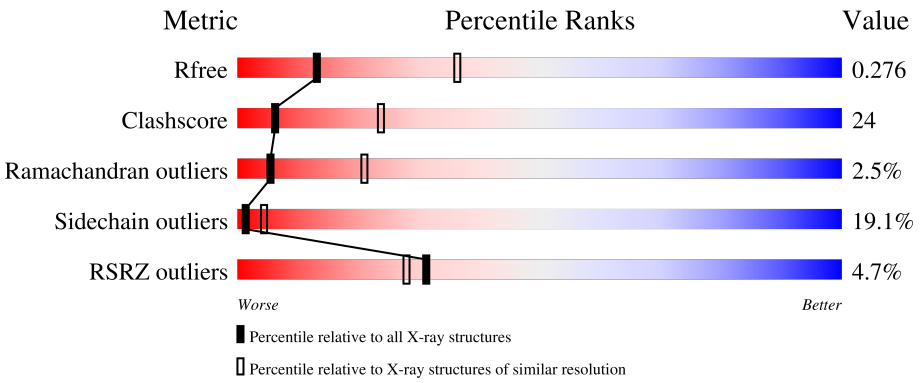
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	299	.% 47% 32% 8% • 12%
1	B	299	4% 44% 33% 9% • 12%
1	C	299	2% 44% 33% 7% • 15%
1	D	299	10% 45% 33% 7% 14%

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
2	MIX	D	3539	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7998 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 Probable serine/threonine-protein kinase pknB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	1994	1249	354	383	8	0	0	0
1	B	262	1991	1247	357	379	8	0	0	0
1	C	254	1931	1211	340	372	8	0	0	0
1	D	258	1954	1225	347	374	8	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	cloning artifact	UNP P0A5S4
A	-18	GLY	-	cloning artifact	UNP P0A5S4
A	-17	SER	-	cloning artifact	UNP P0A5S4
A	-16	SER	-	cloning artifact	UNP P0A5S4
A	-15	HIS	-	cloning artifact	UNP P0A5S4
A	-14	HIS	-	cloning artifact	UNP P0A5S4
A	-13	HIS	-	cloning artifact	UNP P0A5S4
A	-12	HIS	-	cloning artifact	UNP P0A5S4
A	-11	HIS	-	cloning artifact	UNP P0A5S4
A	-10	HIS	-	cloning artifact	UNP P0A5S4
A	-9	SER	-	cloning artifact	UNP P0A5S4
A	-8	SER	-	cloning artifact	UNP P0A5S4
A	-7	GLY	-	cloning artifact	UNP P0A5S4
A	-6	LEU	-	cloning artifact	UNP P0A5S4
A	-5	VAL	-	cloning artifact	UNP P0A5S4
A	-4	PRO	-	cloning artifact	UNP P0A5S4
A	-3	ARG	-	cloning artifact	UNP P0A5S4
A	-2	GLY	-	cloning artifact	UNP P0A5S4
A	-1	SER	-	cloning artifact	UNP P0A5S4
A	0	HIS	-	cloning artifact	UNP P0A5S4
B	-19	MET	-	cloning artifact	UNP P0A5S4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	cloning artifact	UNP P0A5S4
B	-17	SER	-	cloning artifact	UNP P0A5S4
B	-16	SER	-	cloning artifact	UNP P0A5S4
B	-15	HIS	-	cloning artifact	UNP P0A5S4
B	-14	HIS	-	cloning artifact	UNP P0A5S4
B	-13	HIS	-	cloning artifact	UNP P0A5S4
B	-12	HIS	-	cloning artifact	UNP P0A5S4
B	-11	HIS	-	cloning artifact	UNP P0A5S4
B	-10	HIS	-	cloning artifact	UNP P0A5S4
B	-9	SER	-	cloning artifact	UNP P0A5S4
B	-8	SER	-	cloning artifact	UNP P0A5S4
B	-7	GLY	-	cloning artifact	UNP P0A5S4
B	-6	LEU	-	cloning artifact	UNP P0A5S4
B	-5	VAL	-	cloning artifact	UNP P0A5S4
B	-4	PRO	-	cloning artifact	UNP P0A5S4
B	-3	ARG	-	cloning artifact	UNP P0A5S4
B	-2	GLY	-	cloning artifact	UNP P0A5S4
B	-1	SER	-	cloning artifact	UNP P0A5S4
B	0	HIS	-	cloning artifact	UNP P0A5S4
C	-19	MET	-	cloning artifact	UNP P0A5S4
C	-18	GLY	-	cloning artifact	UNP P0A5S4
C	-17	SER	-	cloning artifact	UNP P0A5S4
C	-16	SER	-	cloning artifact	UNP P0A5S4
C	-15	HIS	-	cloning artifact	UNP P0A5S4
C	-14	HIS	-	cloning artifact	UNP P0A5S4
C	-13	HIS	-	cloning artifact	UNP P0A5S4
C	-12	HIS	-	cloning artifact	UNP P0A5S4
C	-11	HIS	-	cloning artifact	UNP P0A5S4
C	-10	HIS	-	cloning artifact	UNP P0A5S4
C	-9	SER	-	cloning artifact	UNP P0A5S4
C	-8	SER	-	cloning artifact	UNP P0A5S4
C	-7	GLY	-	cloning artifact	UNP P0A5S4
C	-6	LEU	-	cloning artifact	UNP P0A5S4
C	-5	VAL	-	cloning artifact	UNP P0A5S4
C	-4	PRO	-	cloning artifact	UNP P0A5S4
C	-3	ARG	-	cloning artifact	UNP P0A5S4
C	-2	GLY	-	cloning artifact	UNP P0A5S4
C	-1	SER	-	cloning artifact	UNP P0A5S4
C	0	HIS	-	cloning artifact	UNP P0A5S4
D	-19	MET	-	cloning artifact	UNP P0A5S4
D	-18	GLY	-	cloning artifact	UNP P0A5S4
D	-17	SER	-	cloning artifact	UNP P0A5S4

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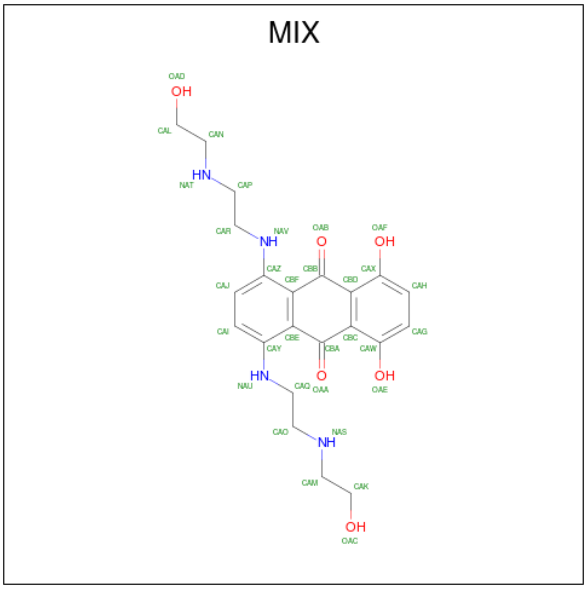
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	cloning artifact	UNP P0A5S4
D	-15	HIS	-	cloning artifact	UNP P0A5S4
D	-14	HIS	-	cloning artifact	UNP P0A5S4
D	-13	HIS	-	cloning artifact	UNP P0A5S4
D	-12	HIS	-	cloning artifact	UNP P0A5S4
D	-11	HIS	-	cloning artifact	UNP P0A5S4
D	-10	HIS	-	cloning artifact	UNP P0A5S4
D	-9	SER	-	cloning artifact	UNP P0A5S4
D	-8	SER	-	cloning artifact	UNP P0A5S4
D	-7	GLY	-	cloning artifact	UNP P0A5S4
D	-6	LEU	-	cloning artifact	UNP P0A5S4
D	-5	VAL	-	cloning artifact	UNP P0A5S4
D	-4	PRO	-	cloning artifact	UNP P0A5S4
D	-3	ARG	-	cloning artifact	UNP P0A5S4
D	-2	GLY	-	cloning artifact	UNP P0A5S4
D	-1	SER	-	cloning artifact	UNP P0A5S4
D	0	HIS	-	cloning artifact	UNP P0A5S4

- Molecule 2 is 1,4-DIHYDROXY-5,8-BIS({2-[(2-HYDROXYETHYL)AMINO]ETHYL}AMINO)-9,10-ANTHRACENEDIONE (three-letter code: MIX) (formula: $C_{22}H_{28}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	32	22	4	6	0	0
			Total	C	N	O		
2	B	1	32	22	4	6	0	0

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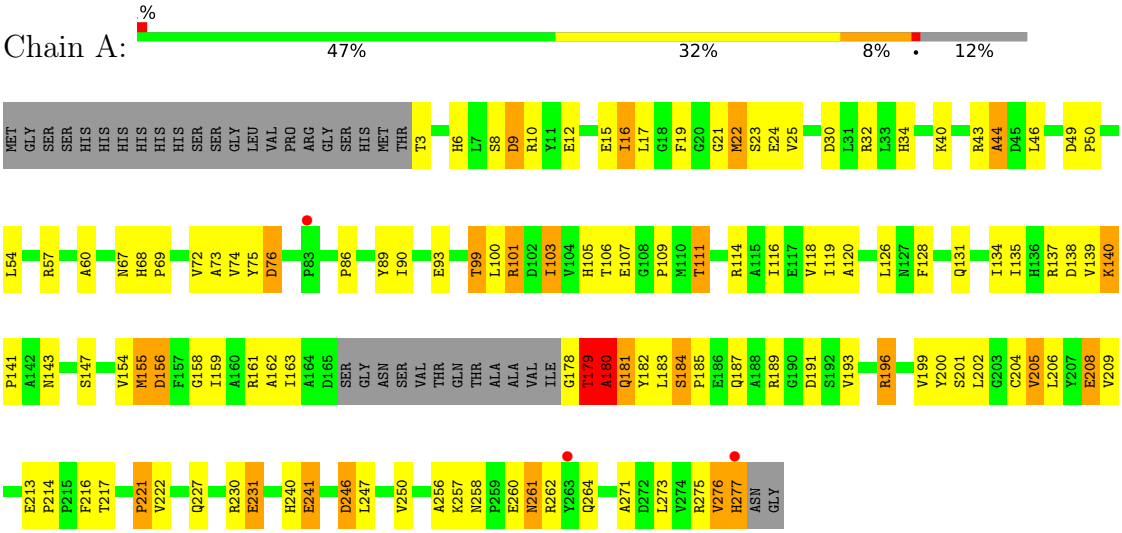
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	32	22	4	6	0	0
			Total	C	N	O		
2	D	1	32	22	4	6	0	0

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.

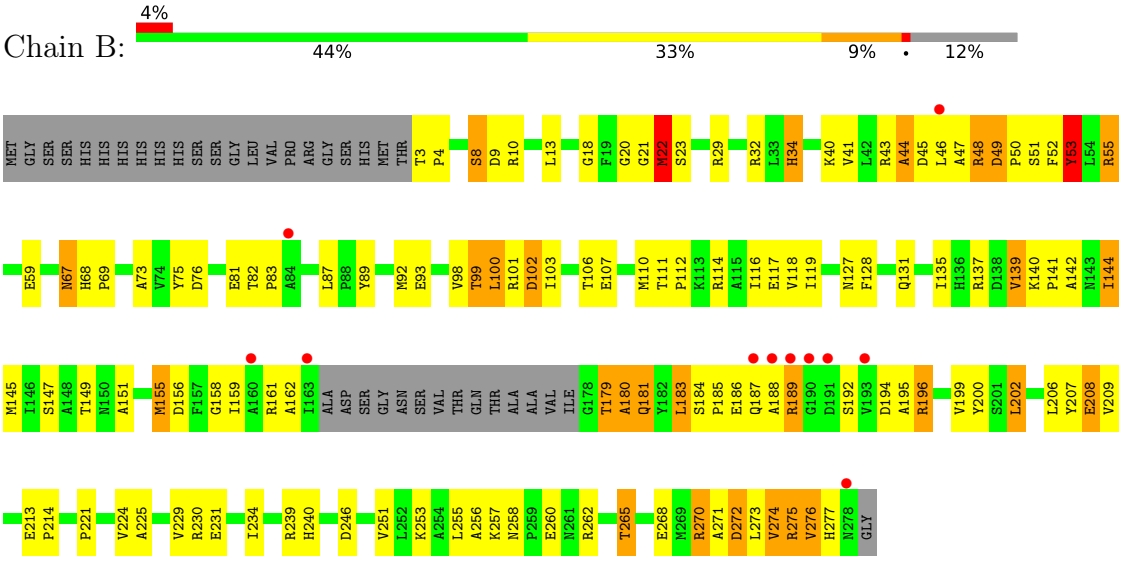
• Molecule 1: Probable serine/threonine-protein kinase pknB

Chain A:



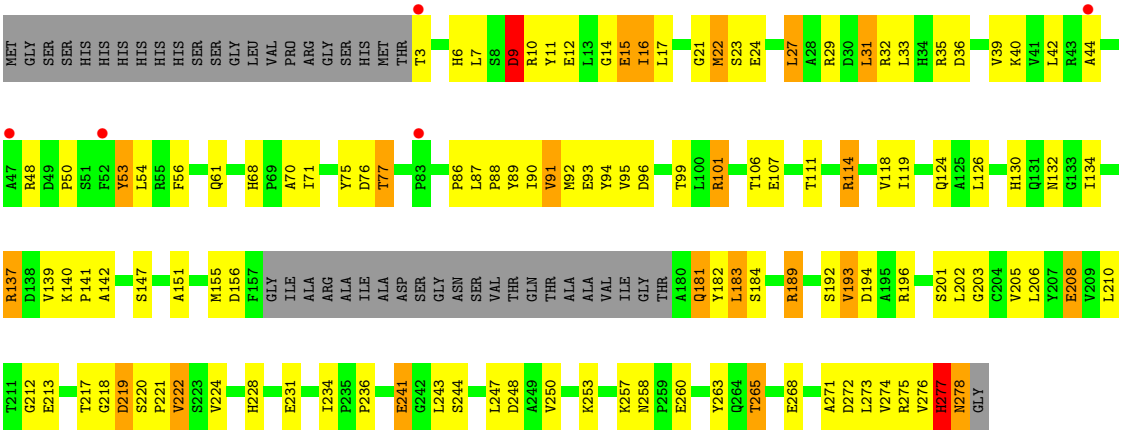
• Molecule 1: Probable serine/threonine-protein kinase pknB

Chain B:



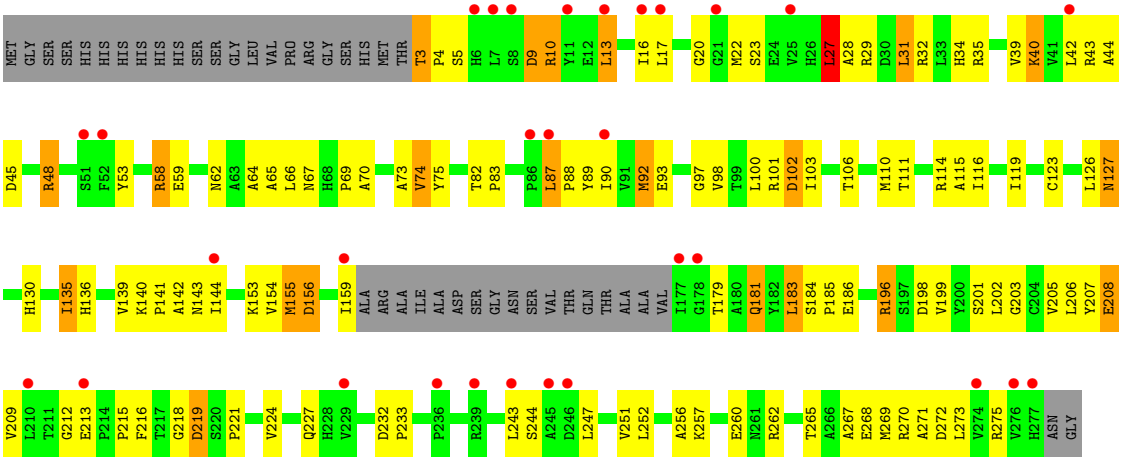
• Molecule 1: Probable serine/threonine-protein kinase pknB

Chain C:



• Molecule 1: Probable serine/threonine-protein kinase pknB

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	116.86Å 116.86Å 260.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.84 – 2.89 58.43 – 2.89	Depositor EDS
% Data completeness (in resolution range)	68.1 (69.84-2.89) 68.1 (58.43-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.218 , 0.278 0.214 , 0.276	Depositor DCC
R_{free} test set	1426 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	97.6	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 114.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7998	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% 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: MIX

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	0.74	0/2035	0.89	1/2775 (0.0%)
1	B	0.78	0/2032	0.93	7/2770 (0.3%)
1	C	0.69	0/1972	0.85	0/2691
1	D	0.63	0/1994	0.76	1/2719 (0.0%)
All	All	0.71	0/8033	0.86	9/10955 (0.1%)

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	A	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	180	ALA	N-CA-C	7.83	132.14	111.00
1	A	179	THR	N-CA-C	7.64	131.64	111.00
1	B	179	THR	N-CA-C	6.64	128.94	111.00
1	B	183	LEU	CB-CG-CD1	-6.29	100.30	111.00
1	B	22	MET	N-CA-C	5.67	126.31	111.00
1	B	92	MET	CB-CG-SD	-5.66	95.43	112.40
1	D	27	LEU	CA-CB-CG	5.39	127.70	115.30
1	B	53	TYR	CB-CA-C	-5.14	100.12	110.40
1	B	87	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLY	Peptide
1	A	180	ALA	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	1994	0	1940	101	0
1	B	1991	0	1944	100	0
1	C	1931	0	1868	86	0
1	D	1954	0	1908	99	0
2	A	32	0	26	2	0
2	B	32	0	27	4	0
2	C	32	0	27	1	0
2	D	32	0	28	6	0
All	All	7998	0	7768	384	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 24.

All (384) 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)
1:D:116:ILE:CD1	1:D:116:ILE:CG1	1.76	1.63
1:B:99:THR:HG21	1:B:142:ALA:HA	1.16	1.16
1:C:189:ARG:HB2	1:C:189:ARG:NH1	1.64	1.12
1:B:180:ALA:HB2	1:B:221:PRO:HA	1.39	1.04
1:C:181:GLN:HG3	1:C:224:VAL:HG11	1.39	1.02
1:C:181:GLN:CG	1:C:224:VAL:HG11	1.92	0.98
1:B:99:THR:CG2	1:B:142:ALA:HA	1.95	0.95
1:A:138:ASP:HB2	1:A:159:ILE:HD11	1.48	0.94
1:B:234:ILE:HD12	1:B:239:ARG:HH11	1.32	0.94
1:D:216:PHE:CD2	1:D:227:GLN:HB3	2.03	0.93
1:D:136:HIS:HE1	1:D:156:ASP:O	1.53	0.89
1:B:99:THR:HG22	1:B:141:PRO:O	1.72	0.89
1:C:189:ARG:HB2	1:C:189:ARG:CZ	2.03	0.88
1:A:10:ARG:NH2	1:B:76:ASP:OD1	2.05	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ARG:NH2	1:D:260:GLU:HG3	1.91	0.86
1:C:137:ARG:HH21	1:C:193:VAL:HG21	1.38	0.86
1:D:136:HIS:CE1	1:D:156:ASP:O	2.29	0.85
1:B:48:ARG:NH1	1:B:48:ARG:HA	1.90	0.85
1:A:50:PRO:HA	1:C:222:VAL:HG21	1.59	0.85
1:A:72:VAL:HG21	1:A:155:MET:HB3	1.57	0.83
1:B:100:LEU:HD22	1:B:144:ILE:HB	1.61	0.82
1:B:49:ASP:HB3	1:B:52:PHE:HD1	1.45	0.82
1:C:68:HIS:HD2	1:C:70:ALA:H	1.26	0.81
1:D:181:GLN:HB2	1:D:224:VAL:HG11	1.61	0.81
1:A:8:SER:O	1:A:9:ASP:HB2	1.80	0.81
1:B:99:THR:HG21	1:B:142:ALA:CA	2.07	0.81
1:B:155:MET:HG2	1:B:156:ASP:N	1.95	0.81
1:C:10:ARG:HG3	1:C:32:ARG:HG3	1.63	0.81
1:C:137:ARG:NH2	1:C:193:VAL:HG21	1.96	0.80
1:B:112:PRO:O	1:B:116:ILE:HG12	1.81	0.80
1:A:43:ARG:CB	1:A:46:LEU:HD23	2.12	0.80
1:D:181:GLN:CB	1:D:224:VAL:HG11	2.12	0.80
1:B:43:ARG:CB	1:B:46:LEU:HD23	2.14	0.78
1:A:100:LEU:HA	1:A:103:ILE:HG22	1.65	0.76
1:B:231:GLU:O	1:B:257:LYS:NZ	2.18	0.76
1:C:189:ARG:CZ	1:C:189:ARG:CB	2.64	0.75
1:C:35:ARG:HD3	1:D:64:ALA:HB1	1.70	0.74
1:D:116:ILE:CD1	1:D:116:ILE:CB	2.66	0.74
1:C:189:ARG:HB2	1:C:189:ARG:HH11	1.53	0.74
1:A:114:ARG:O	1:A:118:VAL:HG23	1.88	0.73
1:D:110:MET:SD	1:D:115:ALA:HA	2.28	0.73
1:D:270:ARG:HA	1:D:273:LEU:HB2	1.71	0.73
1:B:50:PRO:HA	1:B:53:TYR:HB2	1.70	0.73
1:A:111:THR:HG23	1:A:114:ARG:HB2	1.71	0.73
1:A:179:THR:HG23	1:A:180:ALA:N	2.04	0.72
1:C:119:ILE:HG13	1:C:206:LEU:HD13	1.71	0.72
1:A:271:ALA:HB1	1:A:275:ARG:HH22	1.52	0.72
1:C:101:ARG:HH11	1:C:101:ARG:HB3	1.52	0.72
1:D:205:VAL:O	1:D:209:VAL:HG13	1.90	0.72
1:D:256:ALA:O	1:D:262:ARG:HD2	1.89	0.71
1:A:206:LEU:O	1:A:209:VAL:HG22	1.90	0.71
1:D:181:GLN:HA	1:D:183:LEU:CD1	2.21	0.71
1:B:116:ILE:HG21	1:B:277:HIS:HB2	1.72	0.71
1:B:119:ILE:HG23	1:B:202:LEU:CD2	2.21	0.70
1:A:43:ARG:O	1:A:44:ALA:CB	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:HIS:CE1	1:C:12:GLU:HG3	2.28	0.69
1:B:67:ASN:C	1:B:67:ASN:OD1	2.31	0.69
1:B:270:ARG:O	1:B:274:VAL:HG23	1.93	0.69
1:A:140:LYS:HB2	1:A:141:PRO:HD2	1.73	0.68
1:D:247:LEU:O	1:D:251:VAL:HG23	1.94	0.68
1:A:181:GLN:H	1:A:181:GLN:HE21	1.41	0.67
1:D:23:SER:HB3	1:D:40:LYS:HG2	1.76	0.67
1:C:202:LEU:O	1:C:205:VAL:HG12	1.93	0.67
1:C:101:ARG:HB3	1:C:101:ARG:NH1	2.08	0.67
1:A:141:PRO:HD3	1:A:205:VAL:HG13	1.77	0.67
1:D:206:LEU:O	1:D:209:VAL:HG22	1.95	0.67
1:A:73:ALA:H	1:A:93:GLU:HG2	1.59	0.67
1:D:22:MET:HG3	1:D:23:SER:N	2.09	0.66
1:C:220:SER:O	1:C:224:VAL:HG23	1.96	0.66
1:B:140:LYS:HE2	2:B:1539:MIX:HAL2	1.78	0.66
1:A:68:HIS:ND1	1:A:69:PRO:HD2	2.11	0.66
1:B:137:ARG:HH21	1:B:161:ARG:CB	2.09	0.65
1:B:225:ALA:O	1:B:229:VAL:HG23	1.96	0.65
1:A:8:SER:O	1:A:9:ASP:CB	2.42	0.65
1:B:214:PRO:O	1:B:239:ARG:NH2	2.30	0.65
1:C:114:ARG:O	1:C:118:VAL:HG23	1.95	0.65
1:B:184:SER:HA	1:B:200:TYR:CD2	2.32	0.64
1:C:236:PRO:HG2	1:C:248:ASP:OD2	1.98	0.64
1:C:50:PRO:HA	1:C:53:TYR:HD2	1.62	0.64
1:C:94:TYR:C	1:C:94:TYR:CD2	2.71	0.64
1:D:181:GLN:HA	1:D:183:LEU:HD11	1.78	0.64
1:B:68:HIS:ND1	1:B:69:PRO:HD2	2.12	0.63
1:C:94:TYR:CD2	1:C:95:VAL:N	2.66	0.63
1:A:246:ASP:HB2	1:A:276:VAL:HG11	1.80	0.63
1:C:68:HIS:HB3	1:C:71:ILE:HD12	1.78	0.63
1:D:3:THR:HG22	1:D:4:PRO:HD3	1.81	0.63
1:B:43:ARG:O	1:B:44:ALA:CB	2.45	0.63
1:A:72:VAL:CG2	1:A:155:MET:HB3	2.28	0.63
1:C:194:ASP:OD2	1:C:196:ARG:NE	2.24	0.63
1:C:271:ALA:C	1:C:275:ARG:HD2	2.19	0.63
1:A:140:LYS:HB2	1:A:182:TYR:CD2	2.34	0.62
1:B:180:ALA:HB1	1:B:224:VAL:HB	1.81	0.62
1:C:276:VAL:C	1:C:278:ASN:H	2.03	0.62
1:B:102:ASP:OD1	1:B:102:ASP:N	2.33	0.61
1:A:138:ASP:HB2	1:A:159:ILE:CD1	2.27	0.61
1:D:69:PRO:O	1:D:153:LYS:NZ	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:VAL:HB	1:D:102:ASP:OD1	2.01	0.61
1:D:100:LEU:HA	1:D:103:ILE:HD12	1.83	0.61
1:B:48:ARG:HA	1:B:48:ARG:HH11	1.66	0.60
1:A:179:THR:HG23	1:A:180:ALA:H	1.66	0.60
1:D:22:MET:HG3	1:D:23:SER:H	1.65	0.60
1:D:116:ILE:CD1	1:D:116:ILE:HG21	2.32	0.60
2:A:539:MIX:OAA	2:A:539:MIX:NAU	2.33	0.60
1:D:196:ARG:HH22	1:D:260:GLU:HG3	1.67	0.60
1:A:271:ALA:CB	1:A:275:ARG:HH22	2.15	0.59
1:B:181:GLN:H	1:B:181:GLN:HE21	1.51	0.59
1:B:116:ILE:HG23	1:B:273:LEU:CD2	2.33	0.59
1:C:29:ARG:HG2	1:C:36:ASP:OD2	2.02	0.59
1:B:180:ALA:CB	1:B:221:PRO:HA	2.26	0.59
1:B:256:ALA:HB3	1:B:262:ARG:HG3	1.84	0.59
1:A:111:THR:HG23	1:A:114:ARG:CB	2.33	0.59
1:B:49:ASP:HB3	1:B:52:PHE:CD1	2.34	0.59
1:D:42:LEU:HD12	1:D:43:ARG:H	1.67	0.59
1:B:116:ILE:HG23	1:B:273:LEU:HD22	1.84	0.58
1:D:116:ILE:CD1	1:D:116:ILE:CG2	2.81	0.58
1:D:116:ILE:HG21	1:D:116:ILE:HD13	1.85	0.58
1:B:98:VAL:HG23	1:B:103:ILE:HD11	1.84	0.58
1:A:201:SER:O	1:A:205:VAL:HG23	2.03	0.58
1:C:181:GLN:HG2	1:C:224:VAL:HG11	1.83	0.58
1:B:185:PRO:HD3	1:B:200:TYR:CE2	2.39	0.58
1:B:119:ILE:HG23	1:B:202:LEU:HD21	1.85	0.57
1:B:145:MET:SD	1:B:155:MET:HE1	2.45	0.57
1:A:180:ALA:HB2	1:A:221:PRO:HA	1.86	0.56
1:A:60:ALA:HB2	1:A:90:ILE:HG12	1.88	0.56
1:A:271:ALA:HB1	1:A:275:ARG:NH2	2.21	0.56
1:C:29:ARG:O	1:C:31:LEU:HD13	2.06	0.56
1:D:139:VAL:HB	1:D:201:SER:HB2	1.87	0.55
1:D:143:ASN:HD21	2:D:3539:MIX:HAP2	1.72	0.55
1:A:75:TYR:O	1:A:76:ASP:HB2	2.07	0.55
1:C:276:VAL:O	1:C:278:ASN:N	2.37	0.55
1:A:139:VAL:HB	1:A:201:SER:HB3	1.86	0.55
1:A:256:ALA:HB1	1:A:261:ASN:HB2	1.88	0.55
1:D:53:TYR:C	1:D:53:TYR:CD2	2.79	0.55
1:B:34:HIS:ND1	1:B:34:HIS:N	2.53	0.55
1:B:43:ARG:O	1:B:44:ALA:HB2	2.07	0.55
1:C:250:VAL:HG13	1:C:263:TYR:OH	2.07	0.55
1:D:39:VAL:HA	1:D:90:ILE:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2539:MIX:OAB	2:C:2539:MIX:NAV	2.36	0.54
1:D:196:ARG:HH21	1:D:260:GLU:HG3	1.68	0.54
1:A:156:ASP:C	1:A:158:GLY:H	2.11	0.54
1:D:110:MET:SD	1:D:115:ALA:CA	2.95	0.54
1:D:232:ASP:OD1	1:D:233:PRO:HD2	2.07	0.54
1:C:277:HIS:O	1:C:278:ASN:ND2	2.35	0.54
1:D:127:ASN:HD21	1:D:265:THR:HB	1.72	0.54
1:A:43:ARG:O	1:A:44:ALA:HB2	2.08	0.54
1:D:92:MET:HE2	2:D:3539:MIX:HAH	1.90	0.54
1:A:99:THR:OG1	1:A:101:ARG:HB3	2.07	0.54
1:B:258:ASN:ND2	1:B:260:GLU:HB2	2.22	0.54
1:B:155:MET:CG	1:B:156:ASP:N	2.63	0.53
1:B:189:ARG:HB2	1:B:189:ARG:NH1	2.23	0.53
1:A:258:ASN:HB3	1:A:261:ASN:ND2	2.23	0.53
1:A:189:ARG:HH21	1:A:189:ARG:HB2	1.73	0.53
1:B:4:PRO:HG3	1:B:82:THR:HG21	1.89	0.53
2:B:1539:MIX:OAE	2:B:1539:MIX:OAA	2.20	0.53
1:D:98:VAL:HG12	2:D:3539:MIX:HAS	1.73	0.53
1:A:137:ARG:NH2	1:A:161:ARG:CB	2.72	0.53
1:C:139:VAL:HB	1:C:201:SER:HB3	1.91	0.53
1:D:141:PRO:HD3	1:D:205:VAL:HG22	1.91	0.53
1:C:140:LYS:HE2	1:C:142:ALA:HB3	1.91	0.53
1:A:179:THR:CG2	1:A:180:ALA:N	2.70	0.52
1:C:101:ARG:HG3	1:C:141:PRO:HG2	1.91	0.52
1:B:67:ASN:OD1	1:B:67:ASN:O	2.28	0.52
1:B:55:ARG:O	1:B:59:GLU:HB2	2.09	0.52
1:B:147:SER:HB3	1:B:151:ALA:H	1.74	0.52
1:D:179:THR:O	1:D:181:GLN:HG3	2.10	0.52
1:B:135:ILE:HD12	1:B:135:ILE:H	1.75	0.52
1:A:68:HIS:HB2	1:A:128:PHE:CD1	2.45	0.52
1:B:127:ASN:OD1	1:B:265:THR:HG22	2.10	0.52
1:C:22:MET:HB2	1:C:42:LEU:HD12	1.91	0.52
1:C:182:TYR:HE1	1:C:208:GLU:HG3	1.75	0.51
1:C:258:ASN:HD22	1:C:260:GLU:H	1.58	0.51
1:B:272:ASP:O	1:B:276:VAL:HG23	2.10	0.51
1:D:181:GLN:HB2	1:D:224:VAL:CG1	2.38	0.51
1:D:181:GLN:HB3	1:D:224:VAL:HG11	1.92	0.51
1:D:111:THR:O	1:D:114:ARG:HB3	2.10	0.51
1:C:33:LEU:HG	1:D:64:ALA:HB2	1.91	0.51
1:C:181:GLN:HG2	1:C:181:GLN:O	2.11	0.51
1:A:72:VAL:HG23	1:A:154:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:MET:HB2	1:C:42:LEU:CD1	2.41	0.50
1:D:82:THR:HB	1:D:83:PRO:HD2	1.92	0.50
1:D:143:ASN:ND2	2:D:3539:MIX:HAP2	2.26	0.50
1:A:68:HIS:ND1	1:A:69:PRO:CD	2.74	0.50
1:D:70:ALA:O	1:D:154:VAL:HG23	2.11	0.50
1:D:75:TYR:OH	1:D:93:GLU:HB3	2.11	0.50
1:B:181:GLN:HE21	1:B:181:GLN:N	2.09	0.50
1:D:203:GLY:O	1:D:206:LEU:HB3	2.11	0.50
1:A:277:HIS:C	1:A:277:HIS:CD2	2.84	0.50
1:C:147:SER:HB3	1:C:151:ALA:H	1.77	0.50
1:D:87:LEU:HD12	1:D:88:PRO:HD2	1.93	0.50
1:D:216:PHE:HD2	1:D:227:GLN:HB3	1.68	0.50
1:A:6:HIS:CD2	1:A:12:GLU:HG3	2.46	0.50
1:A:119:ILE:HG13	1:A:206:LEU:HD13	1.94	0.50
1:A:179:THR:CG2	1:A:180:ALA:H	2.25	0.50
1:A:189:ARG:HB2	1:A:189:ARG:NH2	2.27	0.50
1:B:100:LEU:HD22	1:B:144:ILE:CB	2.36	0.50
1:A:196:ARG:O	1:A:199:VAL:HB	2.12	0.49
1:A:101:ARG:HH11	1:A:101:ARG:HB2	1.78	0.49
1:A:49:ASP:OD2	1:A:49:ASP:C	2.51	0.49
1:B:194:ASP:OD1	1:B:196:ARG:HD3	2.13	0.49
1:C:10:ARG:HD3	1:C:11:TYR:CE2	2.48	0.49
1:B:40:LYS:O	1:B:89:TYR:HA	2.13	0.48
1:D:119:ILE:HD12	1:D:202:LEU:HD11	1.95	0.48
1:D:184:SER:OG	1:D:186:GLU:OE1	2.31	0.48
1:A:134:ILE:HD13	1:A:162:ALA:HA	1.95	0.48
1:D:64:ALA:HA	1:D:74:VAL:CG2	2.42	0.48
1:B:99:THR:CG2	1:B:141:PRO:O	2.54	0.48
1:D:272:ASP:HA	1:D:275:ARG:HB2	1.96	0.48
1:A:99:THR:HG1	1:A:101:ARG:HB3	1.78	0.48
1:A:185:PRO:HD3	1:A:200:TYR:CE2	2.49	0.48
1:B:75:TYR:O	1:B:76:ASP:HB2	2.12	0.48
1:A:216:PHE:CD2	1:A:227:GLN:HB3	2.49	0.48
1:A:109:PRO:HG3	1:A:240:HIS:CE1	2.49	0.48
1:A:205:VAL:O	1:A:209:VAL:HG13	2.14	0.48
1:B:103:ILE:HG21	1:B:110:MET:CE	2.43	0.48
1:C:61:GLN:OE1	1:D:34:HIS:ND1	2.47	0.48
1:A:231:GLU:O	1:A:257:LYS:HE3	2.13	0.47
1:B:73:ALA:H	1:B:93:GLU:HB2	1.79	0.47
1:B:268:GLU:O	1:B:271:ALA:HB3	2.14	0.47
1:C:94:TYR:HE2	1:C:96:ASP:CA	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ARG:HH11	1:A:101:ARG:CG	2.27	0.47
1:C:268:GLU:O	1:C:271:ALA:HB3	2.13	0.47
1:D:233:PRO:HD3	1:D:257:LYS:HE3	1.95	0.47
1:A:21:GLY:O	1:A:23:SER:N	2.39	0.47
1:B:258:ASN:CG	1:B:260:GLU:HB2	2.34	0.47
1:D:208:GLU:O	1:D:212:GLY:N	2.46	0.47
1:A:86:PRO:HG2	1:A:86:PRO:O	2.14	0.47
1:A:246:ASP:O	1:A:250:VAL:HG23	2.14	0.47
1:B:21:GLY:O	1:B:23:SER:N	2.45	0.47
1:D:126:LEU:HD23	1:D:126:LEU:HA	1.71	0.47
1:A:10:ARG:HD2	1:A:30:ASP:OD2	2.15	0.47
1:A:140:LYS:CB	1:A:141:PRO:HD2	2.38	0.47
1:A:16:ILE:HD11	1:A:24:GLU:HB3	1.97	0.47
1:B:156:ASP:C	1:B:158:GLY:H	2.18	0.47
1:D:119:ILE:HG13	1:D:206:LEU:HD13	1.97	0.47
1:A:196:ARG:HG2	1:A:196:ARG:HH11	1.80	0.46
1:B:260:GLU:HA	1:B:260:GLU:OE2	2.15	0.46
1:C:48:ARG:HG2	1:C:86:PRO:HD2	1.97	0.46
1:C:139:VAL:HB	1:C:201:SER:CB	2.44	0.46
2:A:539:MIX:OAB	2:A:539:MIX:OAF	2.31	0.46
1:B:114:ARG:O	1:B:118:VAL:HG23	2.16	0.46
1:C:272:ASP:HA	1:C:275:ARG:HB2	1.97	0.46
1:D:268:GLU:O	1:D:271:ALA:HB3	2.16	0.46
1:A:101:ARG:CG	1:A:101:ARG:NH1	2.79	0.46
2:D:3539:MIX:OAA	2:D:3539:MIX:NAU	2.46	0.46
1:B:8:SER:O	1:B:9:ASP:HB2	2.15	0.46
1:C:40:LYS:O	1:C:89:TYR:HA	2.16	0.46
1:D:10:ARG:HD3	1:D:32:ARG:HB2	1.98	0.46
1:B:272:ASP:HA	1:B:275:ARG:HE	1.81	0.46
1:C:39:VAL:HA	1:C:90:ILE:O	2.15	0.46
1:D:218:GLY:HA2	1:D:224:VAL:CG2	2.46	0.46
1:A:208:GLU:HG2	1:A:214:PRO:HA	1.97	0.46
1:D:58:ARG:HD2	1:D:58:ARG:C	2.36	0.46
1:B:18:GLY:HA3	2:B:1539:MIX:CAJ	2.46	0.46
1:C:77:THR:O	1:D:32:ARG:NH1	2.49	0.46
1:C:101:ARG:HG3	1:C:141:PRO:CG	2.46	0.46
1:B:139:VAL:HG11	1:B:202:LEU:HD12	1.98	0.45
1:C:9:ASP:OD1	1:C:9:ASP:N	2.48	0.45
1:D:101:ARG:HD2	1:D:142:ALA:HB2	1.96	0.45
1:C:68:HIS:CD2	1:C:70:ALA:H	2.18	0.45
1:D:100:LEU:HG	1:D:144:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:HD23	1:A:247:LEU:O	2.15	0.45
1:B:137:ARG:NH2	1:B:161:ARG:CB	2.78	0.45
1:C:218:GLY:O	1:C:219:ASP:HB2	2.16	0.45
1:D:5:SER:O	1:D:13:LEU:HB2	2.17	0.45
1:A:50:PRO:HA	1:C:222:VAL:CG2	2.36	0.45
1:A:128:PHE:HA	1:A:131:GLN:HG3	1.98	0.45
1:C:15:GLU:HG2	1:C:16:ILE:N	2.32	0.45
1:B:3:THR:HG22	1:B:4:PRO:O	2.17	0.45
1:B:82:THR:HB	1:B:83:PRO:HD2	1.99	0.45
1:B:103:ILE:HG21	1:B:110:MET:HE2	1.99	0.45
1:C:29:ARG:O	1:C:31:LEU:CD1	2.65	0.45
1:C:208:GLU:O	1:C:212:GLY:N	2.49	0.45
1:A:86:PRO:HG3	1:C:220:SER:HB3	1.98	0.45
1:B:55:ARG:HE	1:B:55:ARG:HB2	1.53	0.45
1:C:126:LEU:HB3	1:C:130:HIS:CE1	2.52	0.45
1:D:29:ARG:HG2	1:D:31:LEU:HD13	1.99	0.45
1:D:196:ARG:O	1:D:199:VAL:HB	2.17	0.45
1:B:251:VAL:O	1:B:255:LEU:HD13	2.17	0.45
1:B:10:ARG:NH1	1:B:32:ARG:HH11	2.15	0.45
1:A:100:LEU:HA	1:A:103:ILE:CG2	2.41	0.44
1:B:48:ARG:O	1:B:50:PRO:HD3	2.16	0.44
1:C:14:GLY:HA3	1:C:27:LEU:HD23	1.99	0.44
1:A:100:LEU:HA	1:A:100:LEU:HD23	1.76	0.44
1:D:139:VAL:HB	1:D:201:SER:CB	2.46	0.44
1:A:256:ALA:HB3	1:A:262:ARG:HG3	1.98	0.44
1:C:76:ASP:HB3	1:C:91:VAL:CG2	2.47	0.44
1:A:75:TYR:CE2	1:A:93:GLU:HA	2.53	0.44
1:A:119:ILE:O	1:A:120:ALA:C	2.56	0.44
1:A:201:SER:O	1:A:204:CYS:HB2	2.18	0.44
1:B:20:GLY:O	1:B:40:LYS:NZ	2.50	0.44
1:C:94:TYR:C	1:C:94:TYR:HD2	2.21	0.44
1:D:48:ARG:CZ	1:D:48:ARG:CB	2.94	0.44
1:A:101:ARG:NH1	1:A:101:ARG:HG3	2.32	0.44
1:D:218:GLY:O	1:D:219:ASP:HB2	2.18	0.44
1:A:17:LEU:HB2	1:A:25:VAL:HG12	2.00	0.43
1:B:68:HIS:HB2	1:B:128:PHE:CD1	2.53	0.43
1:A:74:VAL:HG12	1:A:76:ASP:H	1.82	0.43
1:A:143:ASN:HA	1:A:155:MET:CE	2.48	0.43
1:B:208:GLU:HG2	1:B:214:PRO:HA	1.98	0.43
1:B:213:GLU:HB2	1:B:214:PRO:CD	2.48	0.43
1:B:234:ILE:HD12	1:B:239:ARG:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:VAL:HG22	1:C:91:VAL:HG13	1.99	0.43
1:C:203:GLY:O	1:C:206:LEU:HB3	2.17	0.43
1:C:258:ASN:ND2	1:C:260:GLU:H	2.15	0.43
1:B:185:PRO:O	1:B:188:ALA:HB3	2.18	0.43
1:C:181:GLN:HA	1:C:183:LEU:CD2	2.48	0.43
1:D:53:TYR:HE1	1:D:88:PRO:HB3	1.84	0.43
1:D:126:LEU:HB3	1:D:130:HIS:HE1	1.84	0.43
1:A:19:PHE:CD2	1:A:19:PHE:N	2.87	0.43
1:A:196:ARG:NH1	1:A:264:GLN:OE1	2.52	0.43
1:D:40:LYS:O	1:D:89:TYR:HA	2.17	0.43
1:D:181:GLN:HA	1:D:183:LEU:HG	2.00	0.43
1:A:137:ARG:HB2	1:A:159:ILE:CD1	2.49	0.43
1:B:23:SER:HB2	1:B:41:VAL:O	2.18	0.43
1:B:44:ALA:O	1:B:47:ALA:HB3	2.18	0.43
1:B:48:ARG:HA	1:B:48:ARG:CZ	2.46	0.43
1:B:114:ARG:O	1:B:117:GLU:HG2	2.18	0.43
1:B:180:ALA:O	1:B:183:LEU:CD2	2.67	0.43
1:B:189:ARG:HB2	1:B:189:ARG:CZ	2.49	0.43
1:C:7:LEU:N	1:C:7:LEU:HD23	2.33	0.43
1:C:56:PHE:HE2	1:C:90:ILE:HG13	1.84	0.43
1:B:127:ASN:O	1:B:131:GLN:HG3	2.18	0.43
1:A:116:ILE:HG23	1:A:273:LEU:HD22	2.01	0.42
1:B:195:ALA:O	1:B:199:VAL:HG23	2.19	0.42
1:D:272:ASP:OD2	1:D:275:ARG:NH1	2.49	0.42
1:C:228:HIS:O	1:C:257:LYS:HD2	2.19	0.42
1:D:123:CYS:HB3	1:D:270:ARG:HG2	2.00	0.42
1:D:270:ARG:HH21	1:D:270:ARG:HG3	1.85	0.42
1:A:68:HIS:CG	1:A:69:PRO:HD2	2.54	0.42
1:B:184:SER:OG	1:B:187:GLN:HG3	2.19	0.42
1:D:206:LEU:O	1:D:207:TYR:C	2.57	0.42
1:A:100:LEU:CA	1:A:103:ILE:HG22	2.43	0.42
1:B:135:ILE:HD12	1:B:135:ILE:N	2.34	0.42
1:D:126:LEU:HD13	1:D:198:ASP:HB3	2.01	0.42
1:D:207:TYR:CE2	1:D:215:PRO:HA	2.55	0.42
1:A:43:ARG:O	1:A:44:ALA:HB3	2.17	0.42
1:A:111:THR:CG2	1:A:114:ARG:HB2	2.46	0.42
1:C:42:LEU:HD12	1:C:42:LEU:HA	1.86	0.42
1:A:40:LYS:O	1:A:89:TYR:HA	2.19	0.42
1:C:75:TYR:CE2	1:C:93:GLU:HA	2.55	0.42
1:C:94:TYR:HE2	1:C:96:ASP:N	2.18	0.42
1:D:183:LEU:HG	1:D:183:LEU:H	1.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:SER:HA	1:A:200:TYR:CD2	2.54	0.41
1:B:179:THR:HG23	1:B:221:PRO:HD3	2.02	0.41
1:B:180:ALA:HB1	1:B:224:VAL:CB	2.50	0.41
1:A:184:SER:H	1:A:187:GLN:HG3	1.84	0.41
1:B:206:LEU:O	1:B:209:VAL:HG22	2.21	0.41
1:C:87:LEU:HD12	1:C:88:PRO:HD2	2.02	0.41
1:C:210:LEU:HD23	1:C:210:LEU:HA	1.68	0.41
1:C:16:ILE:H	1:C:16:ILE:HG12	1.44	0.41
1:D:127:ASN:OD1	1:D:267:ALA:HB2	2.20	0.41
1:C:231:GLU:OE1	1:C:231:GLU:HA	2.19	0.41
1:A:100:LEU:HB2	1:A:141:PRO:O	2.21	0.41
1:C:132:ASN:HB2	1:C:134:ILE:CD1	2.51	0.41
1:C:241:GLU:N	1:C:241:GLU:OE1	2.53	0.41
1:D:73:ALA:H	1:D:93:GLU:HG2	1.85	0.41
1:D:116:ILE:CG2	1:D:116:ILE:HD13	2.46	0.41
1:D:181:GLN:HA	1:D:183:LEU:CG	2.50	0.41
1:C:276:VAL:C	1:C:278:ASN:N	2.72	0.41
1:A:86:PRO:O	1:A:86:PRO:CG	2.68	0.41
1:A:182:TYR:HE1	1:A:208:GLU:HG3	1.85	0.41
1:A:208:GLU:HA	1:A:213:GLU:O	2.21	0.41
1:C:265:THR:OG1	1:C:268:GLU:HG3	2.21	0.41
1:B:139:VAL:H	1:B:139:VAL:HG23	1.46	0.41
1:B:207:TYR:OH	1:B:239:ARG:HG3	2.21	0.41
1:C:253:LYS:HB3	1:C:263:TYR:CE2	2.55	0.41
1:D:27:LEU:HD22	1:D:28:ALA:H	1.86	0.41
1:D:97:GLY:O	2:D:3539:MIX:HAO2	2.21	0.41
1:A:105:HIS:ND1	1:A:105:HIS:C	2.74	0.41
1:B:183:LEU:HD23	1:B:183:LEU:H	1.86	0.41
1:B:186:GLU:OE1	1:B:186:GLU:N	2.49	0.41
2:B:1539:MIX:OAA	2:B:1539:MIX:NAU	2.52	0.41
1:D:184:SER:OG	1:D:185:PRO:HD2	2.21	0.41
1:A:135:ILE:HG22	1:A:137:ARG:HG2	2.03	0.41
1:D:126:LEU:HB3	1:D:130:HIS:CE1	2.56	0.41
1:D:135:ILE:H	1:D:135:ILE:HG13	1.58	0.41
1:A:277:HIS:HD2	1:A:277:HIS:O	2.04	0.40
1:D:58:ARG:O	1:D:59:GLU:C	2.60	0.40
1:D:155:MET:HE3	1:D:155:MET:HB2	1.98	0.40
1:C:274:VAL:O	1:C:277:HIS:HB2	2.22	0.40
1:A:116:ILE:HG21	1:A:277:HIS:HB2	2.04	0.40
1:D:64:ALA:C	1:D:66:LEU:H	2.25	0.40
1:D:102:ASP:OD2	1:D:102:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:ASP:OD1	1:D:233:PRO:CD	2.68	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	259/299 (87%)	222 (86%)	32 (12%)	5 (2%)	8 28
1	B	258/299 (86%)	223 (86%)	29 (11%)	6 (2%)	6 23
1	C	250/299 (84%)	216 (86%)	26 (10%)	8 (3%)	4 16
1	D	254/299 (85%)	217 (85%)	30 (12%)	7 (3%)	5 19
All	All	1021/1196 (85%)	878 (86%)	117 (12%)	26 (2%)	5 21

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	MET
1	A	44	ALA
1	A	180	ALA
1	B	22	MET
1	B	44	ALA
1	C	9	ASP
1	C	219	ASP
1	C	277	HIS
1	D	219	ASP
1	A	241	GLU
1	B	51	SER
1	C	44	ALA
1	D	44	ALA
1	B	149	THR

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Mol	Chain	Res	Type
1	B	162	ALA
1	C	156	ASP
1	D	65	ALA
1	D	156	ASP
1	C	181	GLN
1	D	9	ASP
1	D	20	GLY
1	D	221	PRO
1	A	76	ASP
1	B	240	HIS
1	C	221	PRO
1	C	21	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	208/242 (86%)	165 (79%)	43 (21%)	1 3
1	B	208/242 (86%)	170 (82%)	38 (18%)	1 5
1	C	203/242 (84%)	161 (79%)	42 (21%)	1 3
1	D	205/242 (85%)	171 (83%)	34 (17%)	2 7
All	All	824/968 (85%)	667 (81%)	157 (19%)	1 4

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	9	ASP
1	A	15	GLU
1	A	16	ILE
1	A	22	MET
1	A	32	ARG
1	A	34	HIS
1	A	54	LEU
1	A	57	ARG

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Mol	Chain	Res	Type
1	A	67	ASN
1	A	99	THR
1	A	101	ARG
1	A	103	ILE
1	A	106	THR
1	A	107	GLU
1	A	111	THR
1	A	126	LEU
1	A	140	LYS
1	A	147	SER
1	A	155	MET
1	A	156	ASP
1	A	163	ILE
1	A	179	THR
1	A	181	GLN
1	A	183	LEU
1	A	184	SER
1	A	191	ASP
1	A	193	VAL
1	A	196	ARG
1	A	202	LEU
1	A	205	VAL
1	A	208	GLU
1	A	217	THR
1	A	221	PRO
1	A	222	VAL
1	A	230	ARG
1	A	231	GLU
1	A	241	GLU
1	A	246	ASP
1	A	260	GLU
1	A	261	ASN
1	A	276	VAL
1	A	277	HIS
1	B	8	SER
1	B	13	LEU
1	B	22	MET
1	B	29	ARG
1	B	34	HIS
1	B	45	ASP
1	B	48	ARG
1	B	49	ASP

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Mol	Chain	Res	Type
1	B	53	TYR
1	B	55	ARG
1	B	67	ASN
1	B	81	GLU
1	B	99	THR
1	B	100	LEU
1	B	101	ARG
1	B	102	ASP
1	B	106	THR
1	B	107	GLU
1	B	111	THR
1	B	139	VAL
1	B	144	ILE
1	B	155	MET
1	B	159	ILE
1	B	181	GLN
1	B	189	ARG
1	B	192	SER
1	B	196	ARG
1	B	202	LEU
1	B	208	GLU
1	B	230	ARG
1	B	246	ASP
1	B	253	LYS
1	B	265	THR
1	B	270	ARG
1	B	272	ASP
1	B	274	VAL
1	B	275	ARG
1	B	276	VAL
1	C	3	THR
1	C	9	ASP
1	C	15	GLU
1	C	16	ILE
1	C	17	LEU
1	C	22	MET
1	C	23	SER
1	C	24	GLU
1	C	27	LEU
1	C	31	LEU
1	C	53	TYR
1	C	54	LEU

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Mol	Chain	Res	Type
1	C	77	THR
1	C	91	VAL
1	C	92	MET
1	C	99	THR
1	C	101	ARG
1	C	106	THR
1	C	107	GLU
1	C	111	THR
1	C	114	ARG
1	C	124	GLN
1	C	137	ARG
1	C	155	MET
1	C	183	LEU
1	C	184	SER
1	C	189	ARG
1	C	192	SER
1	C	193	VAL
1	C	208	GLU
1	C	213	GLU
1	C	217	THR
1	C	222	VAL
1	C	234	ILE
1	C	241	GLU
1	C	243	LEU
1	C	244	SER
1	C	247	LEU
1	C	265	THR
1	C	273	LEU
1	C	277	HIS
1	C	278	ASN
1	D	3	THR
1	D	9	ASP
1	D	10	ARG
1	D	13	LEU
1	D	16	ILE
1	D	17	LEU
1	D	27	LEU
1	D	31	LEU
1	D	35	ARG
1	D	40	LYS
1	D	45	ASP
1	D	48	ARG

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Mol	Chain	Res	Type
1	D	58	ARG
1	D	62	ASN
1	D	67	ASN
1	D	74	VAL
1	D	87	LEU
1	D	92	MET
1	D	102	ASP
1	D	106	THR
1	D	127	ASN
1	D	135	ILE
1	D	140	LYS
1	D	155	MET
1	D	159	ILE
1	D	181	GLN
1	D	183	LEU
1	D	196	ARG
1	D	208	GLU
1	D	213	GLU
1	D	243	LEU
1	D	244	SER
1	D	252	LEU
1	D	269	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	62	ASN
1	A	67	ASN
1	A	127	ASN
1	A	150	ASN
1	A	181	GLN
1	A	240	HIS
1	A	261	ASN
1	A	277	HIS
1	B	62	ASN
1	B	124	GLN
1	B	131	GLN
1	B	132	ASN
1	B	181	GLN
1	B	277	HIS
1	C	62	ASN

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Mol	Chain	Res	Type
1	C	68	HIS
1	C	124	GLN
1	C	132	ASN
1	C	258	ASN
1	D	67	ASN
1	D	127	ASN
1	D	132	ASN
1	D	136	HIS
1	D	143	ASN

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)

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	MIX	C	2539	-	34,34,34	1.06	4 (11%)	44,46,46	1.06	2 (4%)
2	MIX	A	539	-	34,34,34	1.46	4 (11%)	44,46,46	1.03	4 (9%)
2	MIX	D	3539	-	34,34,34	1.08	4 (11%)	44,46,46	0.81	1 (2%)
2	MIX	B	1539	-	34,34,34	1.25	4 (11%)	44,46,46	1.48	6 (13%)

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
2	MIX	C	2539	-	-	6/14/30/30	0/3/3/3
2	MIX	A	539	-	-	7/14/30/30	0/3/3/3
2	MIX	D	3539	-	-	9/14/30/30	0/3/3/3
2	MIX	B	1539	-	-	11/14/30/30	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1539	MIX	CBC-CBA	-3.90	1.38	1.47
2	A	539	MIX	CBD-CBB	-3.79	1.38	1.47
2	A	539	MIX	CBE-CBA	-3.62	1.39	1.47
2	A	539	MIX	CBC-CBA	-3.56	1.39	1.47
2	A	539	MIX	CBF-CBB	-3.13	1.40	1.47
2	C	2539	MIX	CBD-CBB	-2.98	1.40	1.47
2	D	3539	MIX	CBC-CBA	-2.97	1.40	1.47
2	B	1539	MIX	CBD-CBB	-2.91	1.40	1.47
2	C	2539	MIX	CBF-CBB	-2.80	1.41	1.47
2	D	3539	MIX	CBF-CBB	-2.60	1.41	1.47
2	D	3539	MIX	CBE-CBA	-2.52	1.41	1.47
2	D	3539	MIX	CBD-CBB	-2.51	1.41	1.47
2	B	1539	MIX	CBF-CBB	-2.48	1.41	1.47
2	B	1539	MIX	CBE-CBA	-2.41	1.42	1.47
2	C	2539	MIX	CBC-CBA	-2.12	1.42	1.47
2	C	2539	MIX	CBE-CBA	-2.03	1.42	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1539	MIX	CAJ-CAZ-NAV	-4.61	113.94	121.80
2	B	1539	MIX	CBF-CAZ-NAV	4.39	126.53	121.32
2	B	1539	MIX	OAA-CBA-CBC	-2.90	116.74	121.43
2	A	539	MIX	CAJ-CAZ-NAV	-2.63	117.31	121.80
2	A	539	MIX	CAP-CAR-NAV	-2.60	106.04	111.46
2	C	2539	MIX	CBE-CBF-CAZ	2.47	121.38	119.74
2	A	539	MIX	OAB-CBB-CBD	-2.46	117.45	121.43
2	B	1539	MIX	CAW-CBC-CBA	-2.39	116.92	120.59
2	B	1539	MIX	OAB-CBB-CBD	-2.37	117.59	121.43
2	C	2539	MIX	CBF-CAZ-NAV	-2.19	118.73	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3539	MIX	CAJ-CAZ-NAV	-2.10	118.22	121.80
2	A	539	MIX	CAY-CBE-CBA	-2.03	118.26	121.08
2	B	1539	MIX	CAY-CBE-CBA	-2.01	118.30	121.08

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1539	MIX	OAD-CAL-CAN-NAT
2	C	2539	MIX	OAC-CAK-CAM-NAS
2	C	2539	MIX	CAK-CAM-NAS-CAO
2	B	1539	MIX	CAJ-CAZ-NAV-CAR
2	D	3539	MIX	CAI-CAY-NAU-CAQ
2	D	3539	MIX	NAS-CAO-CAQ-NAU
2	D	3539	MIX	NAT-CAP-CAR-NAV
2	A	539	MIX	CAJ-CAZ-NAV-CAR
2	B	1539	MIX	CAI-CAY-NAU-CAQ
2	D	3539	MIX	CBE-CAY-NAU-CAQ
2	A	539	MIX	OAC-CAK-CAM-NAS
2	C	2539	MIX	NAS-CAO-CAQ-NAU
2	A	539	MIX	CAL-CAN-NAT-CAP
2	B	1539	MIX	CAL-CAN-NAT-CAP
2	C	2539	MIX	CAL-CAN-NAT-CAP
2	D	3539	MIX	CAL-CAN-NAT-CAP
2	A	539	MIX	CBF-CAZ-NAV-CAR
2	B	1539	MIX	CBE-CAY-NAU-CAQ
2	B	1539	MIX	CBF-CAZ-NAV-CAR
2	C	2539	MIX	OAD-CAL-CAN-NAT
2	D	3539	MIX	CBF-CAZ-NAV-CAR
2	D	3539	MIX	OAC-CAK-CAM-NAS
2	B	1539	MIX	CAO-CAQ-NAU-CAY
2	D	3539	MIX	CAJ-CAZ-NAV-CAR
2	A	539	MIX	CAR-CAP-NAT-CAN
2	B	1539	MIX	CAQ-CAO-NAS-CAM
2	D	3539	MIX	CAQ-CAO-NAS-CAM
2	B	1539	MIX	CAK-CAM-NAS-CAO
2	A	539	MIX	CAQ-CAO-NAS-CAM
2	C	2539	MIX	CAP-CAR-NAV-CAZ
2	B	1539	MIX	NAS-CAO-CAQ-NAU
2	A	539	MIX	CAK-CAM-NAS-CAO
2	B	1539	MIX	OAC-CAK-CAM-NAS

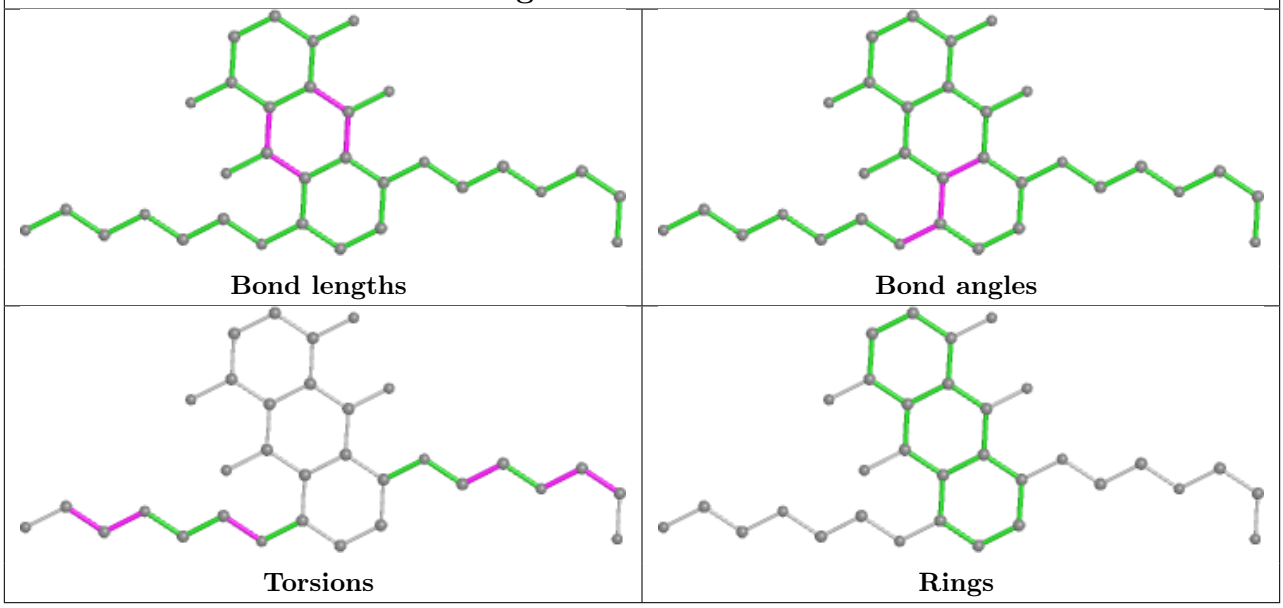
There are no ring outliers.

4 monomers are involved in 13 short contacts:

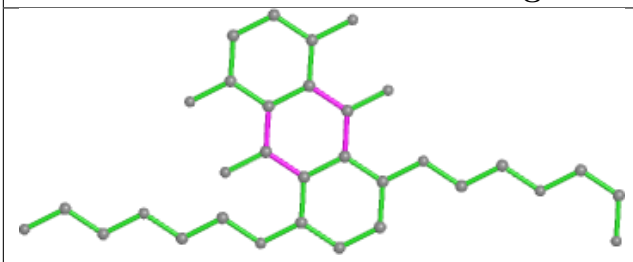
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2539	MIX	1	0
2	A	539	MIX	2	0
2	D	3539	MIX	6	0
2	B	1539	MIX	4	0

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.

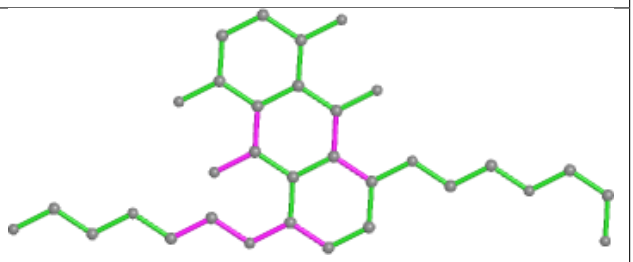
Ligand MIX C 2539



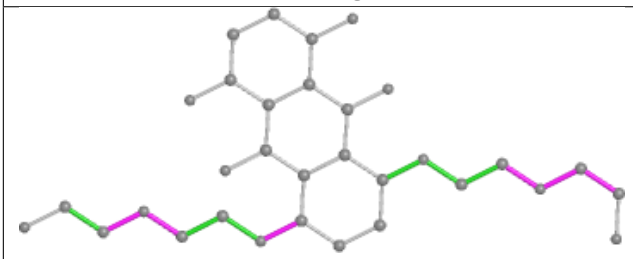
Ligand MIX A 539



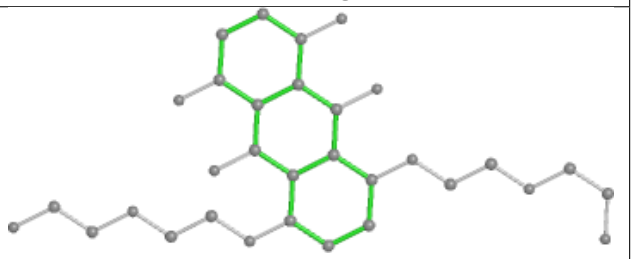
Bond lengths



Bond angles

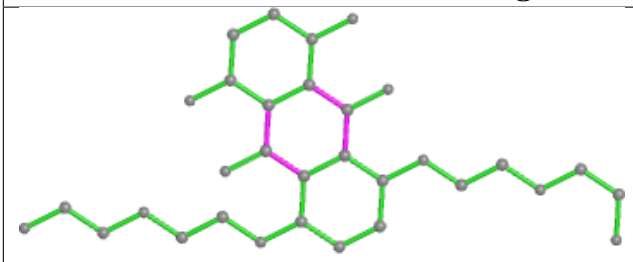


Torsions

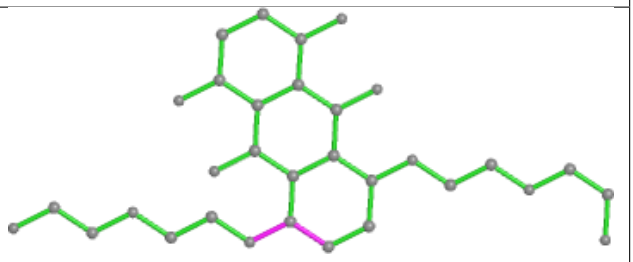


Rings

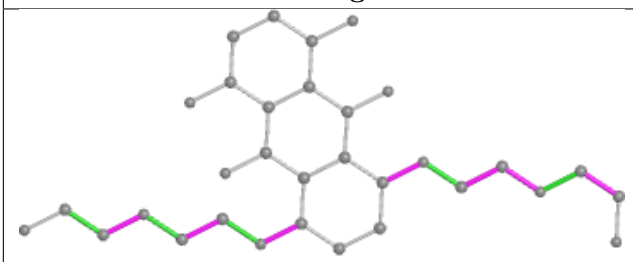
Ligand MIX D 3539



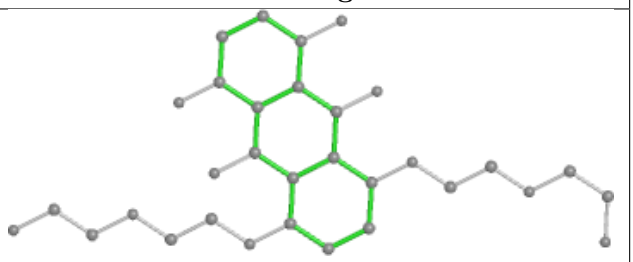
Bond lengths



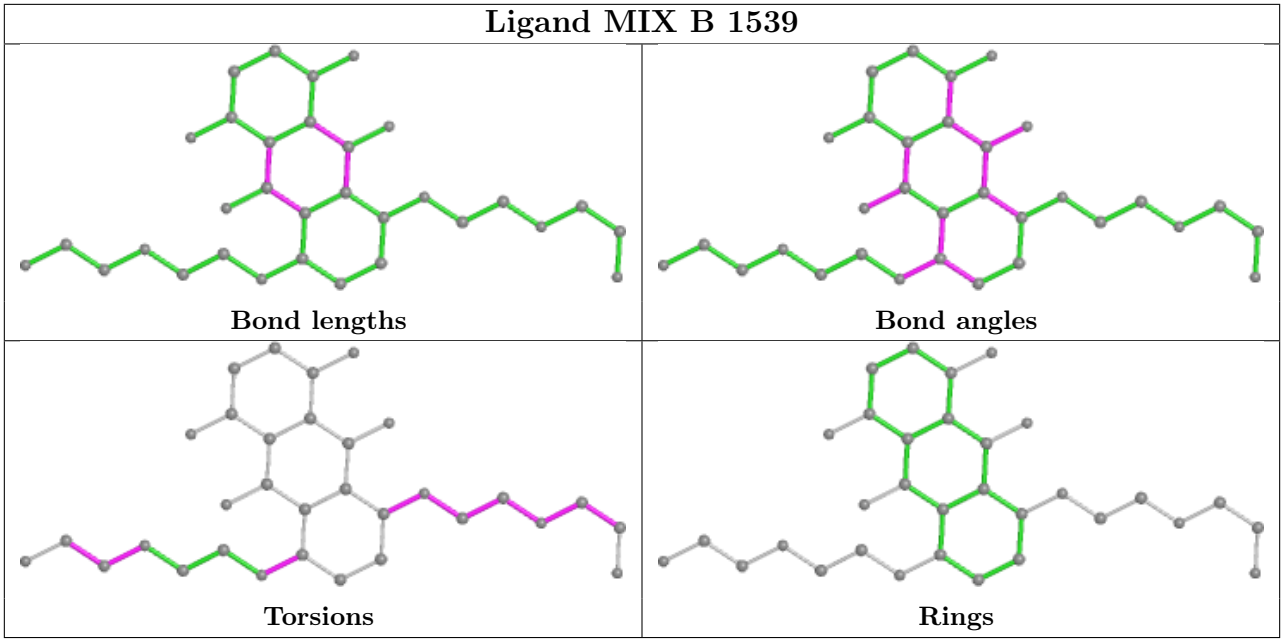
Bond angles



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	263/299 (87%)	0.31	3 (1%)	80	80	76, 79, 83, 89	0
1	B	262/299 (87%)	0.42	11 (4%)	36	32	75, 79, 83, 89	0
1	C	254/299 (84%)	0.27	5 (1%)	65	63	77, 79, 81, 86	0
1	D	258/299 (86%)	0.66	30 (11%)	4	3	76, 79, 82, 86	0
All	All	1037/1196 (86%)	0.42	49 (4%)	31	28	75, 79, 83, 89	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	177	ILE	7.0
1	D	7	LEU	6.3
1	B	84	ALA	4.9
1	D	210	LEU	4.9
1	D	276	VAL	4.6
1	D	13	LEU	4.5
1	A	277	HIS	4.5
1	B	189	ARG	4.0
1	D	245	ALA	3.9
1	D	178	GLY	3.3
1	D	25	VAL	3.2
1	D	246	ASP	3.2
1	B	278	ASN	3.1
1	D	52	PHE	3.1
1	D	17	LEU	3.0
1	C	47	ALA	2.9
1	B	163	ILE	2.9
1	A	83	PRO	2.9
1	D	16	ILE	2.8
1	D	11	TYR	2.8
1	D	86	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	21	GLY	2.8
1	B	187	GLN	2.7
1	B	190	GLY	2.7
1	D	90	ILE	2.5
1	B	191	ASP	2.5
1	D	144	ILE	2.5
1	D	51	SER	2.4
1	D	274	VAL	2.4
1	C	3	THR	2.4
1	C	83	PRO	2.4
1	C	44	ALA	2.4
1	D	8	SER	2.4
1	B	188	ALA	2.4
1	D	236	PRO	2.4
1	D	277	HIS	2.3
1	D	159	ILE	2.3
1	B	160	ALA	2.3
1	D	239	ARG	2.3
1	B	46	LEU	2.2
1	B	193	VAL	2.2
1	D	87	LEU	2.2
1	C	52	PHE	2.2
1	D	6	HIS	2.2
1	D	42	LEU	2.1
1	A	263	TYR	2.1
1	D	213	GLU	2.1
1	D	243	LEU	2.0
1	D	229	VAL	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,

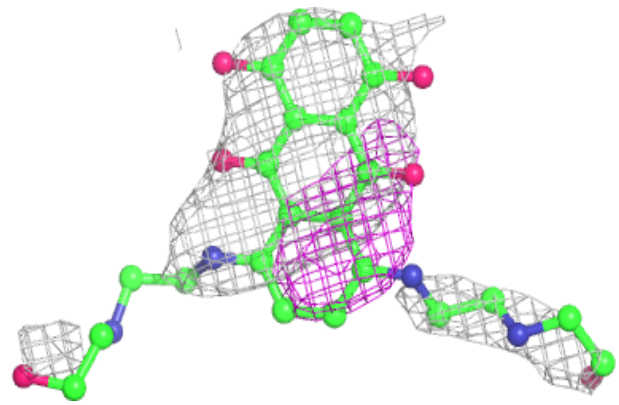
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

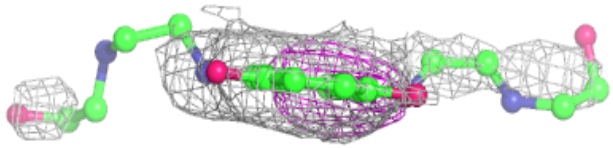
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MIX	D	3539	32/32	0.77	0.54	158,163,164,164	0
2	MIX	C	2539	32/32	0.89	0.19	122,127,130,132	0
2	MIX	A	539	32/32	0.95	0.23	91,91,103,105	0
2	MIX	B	1539	32/32	0.97	0.16	80,81,87,87	0

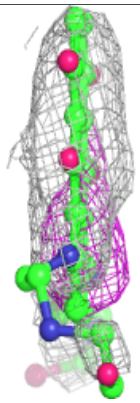
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MIX D 3539:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

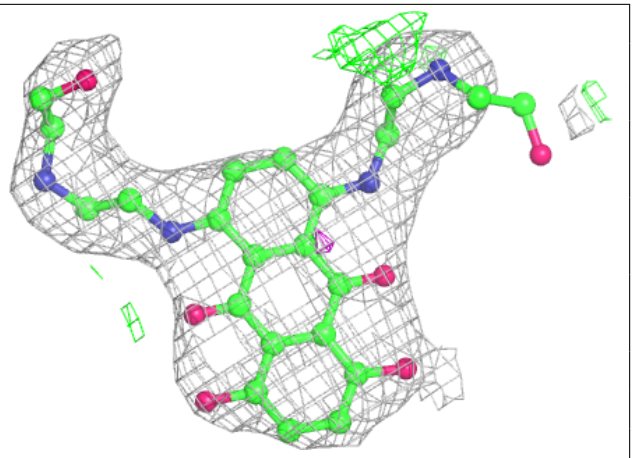


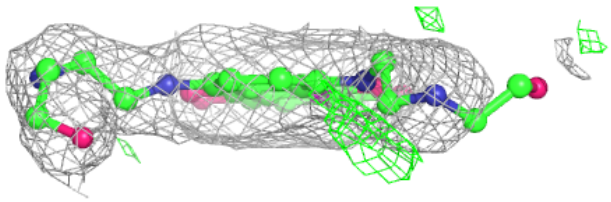


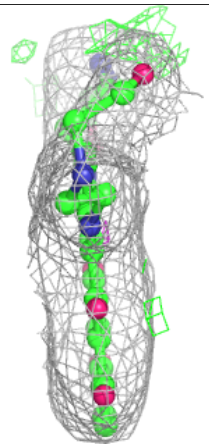


Electron density around MIX C 2539:

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

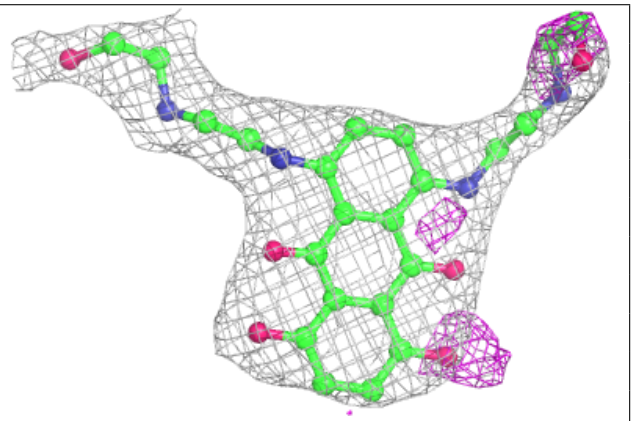


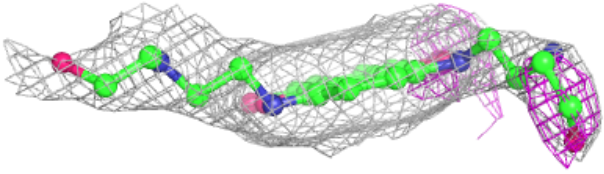


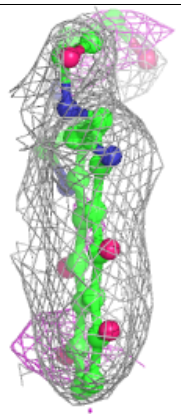


Electron density around MIX A 539:

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

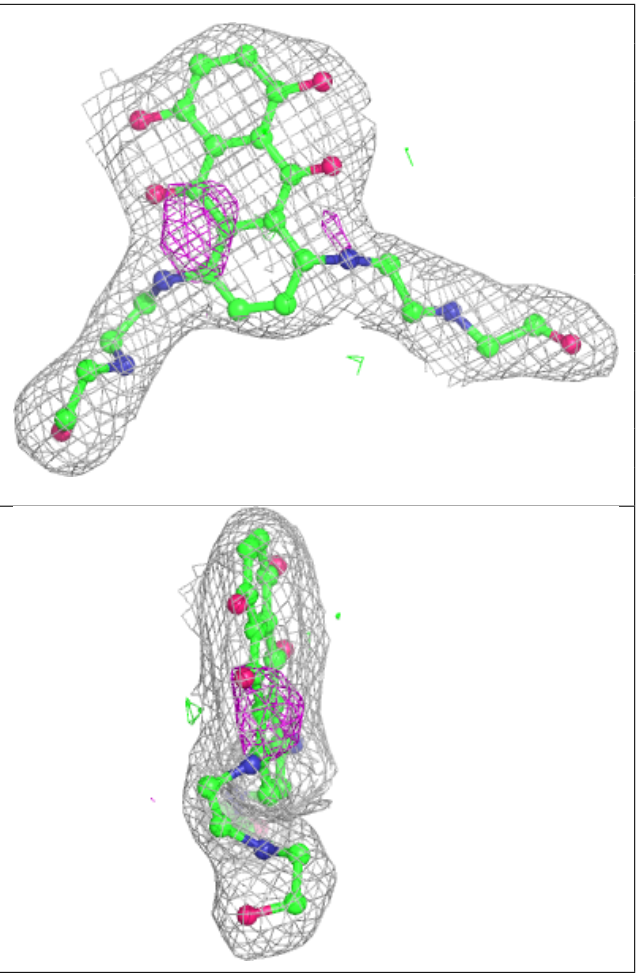






Electron density around MIX B 1539:

$2mF_o$-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.