



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:24 am GMT

PDB ID : 1S64
Title : Rat protein geranylgeranyltransferase type-I complexed with L-778,123 and a sulfate anion
Authors : Reid, T.S.; Long, S.B.; Beese, L.S.
Deposited on : 2004-01-22
Resolution : 2.55 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

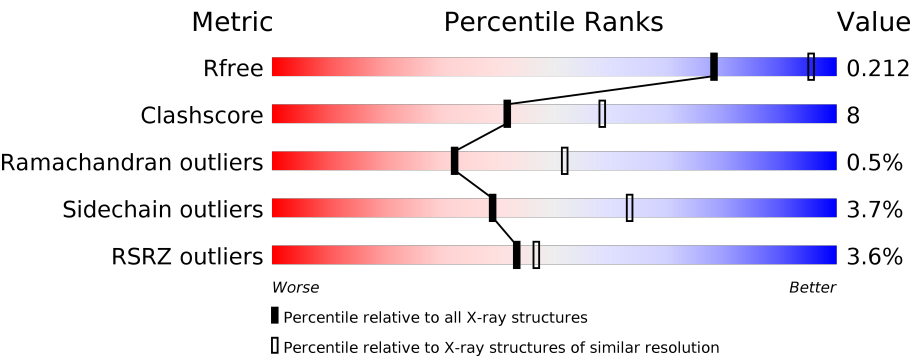
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	100719	4993 (2.58-2.50)
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (2.58-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	377	<div><div>3%</div><div><div></div><div>67%</div><div>15%</div><div>•</div><div>17%</div></div></div>
1	C	377	<div><div>3%</div><div><div></div><div>69%</div><div>14%</div><div>•</div><div>17%</div></div></div>
1	E	377	<div><div>3%</div><div><div></div><div>65%</div><div>17%</div><div>•</div><div>17%</div></div></div>
1	G	377	<div><div>5%</div><div><div></div><div>66%</div><div>18%</div><div></div><div>17%</div></div></div>
1	I	377	<div><div>2%</div><div><div></div><div>67%</div><div>15%</div><div>•</div><div>17%</div></div></div>
1	K	377	<div><div>%</div><div><div></div><div>68%</div><div>14%</div><div>•</div><div>17%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	B	377	
2	D	377	
2	F	377	
2	H	377	
2	J	377	
2	L	377	

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
4	CL	C	378	-	-	-	X
6	778	B	380	-	-	-	X
6	778	L	381	-	-	-	X
7	MES	B	381	-	-	-	X
7	MES	D	382	-	-	-	X
7	MES	F	382	-	-	-	X
7	MES	J	382	-	-	-	X
7	MES	L	382	-	X	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33735 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 Protein farnesyltransferase/geranylgeranyltransferase type I alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2626	1678	463	480	5			
1	C	314	Total	C	N	O	S	0	0	0
			2637	1686	458	488	5			
1	E	314	Total	C	N	O	S	0	0	0
			2642	1686	461	490	5			
1	G	314	Total	C	N	O	S	0	0	0
			2633	1683	459	486	5			
1	I	314	Total	C	N	O	S	0	0	0
			2651	1692	462	492	5			
1	K	314	Total	C	N	O	S	0	0	0
			2667	1700	466	496	5			

- Molecule 2 is a protein called Geranylgeranyl transferase type I beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2693	1704	467	498	24			
2	D	346	Total	C	N	O	S	0	0	0
			2690	1705	463	498	24			
2	F	346	Total	C	N	O	S	0	0	0
			2714	1714	474	502	24			
2	H	346	Total	C	N	O	S	0	0	0
			2688	1701	463	500	24			
2	J	346	Total	C	N	O	S	0	0	0
			2709	1711	471	503	24			
2	L	346	Total	C	N	O	S	0	0	0
			2719	1717	473	505	24			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	L	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

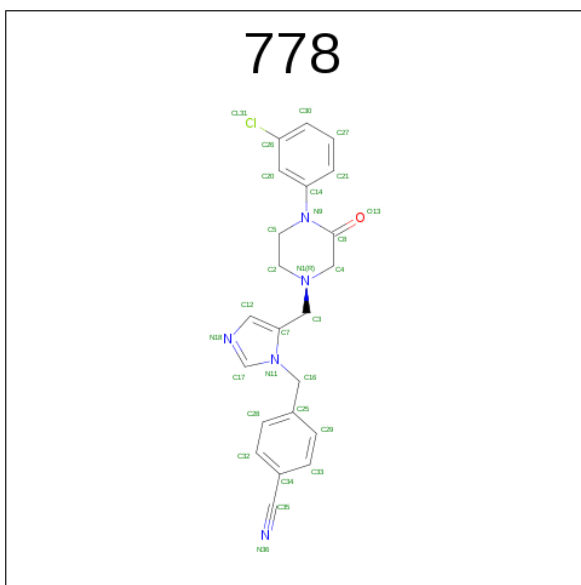
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Cl 1 1	0	0
4	J	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	K	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0
4	I	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	L	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



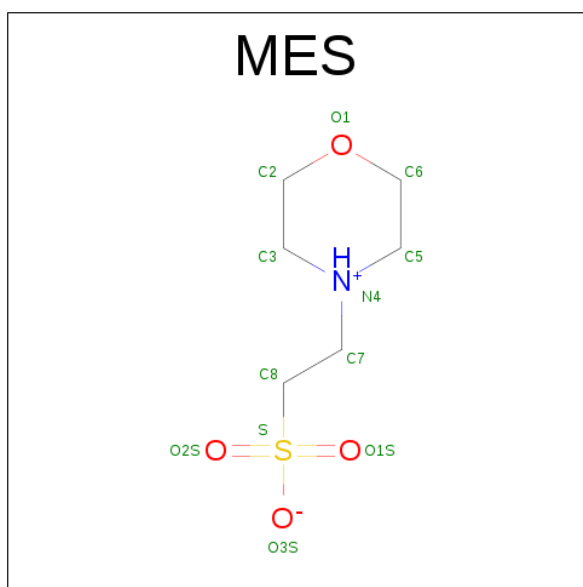
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 4-[(5-{[4-(3-CHLOROPHENYL)-3-OXOPIPERAZIN-1-YL]METHYL}-1H-IMIDAZOL-1-YL)METHYL]BENZONITRILE (three-letter code: 778) (formula: C₂₂H₂₀ClN₅O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Cl	N	O	0	0
			29	22	1	5	1		
6	D	1	Total	C	Cl	N	O	0	0
			29	22	1	5	1		
6	F	1	Total	C	Cl	N	O	0	0
			29	22	1	5	1		
6	H	1	Total	C	Cl	N	O	0	0
			29	22	1	5	1		
6	J	1	Total	C	Cl	N	O	0	0
			29	22	1	5	1		
6	L	1	Total	C	Cl	N	O	0	0
			29	22	1	5	1		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	J	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	L	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 8 is water.

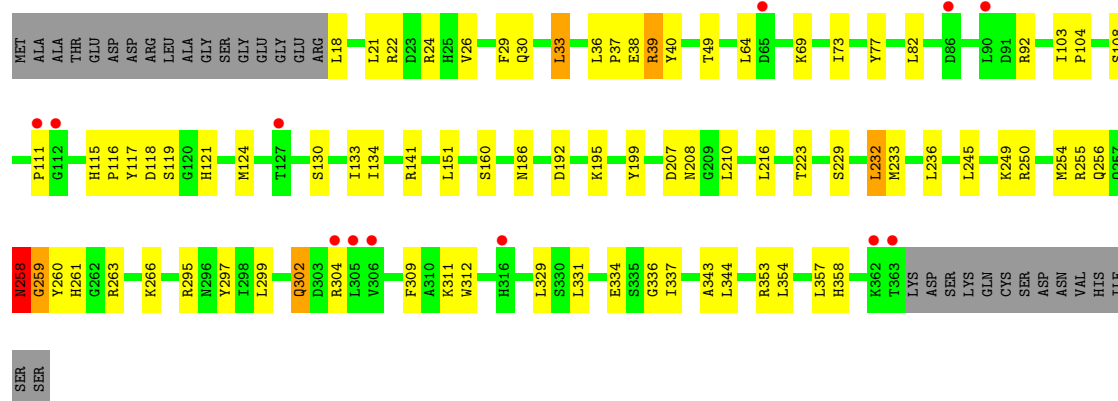
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	95	Total	O	0	0
			95	95		
8	B	74	Total	O	0	0
			74	74		
8	C	102	Total	O	0	0
			102	102		
8	D	123	Total	O	0	0
			123	123		
8	E	97	Total	O	0	0
			97	97		
8	F	114	Total	O	0	0
			114	114		

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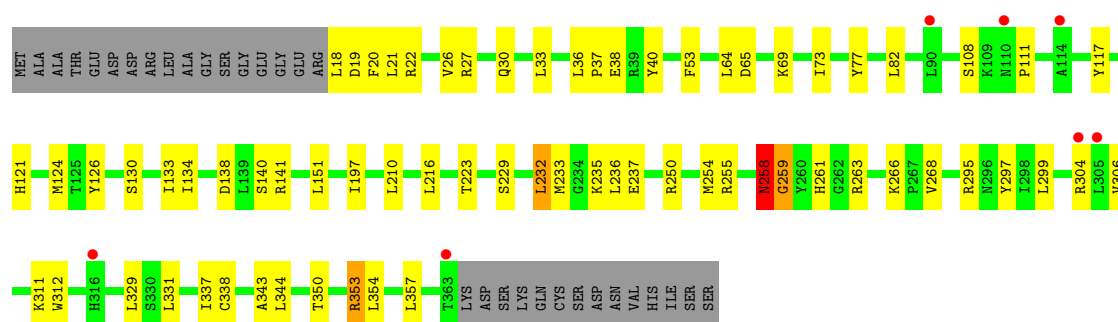
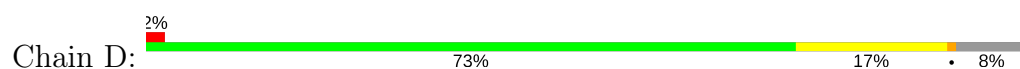
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	96	Total 96	O 96	0	0
8	H	65	Total 65	O 65	0	0
8	I	134	Total 134	O 134	0	0
8	J	102	Total 102	O 102	0	0
8	K	207	Total 207	O 207	0	0
8	L	166	Total 166	O 166	0	0

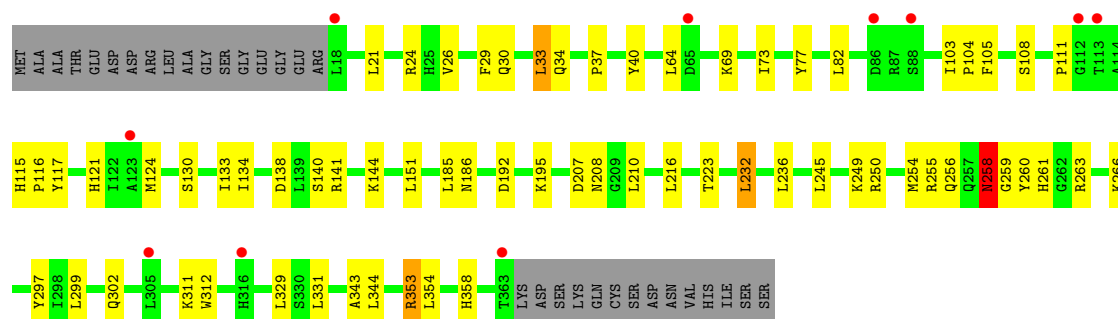
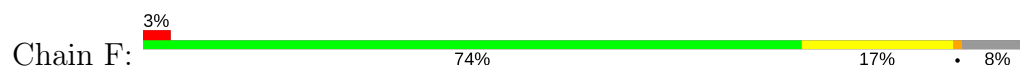




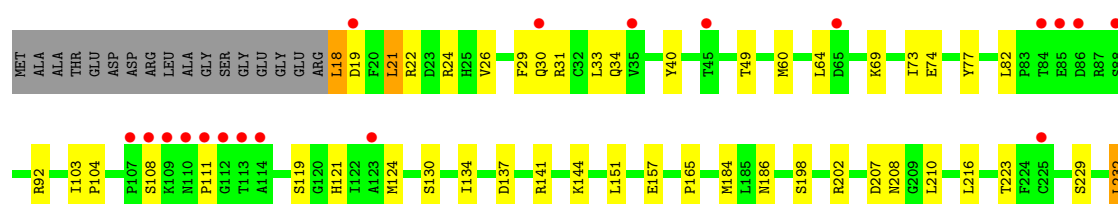
• Molecule 2: Geranylgeranyl transferase type I beta subunit

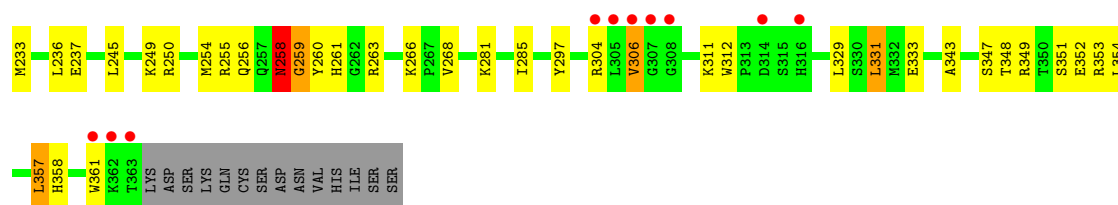


• Molecule 2: Geranylgeranyl transferase type I beta subunit

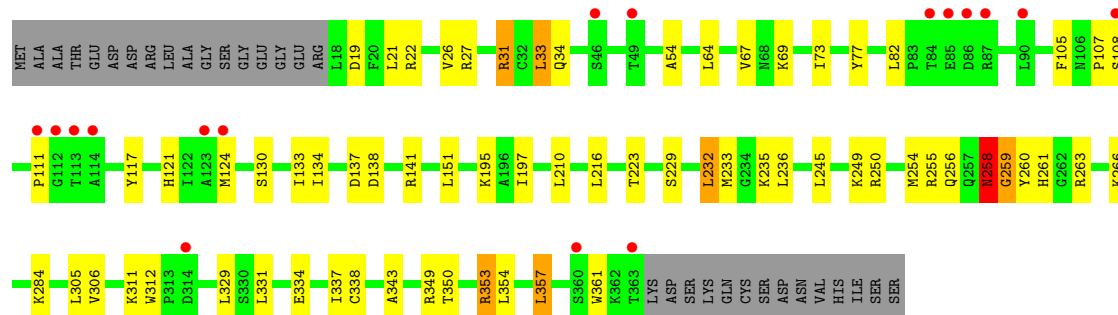
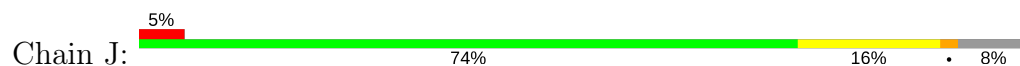


• Molecule 2: Geranylgeranyl transferase type I beta subunit

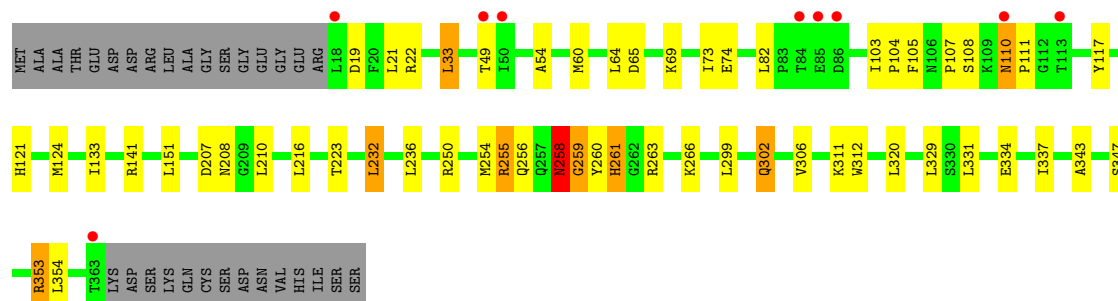




• Molecule 2: Geranylgeranyl transferase type I beta subunit



• Molecule 2: Geranylgeranyl transferase type I beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	271.15Å 268.68Å 184.62Å 90.00° 131.55° 90.00°	Depositor
Resolution (Å)	30.00 – 2.55 39.18 – 2.54	Depositor EDS
% Data completeness (in resolution range)	93.4 (30.00-2.55) 93.1 (39.18-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.54Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.192 , 0.213 0.195 , 0.212	Depositor DCC
R_{free} test set	15041 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.086 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33735	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN, 778, MES, CL

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	0.34	0/2692	0.51	0/3664
1	C	0.35	0/2703	0.52	0/3677
1	E	0.34	0/2708	0.53	0/3684
1	G	0.34	0/2699	0.51	0/3672
1	I	0.36	0/2717	0.52	0/3694
1	K	0.40	0/2733	0.54	0/3713
2	B	0.35	0/2754	0.59	2/3725 (0.1%)
2	D	0.36	0/2751	0.60	2/3720 (0.1%)
2	F	0.37	0/2775	0.60	2/3750 (0.1%)
2	H	0.34	0/2749	0.59	2/3720 (0.1%)
2	J	0.35	0/2770	0.60	2/3745 (0.1%)
2	L	0.39	0/2780	0.61	2/3756 (0.1%)
All	All	0.36	0/32831	0.56	12/44520 (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
2	B	0	1
2	F	0	1
All	All	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	259	GLY	N-CA-C	-6.06	97.95	113.10
2	H	259	GLY	N-CA-C	-5.96	98.21	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	259	GLY	N-CA-C	-5.90	98.34	113.10
2	D	259	GLY	N-CA-C	-5.87	98.44	113.10
2	L	259	GLY	N-CA-C	-5.84	98.50	113.10
2	B	259	GLY	N-CA-C	-5.73	98.77	113.10
2	J	258	ASN	N-CA-C	-5.61	95.85	111.00
2	B	258	ASN	N-CA-C	-5.48	96.21	111.00
2	D	258	ASN	N-CA-C	-5.43	96.33	111.00
2	F	258	ASN	N-CA-C	-5.43	96.35	111.00
2	L	258	ASN	N-CA-C	-5.39	96.46	111.00
2	H	258	ASN	N-CA-C	-5.35	96.54	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	297	TYR	Sidechain
2	F	297	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	2626	0	2518	43	0
1	C	2637	0	2529	36	0
1	E	2642	0	2534	48	0
1	G	2633	0	2524	49	0
1	I	2651	0	2551	40	0
1	K	2667	0	2577	36	0
2	B	2693	0	2589	57	0
2	D	2690	0	2588	39	0
2	F	2714	0	2624	39	0
2	H	2688	0	2573	60	0
2	J	2709	0	2610	40	0
2	L	2719	0	2632	33	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	1	0
4	H	1	0	0	0	0
4	I	1	0	0	1	0
4	J	1	0	0	0	0
4	K	1	0	0	1	0
4	L	1	0	0	0	0
5	B	5	0	0	0	0
5	D	5	0	0	0	0
5	F	5	0	0	0	0
5	H	5	0	0	0	0
5	J	5	0	0	0	0
5	L	5	0	0	0	0
6	B	29	0	20	0	0
6	D	29	0	20	0	0
6	F	29	0	20	0	0
6	H	29	0	20	0	0
6	J	29	0	20	0	0
6	L	29	0	20	0	0
7	B	12	0	13	0	0
7	D	12	0	13	2	0
7	F	12	0	13	0	0
7	H	12	0	13	0	0
7	J	12	0	13	0	0
7	L	12	0	13	0	0
8	A	95	0	0	2	0
8	B	74	0	0	2	0
8	C	102	0	0	2	0
8	D	123	0	0	3	0
8	E	97	0	0	1	0
8	F	114	0	0	1	0
8	G	96	0	0	3	0
8	H	65	0	0	3	0
8	I	134	0	0	3	0
8	J	102	0	0	2	0
8	K	207	0	0	5	0
8	L	166	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	33735	0	31047	504	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 8.

All (504) 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:E:156:ILE:HG12	1:E:172:ARG:HH12	1.10	1.13
1:A:156:ILE:HG12	1:A:172:ARG:HH12	0.97	1.12
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.05	1.11
1:K:156:ILE:HG12	1:K:172:ARG:HH12	0.99	1.07
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.20	1.05
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.22	1.01
1:K:156:ILE:HG12	1:K:172:ARG:NH1	1.83	0.93
1:A:156:ILE:HG12	1:A:172:ARG:NH1	1.83	0.92
2:B:39:ARG:HB3	2:B:39:ARG:HH11	1.33	0.90
4:G:378:CL:CL	8:G:385:HOH:O	2.31	0.86
1:I:156:ILE:HG12	1:I:172:ARG:NH1	1.91	0.86
2:H:18:LEU:HA	2:H:304:ARG:NH2	1.93	0.83
1:E:156:ILE:HG12	1:E:172:ARG:NH1	1.94	0.82
1:K:156:ILE:CG1	1:K:172:ARG:HH12	1.88	0.81
2:H:348:THR:O	2:H:352:GLU:HG2	1.80	0.80
1:A:152:MET:O	1:A:156:ILE:HG13	1.81	0.80
1:G:152:MET:O	1:G:156:ILE:HG13	1.83	0.78
1:K:152:MET:O	1:K:156:ILE:HG13	1.83	0.78
1:E:318:ILE:HG22	1:E:322:MET:HE3	1.66	0.75
1:I:152:MET:O	1:I:156:ILE:HG13	1.87	0.75
1:I:91:ILE:HD12	1:I:91:ILE:O	1.86	0.74
1:E:156:ILE:CG1	1:E:172:ARG:HH12	1.96	0.74
1:E:189:ILE:HD11	1:E:205:HIS:HD2	1.53	0.74
2:H:229:SER:O	2:H:233:MET:HG3	1.86	0.74
1:E:152:MET:O	1:E:156:ILE:HG13	1.87	0.74
1:A:214:ARG:HG2	1:G:180:LYS:HB2	1.69	0.73
1:G:91:ILE:HD12	1:G:91:ILE:O	1.89	0.72
1:K:189:ILE:HD11	1:K:205:HIS:HD2	1.54	0.72
1:C:189:ILE:HD11	1:C:205:HIS:HD2	1.55	0.72
2:B:69:LYS:O	2:B:73:ILE:HG13	1.89	0.72
1:E:353:LYS:HE2	1:E:357:ARG:HH12	1.55	0.71
1:E:214:ARG:O	1:E:214:ARG:HG3	1.91	0.71
1:K:298:GLN:HG2	8:K:529:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:ILE:HD11	1:G:205:HIS:HD2	1.56	0.71
1:C:152:MET:O	1:C:156:ILE:HG13	1.88	0.70
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.57	0.70
2:H:92:ARG:HG2	2:H:165:PRO:HG3	1.74	0.69
1:G:100:TYR:O	1:G:104:ARG:HG3	1.91	0.69
1:A:91:ILE:O	1:A:91:ILE:HD12	1.92	0.69
1:E:353:LYS:HE3	1:E:357:ARG:HH22	1.58	0.69
1:G:97:ARG:HG2	1:G:101:ASP:OD2	1.92	0.69
2:B:353:ARG:HH11	2:B:353:ARG:HG2	1.57	0.69
2:B:133:ILE:HD13	2:B:354:LEU:HD13	1.75	0.68
1:I:189:ILE:HD11	1:I:205:HIS:HD2	1.58	0.68
2:F:69:LYS:O	2:F:73:ILE:HG13	1.93	0.68
1:E:91:ILE:O	1:E:91:ILE:HD12	1.94	0.68
1:K:91:ILE:O	1:K:91:ILE:HD12	1.94	0.68
1:A:339:GLU:O	1:A:343:ILE:HG13	1.95	0.67
2:H:18:LEU:N	2:H:18:LEU:HD22	2.09	0.67
2:D:69:LYS:O	2:D:73:ILE:HG13	1.95	0.67
2:F:133:ILE:HD13	2:F:354:LEU:HD13	1.77	0.66
1:C:91:ILE:HD12	1:C:91:ILE:O	1.95	0.66
2:J:232:LEU:HD13	2:J:343:ALA:HB1	1.76	0.66
2:H:18:LEU:HA	2:H:304:ARG:HH22	1.61	0.66
1:G:87:VAL:HG12	1:G:88:VAL:HG23	1.76	0.66
2:D:353:ARG:HH11	2:D:357:LEU:HG	1.61	0.65
4:K:378:CL:CL	8:K:389:HOH:O	2.51	0.65
2:D:65:ASP:HA	8:D:457:HOH:O	1.96	0.65
2:H:21:LEU:HD21	2:H:304:ARG:HG2	1.77	0.65
2:H:69:LYS:O	2:H:73:ILE:HG13	1.96	0.65
2:F:37:PRO:HD2	2:F:40:TYR:CD1	2.32	0.65
2:H:21:LEU:HD23	2:H:24:ARG:HE	1.63	0.64
1:E:198:LYS:HD3	2:F:266:LYS:HD3	1.80	0.64
2:L:232:LEU:HD13	2:L:343:ALA:HB1	1.80	0.64
1:K:87:VAL:HG12	1:K:88:VAL:HG23	1.80	0.64
1:G:334:LEU:HD22	1:G:367:HIS:O	1.97	0.63
1:I:156:ILE:CG1	1:I:172:ARG:HH12	1.96	0.63
1:G:343:ILE:HG22	1:G:348:LYS:HG3	1.81	0.63
1:A:214:ARG:O	1:A:214:ARG:HG3	1.98	0.62
2:J:133:ILE:HD13	2:J:354:LEU:HD13	1.79	0.62
2:L:133:ILE:HD13	2:L:354:LEU:HD13	1.82	0.62
1:C:334:LEU:HD22	1:C:367:HIS:O	1.99	0.61
1:E:255:VAL:HG13	1:E:258:ARG:NH2	2.16	0.61
2:H:26:VAL:O	2:H:30:GLN:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:92:ARG:HD2	2:H:119:SER:HB3	1.82	0.60
1:E:312:ILE:HG23	1:E:340:LEU:HD22	1.84	0.60
2:H:245:LEU:O	2:H:249:LYS:HG3	2.01	0.60
1:G:101:ASP:HA	1:G:104:ARG:NH1	2.17	0.60
1:E:87:VAL:HG12	1:E:88:VAL:HG23	1.84	0.59
1:A:87:VAL:HG12	1:A:88:VAL:HG23	1.82	0.59
1:C:303:GLN:O	1:C:307:SER:HB2	2.01	0.59
1:E:92:TYR:O	1:E:97:ARG:NH2	2.35	0.59
2:B:258:ASN:OD1	2:B:259:GLY:N	2.33	0.59
2:F:37:PRO:HD2	2:F:40:TYR:CE1	2.37	0.59
2:H:263:ARG:HG3	2:H:266:LYS:HG3	1.85	0.59
2:B:92:ARG:NH1	2:B:119:SER:HB3	2.17	0.59
2:F:26:VAL:O	2:F:30:GLN:HG3	2.03	0.58
2:H:144:LYS:HE2	8:H:439:HOH:O	2.02	0.58
2:H:210:LEU:HB2	2:H:223:THR:HA	1.85	0.58
2:F:263:ARG:HG3	2:F:266:LYS:HG3	1.84	0.58
2:F:353:ARG:HG3	8:F:406:HOH:O	2.03	0.58
1:E:353:LYS:CE	1:E:357:ARG:HH12	2.15	0.58
2:H:232:LEU:HD13	2:H:343:ALA:HB1	1.83	0.58
2:J:210:LEU:HB2	2:J:223:THR:HA	1.84	0.58
1:C:69:ARG:HB3	1:C:71:GLU:OE1	2.03	0.58
1:C:87:VAL:HG12	1:C:88:VAL:HG23	1.85	0.58
2:L:210:LEU:HB2	2:L:223:THR:HA	1.85	0.58
2:B:186:ASN:HB2	2:B:358:HIS:CE1	2.39	0.58
2:D:263:ARG:HG3	2:D:266:LYS:HG3	1.86	0.58
2:B:210:LEU:HB2	2:B:223:THR:HA	1.85	0.58
1:A:334:LEU:HD22	1:A:367:HIS:O	2.04	0.57
1:C:328:ASP:O	1:C:329:ASN:HB2	2.04	0.57
1:I:334:LEU:HD22	1:I:367:HIS:O	2.03	0.57
2:B:295:ARG:HD3	8:B:438:HOH:O	2.05	0.57
1:G:101:ASP:HA	1:G:104:ARG:HH11	1.68	0.57
2:B:26:VAL:O	2:B:30:GLN:HG3	2.04	0.57
1:A:303:GLN:O	1:A:307:SER:HB2	2.04	0.57
2:F:210:LEU:HB2	2:F:223:THR:HA	1.86	0.57
2:J:263:ARG:HG3	2:J:266:LYS:HG3	1.87	0.57
1:I:69:ARG:HB3	1:I:71:GLU:OE1	2.04	0.57
1:K:107:LEU:HD22	2:L:117:TYR:CD2	2.40	0.57
2:B:39:ARG:HH11	2:B:39:ARG:CB	2.12	0.57
1:E:82:ASP:HB2	1:E:86:PRO:HB3	1.87	0.56
1:A:78:VAL:O	1:A:104:ARG:HD2	2.05	0.56
2:D:210:LEU:HB2	2:D:223:THR:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:60:MET:HE2	2:L:347:SER:HB3	1.88	0.56
2:L:263:ARG:HG3	2:L:266:LYS:HG3	1.87	0.56
2:B:334:GLU:HB3	2:B:337:ILE:HD12	1.88	0.56
2:B:353:ARG:HG2	2:B:353:ARG:NH1	2.17	0.56
1:C:339:GLU:O	1:C:343:ILE:HG13	2.05	0.56
2:J:22:ARG:O	2:J:26:VAL:HG23	2.05	0.56
1:G:303:GLN:O	1:G:307:SER:HB2	2.06	0.56
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.86	0.56
1:I:87:VAL:HG12	1:I:88:VAL:HG23	1.87	0.56
1:G:328:ASP:O	1:G:329:ASN:HB2	2.06	0.55
1:K:334:LEU:HD22	1:K:367:HIS:O	2.06	0.55
2:B:263:ARG:HG3	2:B:266:LYS:HG3	1.87	0.55
1:I:107:LEU:HD22	2:J:117:TYR:CD2	2.41	0.55
2:B:353:ARG:HH12	2:B:357:LEU:HG	1.72	0.55
1:C:156:ILE:HG12	1:C:172:ARG:NH1	2.06	0.55
2:D:295:ARG:CZ	2:D:299:LEU:HD11	2.37	0.55
1:E:339:GLU:O	1:E:343:ILE:HG13	2.07	0.55
1:A:251:SER:HA	1:A:287:ARG:HH22	1.70	0.55
1:G:261:GLN:O	1:G:265:GLU:HG2	2.07	0.55
1:E:78:VAL:O	1:E:104:ARG:HD2	2.06	0.55
1:A:156:ILE:CG1	1:A:172:ARG:HH12	1.92	0.54
1:K:303:GLN:O	1:K:307:SER:HB2	2.08	0.54
2:D:133:ILE:HD13	2:D:354:LEU:HD13	1.89	0.54
2:D:26:VAL:O	2:D:30:GLN:HG3	2.08	0.54
1:G:97:ARG:HH11	1:G:97:ARG:HB3	1.73	0.54
1:I:348:LYS:HD2	8:I:473:HOH:O	2.07	0.54
1:K:189:ILE:HD11	1:K:205:HIS:CD2	2.41	0.54
1:G:339:GLU:O	1:G:343:ILE:HG13	2.07	0.54
1:I:303:GLN:O	1:I:307:SER:HB2	2.08	0.54
1:C:318:ILE:HG22	1:C:322:MET:HE3	1.90	0.54
1:E:303:GLN:O	1:E:307:SER:HB2	2.07	0.54
1:C:156:ILE:HD12	8:C:433:HOH:O	2.07	0.54
2:H:349:ARG:O	2:H:352:GLU:HB2	2.08	0.54
1:E:261:GLN:O	1:E:265:GLU:HG2	2.07	0.53
2:J:197:ILE:HD11	2:J:235:LYS:HD3	1.91	0.53
4:I:378:CL:CL	8:I:512:HOH:O	2.56	0.53
1:K:265:GLU:O	1:K:269:LEU:HD13	2.09	0.53
1:C:261:GLN:O	1:C:265:GLU:HG2	2.08	0.53
1:G:318:ILE:HG22	1:G:322:MET:CE	2.39	0.53
2:H:202:ARG:HD2	8:H:440:HOH:O	2.08	0.53
2:B:18:LEU:HD12	2:B:304:ARG:CZ	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27:ARG:HA	2:D:30:GLN:HE21	1.73	0.53
1:G:79:PRO:HA	1:G:101:ASP:OD1	2.09	0.53
1:E:318:ILE:HG22	1:E:322:MET:CE	2.38	0.53
2:D:338:CYS:HB3	8:D:402:HOH:O	2.08	0.53
2:H:22:ARG:HG2	2:H:22:ARG:HH11	1.73	0.53
2:J:138:ASP:HA	2:J:357:LEU:HD11	1.91	0.53
2:L:60:MET:CE	2:L:347:SER:HB3	2.38	0.53
2:B:229:SER:O	2:B:233:MET:HG3	2.08	0.53
1:I:311:LEU:C	1:I:311:LEU:HD23	2.29	0.53
2:J:69:LYS:O	2:J:73:ILE:HG13	2.08	0.52
2:F:232:LEU:HD13	2:F:343:ALA:HB1	1.91	0.52
2:B:245:LEU:O	2:B:249:LYS:HG3	2.09	0.52
2:H:186:ASN:HB2	2:H:358:HIS:CE1	2.44	0.52
2:B:37:PRO:HD2	2:B:40:TYR:CE1	2.44	0.52
2:D:353:ARG:NH1	2:D:357:LEU:HG	2.22	0.52
2:B:258:ASN:CG	2:B:259:GLY:H	2.12	0.52
2:B:37:PRO:HD2	2:B:40:TYR:CD1	2.44	0.52
1:G:156:ILE:HD12	8:G:459:HOH:O	2.08	0.52
1:A:328:ASP:O	1:A:329:ASN:HB2	2.10	0.52
1:I:189:ILE:HD11	1:I:205:HIS:CD2	2.43	0.52
1:I:218:ASN:HB3	8:I:510:HOH:O	2.10	0.52
1:E:255:VAL:HG13	1:E:258:ARG:HH21	1.75	0.52
1:C:198:LYS:HD3	2:D:266:LYS:HD3	1.91	0.52
1:E:214:ARG:O	1:E:214:ARG:CG	2.57	0.52
1:C:312:ILE:HG23	1:C:340:LEU:HD22	1.92	0.51
1:E:156:ILE:HD11	1:E:172:ARG:HH22	1.76	0.51
2:D:229:SER:O	2:D:233:MET:HG3	2.11	0.51
2:D:232:LEU:HD13	2:D:343:ALA:HB1	1.92	0.51
1:G:156:ILE:HG12	1:G:172:ARG:NH1	2.05	0.51
2:H:64:LEU:HD11	2:H:134:ILE:HG22	1.93	0.51
1:I:157:ALA:O	1:I:161:GLU:HG3	2.10	0.51
2:D:311:LYS:HG3	2:D:312:TRP:CD2	2.46	0.51
1:G:318:ILE:HG22	1:G:322:MET:HE2	1.93	0.51
2:L:69:LYS:O	2:L:73:ILE:HG13	2.12	0.51
1:G:312:ILE:HG23	1:G:340:LEU:HD22	1.93	0.50
1:A:265:GLU:O	1:A:269:LEU:HD13	2.11	0.50
2:B:92:ARG:HH11	2:B:119:SER:HB3	1.75	0.50
1:C:156:ILE:CG1	1:C:172:ARG:HH12	2.08	0.50
1:E:265:GLU:O	1:E:269:LEU:HD13	2.11	0.50
1:A:214:ARG:CG	1:A:214:ARG:O	2.58	0.50
1:C:189:ILE:HD11	1:C:205:HIS:CD2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:18:LEU:HD12	2:D:304:ARG:NH1	2.26	0.50
2:H:202:ARG:HG3	2:H:202:ARG:HH11	1.76	0.50
2:F:311:LYS:HG3	2:F:312:TRP:CD2	2.47	0.50
2:D:138:ASP:OD1	2:D:140:SER:HB3	2.12	0.50
1:E:189:ILE:HD11	1:E:205:HIS:CD2	2.40	0.50
1:A:189:ILE:HD11	1:A:205:HIS:CD2	2.43	0.49
2:F:30:GLN:O	2:F:34:GLN:HG3	2.12	0.49
2:B:29:PHE:O	2:B:33:LEU:HD22	2.12	0.49
1:C:148:LEU:HB2	1:C:179:LEU:HD21	1.93	0.49
1:G:286:ASP:HB2	8:G:426:HOH:O	2.13	0.49
2:H:77:TYR:CZ	2:H:141:ARG:HB2	2.47	0.49
2:J:284:LYS:HE3	8:J:461:HOH:O	2.10	0.49
2:L:353:ARG:HD3	2:L:353:ARG:O	2.12	0.49
1:E:117:PHE:CE2	1:E:146:LYS:HE2	2.48	0.49
1:I:106:VAL:HG11	1:I:116:ALA:HB1	1.95	0.49
2:J:133:ILE:CD1	2:J:354:LEU:HD13	2.42	0.49
2:L:133:ILE:CD1	2:L:354:LEU:HD13	2.42	0.49
1:C:82:ASP:HB2	1:C:86:PRO:HB3	1.94	0.49
2:D:77:TYR:CZ	2:D:141:ARG:HB2	2.48	0.49
1:K:214:ARG:HH11	1:K:214:ARG:HG3	1.78	0.49
1:K:312:ILE:HG23	1:K:340:LEU:HD22	1.94	0.49
2:L:103:ILE:HG23	2:L:104:PRO:HD2	1.93	0.49
2:J:258:ASN:OD1	2:J:259:GLY:N	2.38	0.49
2:L:110:ASN:H	2:L:110:ASN:ND2	2.11	0.49
2:F:121:HIS:HB3	2:F:124:MET:HG2	1.95	0.49
2:H:311:LYS:HG3	2:H:312:TRP:CD2	2.48	0.49
2:B:336:GLY:HA2	2:J:305:LEU:CD1	2.43	0.49
1:A:92:TYR:O	1:A:97:ARG:NH2	2.46	0.48
2:B:77:TYR:CZ	2:B:141:ARG:HB2	2.48	0.48
1:E:334:LEU:HD22	1:E:367:HIS:O	2.12	0.48
1:K:104:ARG:NH2	8:K:393:HOH:O	2.46	0.48
1:I:328:ASP:O	1:I:329:ASN:HB2	2.13	0.48
1:E:107:LEU:HD22	2:F:117:TYR:CD2	2.48	0.48
2:F:245:LEU:O	2:F:249:LYS:HG3	2.13	0.48
1:E:338:LEU:HD11	1:E:364:GLN:HG3	1.95	0.48
1:E:58:LEU:HD22	1:E:95:LYS:HD3	1.95	0.48
1:G:189:ILE:HD11	1:G:205:HIS:CD2	2.42	0.48
2:H:29:PHE:O	2:H:33:LEU:HD22	2.12	0.48
1:E:97:ARG:HG2	1:E:101:ASP:OD2	2.14	0.48
1:E:148:LEU:HB2	1:E:179:LEU:HD21	1.94	0.48
1:K:192:ILE:O	1:K:195:GLN:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:311:LYS:HG3	2:L:312:TRP:CD2	2.48	0.48
2:H:74:GLU:CD	2:H:141:ARG:HH22	2.16	0.48
2:B:64:LEU:HD11	2:B:134:ILE:HG22	1.94	0.48
2:H:21:LEU:CD1	2:H:21:LEU:N	2.75	0.48
2:B:299:LEU:O	2:B:302:GLN:HB2	2.14	0.48
1:C:286:ASP:HB2	8:C:437:HOH:O	2.14	0.48
1:C:311:LEU:HD23	1:C:311:LEU:C	2.34	0.48
2:F:186:ASN:HB2	2:F:358:HIS:NE2	2.29	0.48
1:G:148:LEU:HB2	1:G:179:LEU:HD21	1.95	0.48
2:L:74:GLU:CD	2:L:141:ARG:HH22	2.16	0.48
1:A:287:ARG:O	1:A:291:ARG:HD3	2.14	0.48
2:B:311:LYS:HG3	2:B:312:TRP:CD2	2.47	0.48
1:C:265:GLU:O	1:C:269:LEU:HD13	2.14	0.48
1:C:329:ASN:HB3	1:C:332:ASP:HB3	1.96	0.48
2:F:37:PRO:HD2	2:F:40:TYR:HD1	1.79	0.48
1:G:344:LEU:HD13	1:G:356:TRP:CE2	2.49	0.48
1:E:58:LEU:HD23	1:E:63:TYR:CE2	2.49	0.47
1:I:329:ASN:HB3	1:I:332:ASP:HB3	1.96	0.47
1:K:311:LEU:HD23	1:K:311:LEU:C	2.34	0.47
1:A:71:GLU:CD	1:A:71:GLU:H	2.16	0.47
1:E:106:VAL:HG11	1:E:116:ALA:HB1	1.96	0.47
1:G:330:LYS:HE2	1:G:367:HIS:HB3	1.94	0.47
2:H:130:SER:O	2:H:134:ILE:HG13	2.14	0.47
1:I:148:LEU:HB2	1:I:179:LEU:HD21	1.96	0.47
1:I:88:VAL:HG12	1:I:88:VAL:O	2.14	0.47
1:K:311:LEU:HD23	1:K:311:LEU:O	2.14	0.47
2:D:121:HIS:HB3	2:D:124:MET:HG2	1.96	0.47
1:G:350:THR:O	1:G:353:LYS:HB3	2.14	0.47
1:C:106:VAL:HG11	1:C:116:ALA:HB1	1.96	0.47
2:J:334:GLU:HB3	2:J:337:ILE:HD12	1.96	0.47
1:E:103:PHE:CZ	1:E:133:VAL:HG22	2.50	0.47
1:G:265:GLU:O	1:G:269:LEU:HD13	2.15	0.47
1:A:97:ARG:HD3	8:A:437:HOH:O	2.14	0.47
2:B:250:ARG:O	2:B:254:MET:HG2	2.13	0.47
1:E:105:ALA:O	1:E:109:ARG:HG3	2.15	0.47
2:F:103:ILE:HG23	2:F:104:PRO:HD2	1.96	0.47
1:I:344:LEU:HD13	1:I:356:TRP:CE2	2.50	0.47
2:J:121:HIS:HB3	2:J:124:MET:HG2	1.96	0.47
2:J:311:LYS:HG3	2:J:312:TRP:CD2	2.50	0.47
2:H:281:LYS:HE3	2:H:331:LEU:HD12	1.97	0.47
2:D:82:LEU:HD11	2:D:108:SER:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:PHE:O	2:F:33:LEU:HD22	2.14	0.47
1:E:100:TYR:O	1:E:104:ARG:HG3	2.15	0.46
1:E:294:ASN:O	1:E:298:GLN:HG3	2.15	0.46
2:F:130:SER:O	2:F:134:ILE:HG13	2.15	0.46
1:I:350:THR:O	1:I:353:LYS:HB3	2.16	0.46
2:J:245:LEU:O	2:J:249:LYS:HG3	2.16	0.46
2:L:299:LEU:O	2:L:302:GLN:HB2	2.14	0.46
1:G:65:LEU:O	1:G:69:ARG:HG3	2.16	0.46
1:A:117:PHE:CE2	1:A:146:LYS:HE2	2.51	0.46
2:H:22:ARG:HG2	2:H:22:ARG:NH1	2.29	0.46
2:J:77:TYR:CE1	2:J:141:ARG:HB2	2.50	0.46
1:G:311:LEU:HD23	1:G:311:LEU:C	2.36	0.46
1:I:100:TYR:O	1:I:104:ARG:HG3	2.16	0.46
2:J:105:PHE:CE2	2:J:107:PRO:HD3	2.51	0.46
2:B:22:ARG:HH11	2:B:22:ARG:HG2	1.81	0.46
1:C:91:ILE:HG13	2:D:36:LEU:O	2.15	0.46
1:G:106:VAL:HG11	1:G:116:ALA:HB1	1.97	0.46
2:H:207:ASP:O	2:H:208:ASN:HB2	2.16	0.46
1:A:106:VAL:HG11	1:A:116:ALA:HB1	1.97	0.46
2:F:299:LEU:O	2:F:302:GLN:HB2	2.16	0.46
2:L:121:HIS:HB3	2:L:124:MET:HG2	1.98	0.46
2:B:192:ASP:OD1	2:B:195:LYS:HE3	2.16	0.46
2:B:207:ASP:O	2:B:208:ASN:HB2	2.16	0.46
1:K:151:GLU:HG3	1:K:175:LEU:HD11	1.97	0.46
2:B:336:GLY:HA2	2:J:305:LEU:HD13	1.98	0.45
2:B:232:LEU:HD13	2:B:343:ALA:HB1	1.98	0.45
1:C:97:ARG:HG2	1:C:101:ASP:OD2	2.15	0.45
1:I:265:GLU:O	1:I:269:LEU:HD13	2.16	0.45
1:K:106:VAL:HG11	1:K:116:ALA:HB1	1.98	0.45
2:D:258:ASN:OD1	2:D:259:GLY:N	2.37	0.45
1:A:114:GLU:HB2	8:A:459:HOH:O	2.16	0.45
1:A:318:ILE:O	1:A:322:MET:HG3	2.16	0.45
2:H:121:HIS:HB3	2:H:124:MET:HG2	1.98	0.45
1:K:328:ASP:O	1:K:329:ASN:HB2	2.16	0.45
2:L:22:ARG:HH11	2:L:22:ARG:HG2	1.81	0.45
1:A:107:LEU:HD22	2:B:117:TYR:CD2	2.51	0.45
2:D:250:ARG:O	2:D:254:MET:HG2	2.17	0.45
2:F:353:ARG:HD3	2:F:353:ARG:O	2.17	0.45
2:H:357:LEU:HD22	2:H:361:TRP:CZ2	2.51	0.45
2:H:258:ASN:OD1	2:H:259:GLY:N	2.44	0.45
1:A:311:LEU:HD23	1:A:311:LEU:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:LEU:HD11	2:B:108:SER:HA	1.98	0.45
2:B:311:LYS:HG3	2:B:312:TRP:CE2	2.51	0.45
2:F:77:TYR:CZ	2:F:141:ARG:HB2	2.52	0.45
2:H:82:LEU:HD11	2:H:108:SER:HA	1.99	0.45
1:I:65:LEU:O	1:I:69:ARG:HG3	2.16	0.45
2:L:250:ARG:O	2:L:254:MET:HG2	2.17	0.45
2:J:229:SER:O	2:J:233:MET:HG3	2.17	0.45
2:L:311:LYS:HG3	2:L:312:TRP:CE2	2.52	0.45
1:G:90:ILE:HD13	2:H:40:TYR:O	2.17	0.44
2:H:354:LEU:HD11	2:H:358:HIS:HE2	1.82	0.44
1:I:353:LYS:HG2	1:I:354:GLU:N	2.31	0.44
1:A:261:GLN:O	1:A:265:GLU:HG2	2.17	0.44
2:F:64:LEU:HD23	2:F:64:LEU:HA	1.86	0.44
1:K:82:ASP:HB2	1:K:86:PRO:HB3	1.99	0.44
1:A:91:ILE:HG13	2:B:36:LEU:O	2.18	0.44
1:A:67:ARG:NH2	1:A:94:GLU:OE1	2.51	0.44
2:B:121:HIS:HB3	2:B:124:MET:HG2	2.00	0.44
2:D:197:ILE:HD11	2:D:235:LYS:HD3	1.98	0.44
2:F:82:LEU:HD11	2:F:108:SER:HA	1.99	0.44
1:I:325:ASN:O	1:I:326:GLN:C	2.55	0.44
1:I:339:GLU:O	1:I:343:ILE:HG13	2.17	0.44
2:J:77:TYR:CZ	2:J:141:ARG:HB2	2.52	0.44
1:K:173:ARG:HD2	8:K:461:HOH:O	2.17	0.44
2:L:22:ARG:HG2	2:L:22:ARG:NH1	2.32	0.44
2:B:103:ILE:HG23	2:B:104:PRO:HD2	1.98	0.44
2:B:344:LEU:HD12	2:B:344:LEU:HA	1.84	0.44
2:H:237:GLU:HG2	8:H:415:HOH:O	2.17	0.44
2:H:31:ARG:HH22	2:H:306:VAL:HB	1.83	0.44
2:H:354:LEU:HD11	2:H:358:HIS:NE2	2.33	0.44
1:I:151:GLU:HG3	1:I:175:LEU:HD11	2.00	0.44
2:J:77:TYR:HE2	2:J:137:ASP:OD2	2.01	0.44
2:L:82:LEU:HD11	2:L:108:SER:HA	1.99	0.44
2:B:38:GLU:HG2	2:B:38:GLU:O	2.18	0.44
2:D:130:SER:O	2:D:134:ILE:HG13	2.18	0.44
1:G:290:SER:HB2	1:G:322:MET:HG2	2.00	0.44
1:I:311:LEU:HD23	1:I:311:LEU:O	2.17	0.44
2:H:21:LEU:CD2	2:H:304:ARG:HG2	2.45	0.44
1:A:156:ILE:HD11	1:A:172:ARG:HH22	1.83	0.44
1:G:325:ASN:O	1:G:326:GLN:C	2.56	0.44
2:H:18:LEU:N	2:H:18:LEU:CD2	2.79	0.44
2:H:353:ARG:O	2:H:357:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HB2	1:A:179:LEU:HD21	2.00	0.44
2:F:311:LYS:HG3	2:F:312:TRP:CE2	2.53	0.44
1:G:65:LEU:HD12	1:G:67:ARG:HH11	1.83	0.44
2:H:103:ILE:HG23	2:H:104:PRO:HD2	1.99	0.44
2:L:105:PHE:CE2	2:L:107:PRO:HD3	2.52	0.43
1:A:325:ASN:O	1:A:326:GLN:C	2.56	0.43
2:D:311:LYS:HG3	2:D:312:TRP:CE2	2.53	0.43
1:G:219:GLU:OE1	1:G:219:GLU:HA	2.18	0.43
2:H:198:SER:OG	2:H:202:ARG:NH1	2.51	0.43
2:H:250:ARG:O	2:H:254:MET:HG2	2.18	0.43
2:J:64:LEU:O	2:J:67:VAL:HG22	2.17	0.43
1:K:83:GLY:HA3	2:L:105:PHE:CD1	2.53	0.43
1:C:287:ARG:H	1:C:287:ARG:HG2	1.59	0.43
1:G:329:ASN:HB3	1:G:332:ASP:HB3	1.99	0.43
2:H:311:LYS:HG3	2:H:312:TRP:CE2	2.53	0.43
2:J:19:ASP:OD2	2:J:19:ASP:N	2.51	0.43
2:B:115:HIS:HA	2:B:116:PRO:HD3	1.90	0.43
1:C:78:VAL:O	1:C:104:ARG:HD2	2.17	0.43
2:F:138:ASP:OD1	2:F:140:SER:HB3	2.18	0.43
2:F:207:ASP:O	2:F:208:ASN:HB2	2.18	0.43
2:H:22:ARG:O	2:H:26:VAL:HG23	2.18	0.43
8:B:441:HOH:O	2:J:31:ARG:HD3	2.18	0.43
1:A:103:PHE:CZ	1:A:133:VAL:HG22	2.54	0.43
2:B:36:LEU:HA	2:B:37:PRO:HD3	1.86	0.43
2:D:19:ASP:OD2	2:D:19:ASP:N	2.43	0.43
2:H:77:TYR:HE2	2:H:137:ASP:OD2	2.02	0.43
1:C:318:ILE:HG22	1:C:322:MET:CE	2.48	0.43
1:G:353:LYS:CG	1:G:354:GLU:N	2.81	0.43
2:J:311:LYS:HG3	2:J:312:TRP:CE2	2.53	0.43
2:F:250:ARG:O	2:F:254:MET:HG2	2.18	0.43
2:H:249:LYS:HB3	2:H:285:ILE:HD13	2.00	0.43
2:H:92:ARG:HG2	2:H:165:PRO:CG	2.46	0.43
2:J:133:ILE:HG22	2:J:350:THR:HG23	1.99	0.43
2:J:82:LEU:HD11	2:J:108:SER:HA	1.99	0.43
2:L:334:GLU:HB3	2:L:337:ILE:HD12	2.00	0.43
1:C:107:LEU:HD22	2:D:117:TYR:CD2	2.54	0.43
1:G:105:ALA:O	1:G:109:ARG:HG3	2.18	0.43
2:H:30:GLN:O	2:H:34:GLN:HG3	2.19	0.43
1:E:83:GLY:HA3	2:F:105:PHE:CD1	2.55	0.42
2:F:133:ILE:CD1	2:F:354:LEU:HD13	2.48	0.42
2:F:256:GLN:HB2	2:F:260:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:64:LEU:HB3	2:J:69:LYS:HE2	2.01	0.42
2:L:33:LEU:HD22	2:L:54:ALA:HB1	2.02	0.42
1:E:312:ILE:O	1:E:316:VAL:HG23	2.20	0.42
2:J:130:SER:O	2:J:134:ILE:HG13	2.19	0.42
2:J:338:CYS:SG	2:J:349:ARG:NH2	2.92	0.42
1:K:148:LEU:HB2	1:K:179:LEU:HD21	2.00	0.42
2:L:64:LEU:HB3	2:L:69:LYS:HE2	2.02	0.42
1:C:311:LEU:O	1:C:311:LEU:HD23	2.18	0.42
2:B:22:ARG:NH1	2:B:22:ARG:HG2	2.34	0.42
2:B:133:ILE:CD1	2:B:354:LEU:HD13	2.47	0.42
2:B:77:TYR:CE1	2:B:141:ARG:HB2	2.54	0.42
2:L:256:GLN:HB2	2:L:260:TYR:CE2	2.55	0.42
2:B:256:GLN:HB2	2:B:260:TYR:CE2	2.55	0.42
2:D:37:PRO:HD2	2:D:40:TYR:CE1	2.54	0.42
1:I:338:LEU:HD11	1:I:364:GLN:HG2	2.00	0.42
1:K:330:LYS:HE2	1:K:367:HIS:HB3	2.02	0.42
2:L:49:THR:HG23	2:L:124:MET:SD	2.59	0.42
2:B:21:LEU:CD1	2:B:21:LEU:N	2.81	0.42
2:B:22:ARG:O	2:B:26:VAL:HG23	2.19	0.42
2:F:192:ASP:CG	2:F:195:LYS:HG3	2.40	0.42
1:K:167:GLN:NE2	8:K:569:HOH:O	2.52	0.42
1:A:274:GLU:HG3	1:A:310:TYR:CE2	2.55	0.42
1:E:151:GLU:HG3	1:E:175:LEU:HD11	2.02	0.42
1:E:361:ARG:HD3	8:E:456:HOH:O	2.20	0.42
1:I:198:LYS:HD3	2:J:266:LYS:HD3	2.02	0.42
1:I:351:ILE:CD1	2:J:256:GLN:HG2	2.50	0.42
1:K:96:PHE:CE1	1:K:126:LEU:HB3	2.55	0.42
1:A:151:GLU:HG3	1:A:175:LEU:HD11	2.02	0.42
2:B:64:LEU:HD23	2:B:64:LEU:HA	1.85	0.42
2:H:19:ASP:O	2:H:21:LEU:HD13	2.19	0.42
2:H:268:VAL:HG23	2:H:297:TYR:CZ	2.55	0.42
2:D:22:ARG:HG2	2:D:22:ARG:HH11	1.86	0.41
2:D:53:PHE:HZ	7:D:382:MES:H71	1.85	0.41
1:E:69:ARG:HB3	1:E:71:GLU:OE1	2.20	0.41
1:C:91:ILE:HD11	2:D:38:GLU:H	1.85	0.41
1:K:339:GLU:O	1:K:343:ILE:HG13	2.20	0.41
2:B:192:ASP:OD1	2:B:195:LYS:CE	2.68	0.41
2:L:258:ASN:OD1	2:L:259:GLY:N	2.43	0.41
2:B:130:SER:O	2:B:134:ILE:HG13	2.19	0.41
1:C:103:PHE:CZ	1:C:133:VAL:HG22	2.55	0.41
2:F:77:TYR:CE1	2:F:141:ARG:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:344:LEU:HA	2:F:344:LEU:HD12	1.73	0.41
2:B:92:ARG:NH1	2:B:118:ASP:O	2.54	0.41
1:G:334:LEU:O	1:G:338:LEU:HG	2.20	0.41
2:H:256:GLN:HB2	2:H:260:TYR:CE2	2.56	0.41
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.55	0.41
1:C:74:ASP:N	1:C:74:ASP:OD2	2.52	0.41
1:E:287:ARG:HG2	1:E:287:ARG:H	1.48	0.41
2:F:144:LYS:HG2	2:F:185:LEU:HD22	2.03	0.41
1:I:330:LYS:HE2	1:I:367:HIS:HB3	2.01	0.41
1:K:117:PHE:CE2	1:K:146:LYS:HE2	2.55	0.41
1:K:353:LYS:HB2	1:K:353:LYS:HE3	1.78	0.41
2:B:160:SER:HB3	2:B:199:TYR:CE1	2.56	0.41
2:B:302:GLN:HG3	2:B:309:PHE:CE2	2.55	0.41
1:G:117:PHE:CE2	1:G:146:LYS:HE2	2.56	0.41
1:G:97:ARG:NH1	1:G:97:ARG:CB	2.83	0.41
2:L:19:ASP:N	2:L:19:ASP:OD2	2.51	0.41
2:D:237:GLU:HG2	8:D:418:HOH:O	2.21	0.41
2:D:20:PHE:CZ	2:D:337:ILE:HD11	2.56	0.41
2:F:115:HIS:HA	2:F:116:PRO:HD3	1.92	0.41
1:I:101:ASP:HA	1:I:104:ARG:HH11	1.86	0.41
1:K:78:VAL:O	1:K:104:ARG:HD2	2.21	0.41
2:L:255:ARG:HD3	2:L:261:HIS:CD2	2.56	0.41
1:E:325:ASN:O	1:E:326:GLN:C	2.58	0.41
1:E:348:LYS:HD3	1:E:348:LYS:HA	1.89	0.41
2:F:186:ASN:HB2	2:F:358:HIS:CE1	2.56	0.41
1:C:96:PHE:CE1	1:C:126:LEU:HB3	2.56	0.41
2:D:133:ILE:HG22	2:D:350:THR:HG23	2.02	0.41
1:G:127:ASN:ND2	1:G:130:ASN:HB2	2.36	0.41
1:A:212:GLU:O	1:G:180:LYS:HE3	2.21	0.41
1:G:319:TYR:HA	1:G:322:MET:HE3	2.02	0.41
2:H:184:MET:HA	2:H:354:LEU:HD21	2.03	0.41
1:I:219:GLU:HA	1:I:219:GLU:OE1	2.21	0.41
2:J:195:LYS:NZ	8:J:415:HOH:O	2.54	0.41
1:A:355:TYR:O	1:A:358:TYR:HB3	2.21	0.40
1:I:103:PHE:CZ	1:I:133:VAL:HG22	2.56	0.40
2:J:250:ARG:O	2:J:254:MET:HG2	2.21	0.40
2:D:126:TYR:HE2	7:D:382:MES:C6	2.34	0.40
2:D:268:VAL:HG23	2:D:297:TYR:CZ	2.57	0.40
1:G:156:ILE:HD11	1:G:172:ARG:HH22	1.87	0.40
1:I:312:ILE:HG23	1:I:340:LEU:HD22	2.03	0.40
2:J:357:LEU:HD22	2:J:361:TRP:CZ2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:103:PHE:CZ	1:K:133:VAL:HG22	2.56	0.40
1:K:294:ASN:O	1:K:298:GLN:HB2	2.21	0.40
2:L:320:LEU:C	2:L:320:LEU:HD23	2.42	0.40
1:A:267:ILE:HD13	1:A:277:TRP:CE2	2.57	0.40
1:A:348:LYS:HA	1:A:348:LYS:HD3	1.82	0.40
2:B:49:THR:HG23	2:B:124:MET:SD	2.62	0.40
2:D:64:LEU:HD11	2:D:134:ILE:HG22	2.03	0.40
2:D:344:LEU:HA	2:D:344:LEU:HD12	1.84	0.40
2:F:192:ASP:OD1	2:F:195:LYS:HG3	2.22	0.40
2:J:33:LEU:HD22	2:J:54:ALA:HB1	2.02	0.40
2:H:348:THR:HA	2:H:351:SER:OG	2.21	0.40
2:H:357:LEU:HD22	2:H:361:TRP:CE2	2.57	0.40
1:I:287:ARG:H	1:I:287:ARG:HG2	1.57	0.40
2:J:256:GLN:HB2	2:J:260:TYR:CE2	2.57	0.40
2:J:353:ARG:HH11	2:J:353:ARG:HG2	1.87	0.40
2:L:207:ASP:O	2:L:208:ASN:HB2	2.22	0.40
1:G:96:PHE:CE1	1:G:126:LEU:HB3	2.56	0.40
2:H:60:MET:HE2	2:H:347:SER:HB3	2.04	0.40
2:H:49:THR:HG23	2:H:124:MET:SD	2.62	0.40
1:K:156:ILE:HD11	1:K:172:ARG:HH22	1.87	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	312/377 (83%)	289 (93%)	22 (7%)	1 (0%)	44	64
1	C	312/377 (83%)	294 (94%)	17 (5%)	1 (0%)	44	64
1	E	312/377 (83%)	288 (92%)	24 (8%)	0	100	100
1	G	312/377 (83%)	291 (93%)	21 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	312/377 (83%)	292 (94%)	18 (6%)	2 (1%)	28	46
1	K	312/377 (83%)	294 (94%)	17 (5%)	1 (0%)	44	64
2	B	344/377 (91%)	325 (94%)	17 (5%)	2 (1%)	28	46
2	D	344/377 (91%)	329 (96%)	13 (4%)	2 (1%)	28	46
2	F	344/377 (91%)	327 (95%)	15 (4%)	2 (1%)	28	46
2	H	344/377 (91%)	326 (95%)	15 (4%)	3 (1%)	20	34
2	J	344/377 (91%)	329 (96%)	12 (4%)	3 (1%)	20	34
2	L	344/377 (91%)	332 (96%)	10 (3%)	2 (1%)	28	46
All	All	3936/4524 (87%)	3716 (94%)	201 (5%)	19 (0%)	32	52

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	GLN
2	B	258	ASN
1	C	326	GLN
2	D	258	ASN
2	H	258	ASN
2	H	333	GLU
1	I	306	HIS
2	J	258	ASN
2	L	258	ASN
2	F	258	ASN
1	I	326	GLN
2	J	34	GLN
1	K	306	HIS
2	H	111	PRO
2	F	111	PRO
2	J	111	PRO
2	B	111	PRO
2	D	111	PRO
2	L	111	PRO

5.3.2 Protein sidechains ⓘ

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	279/338 (82%)	273 (98%)	6 (2%)	57	80
1	C	282/338 (83%)	274 (97%)	8 (3%)	49	74
1	E	284/338 (84%)	277 (98%)	7 (2%)	53	77
1	G	281/338 (83%)	276 (98%)	5 (2%)	64	84
1	I	286/338 (85%)	278 (97%)	8 (3%)	49	74
1	K	290/338 (86%)	281 (97%)	9 (3%)	45	70
2	B	287/326 (88%)	275 (96%)	12 (4%)	34	57
2	D	286/326 (88%)	273 (96%)	13 (4%)	32	54
2	F	292/326 (90%)	279 (96%)	13 (4%)	32	54
2	H	286/326 (88%)	272 (95%)	14 (5%)	29	50
2	J	291/326 (89%)	276 (95%)	15 (5%)	27	47
2	L	294/326 (90%)	278 (95%)	16 (5%)	26	44
All	All	3438/3984 (86%)	3312 (96%)	126 (4%)	39	63

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	PHE
1	A	67	ARG
1	A	71	GLU
1	A	81	ASN
1	A	214	ARG
1	A	287	ARG
2	B	24	ARG
2	B	33	LEU
2	B	39	ARG
2	B	151	LEU
2	B	216	LEU
2	B	232	LEU
2	B	236	LEU
2	B	255	ARG
2	B	261	HIS
2	B	302	GLN
2	B	329	LEU
2	B	331	LEU
1	C	55	PHE

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Mol	Chain	Res	Type
1	C	59	ASP
1	C	71	GLU
1	C	76	ASP
1	C	182	PRO
1	C	287	ARG
1	C	324	GLU
1	C	364	GLN
2	D	21	LEU
2	D	33	LEU
2	D	151	LEU
2	D	216	LEU
2	D	232	LEU
2	D	236	LEU
2	D	255	ARG
2	D	258	ASN
2	D	261	HIS
2	D	306	VAL
2	D	329	LEU
2	D	331	LEU
2	D	353	ARG
1	E	55	PHE
1	E	67	ARG
1	E	71	GLU
1	E	194	ASN
1	E	214	ARG
1	E	287	ARG
1	E	324	GLU
2	F	21	LEU
2	F	24	ARG
2	F	33	LEU
2	F	151	LEU
2	F	216	LEU
2	F	232	LEU
2	F	236	LEU
2	F	255	ARG
2	F	258	ASN
2	F	261	HIS
2	F	329	LEU
2	F	331	LEU
2	F	353	ARG
1	G	71	GLU
1	G	214	ARG

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Mol	Chain	Res	Type
1	G	224	ASP
1	G	287	ARG
1	G	324	GLU
2	H	18	LEU
2	H	21	LEU
2	H	151	LEU
2	H	157	GLU
2	H	216	LEU
2	H	232	LEU
2	H	236	LEU
2	H	255	ARG
2	H	258	ASN
2	H	261	HIS
2	H	306	VAL
2	H	329	LEU
2	H	331	LEU
2	H	357	LEU
1	I	55	PHE
1	I	71	GLU
1	I	194	ASN
1	I	195	GLN
1	I	287	ARG
1	I	324	GLU
1	I	353	LYS
1	I	364	GLN
2	J	21	LEU
2	J	27	ARG
2	J	31	ARG
2	J	33	LEU
2	J	151	LEU
2	J	216	LEU
2	J	232	LEU
2	J	236	LEU
2	J	255	ARG
2	J	261	HIS
2	J	306	VAL
2	J	329	LEU
2	J	331	LEU
2	J	353	ARG
2	J	357	LEU
1	K	55	PHE
1	K	67	ARG

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Mol	Chain	Res	Type
1	K	71	GLU
1	K	142	ARG
1	K	194	ASN
1	K	195	GLN
1	K	287	ARG
1	K	298	GLN
1	K	324	GLU
2	L	21	LEU
2	L	33	LEU
2	L	65	ASP
2	L	110	ASN
2	L	151	LEU
2	L	216	LEU
2	L	232	LEU
2	L	236	LEU
2	L	255	ARG
2	L	258	ASN
2	L	261	HIS
2	L	302	GLN
2	L	306	VAL
2	L	329	LEU
2	L	331	LEU
2	L	353	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	184	GLN
1	A	201	HIS
1	A	285	GLN
1	A	329	ASN
2	B	208	ASN
1	C	108	GLN
1	C	218	ASN
1	C	298	GLN
1	C	335	ASN
1	C	364	GLN
2	D	30	GLN
2	D	246	ASN
1	E	81	ASN
1	E	184	GLN

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Mol	Chain	Res	Type
1	E	298	GLN
2	F	30	GLN
2	F	246	ASN
1	G	80	GLN
1	G	81	ASN
1	G	89	GLN
1	G	162	GLN
1	G	184	GLN
1	G	297	ASN
1	G	325	ASN
2	H	246	ASN
1	I	89	GLN
1	I	285	GLN
1	I	364	GLN
2	J	30	GLN
2	J	208	ASN
2	J	246	ASN
1	K	81	ASN
1	K	218	ASN
2	L	110	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 15 are monoatomic - leaving 18 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
5	SO4	B	379	-	4,4,4	0.34	0	6,6,6	0.07	0
6	778	B	380	3	29,32,32	2.45	17 (58%)	37,44,44	2.04	9 (24%)
7	MES	B	381	-	12,12,12	9.15	8 (66%)	14,16,16	3.32	6 (42%)
5	SO4	D	380	-	4,4,4	0.34	0	6,6,6	0.10	0
6	778	D	381	3	29,32,32	2.37	17 (58%)	37,44,44	2.05	9 (24%)
7	MES	D	382	-	12,12,12	9.29	8 (66%)	14,16,16	3.19	7 (50%)
5	SO4	F	380	-	4,4,4	0.29	0	6,6,6	0.24	0
6	778	F	381	3	29,32,32	2.40	16 (55%)	37,44,44	2.08	10 (27%)
7	MES	F	382	-	12,12,12	9.06	8 (66%)	14,16,16	3.38	7 (50%)
5	SO4	H	380	-	4,4,4	0.34	0	6,6,6	0.18	0
6	778	H	381	3	29,32,32	2.34	15 (51%)	37,44,44	2.05	9 (24%)
7	MES	H	382	-	12,12,12	9.28	8 (66%)	14,16,16	3.09	6 (42%)
5	SO4	J	380	-	4,4,4	0.30	0	6,6,6	0.21	0
6	778	J	381	3	29,32,32	2.34	14 (48%)	37,44,44	2.05	9 (24%)
7	MES	J	382	-	12,12,12	9.23	8 (66%)	14,16,16	3.30	7 (50%)
5	SO4	L	380	-	4,4,4	0.29	0	6,6,6	0.19	0
6	778	L	381	3	29,32,32	2.39	15 (51%)	37,44,44	2.05	8 (21%)
7	MES	L	382	-	12,12,12	9.45	9 (75%)	14,16,16	3.37	7 (50%)

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
5	SO4	B	379	-	-	0/0/0/0	0/0/0/0
6	778	B	380	3	-	0/14/27/27	0/4/4/4
7	MES	B	381	-	-	0/6/14/14	0/1/1/1
5	SO4	D	380	-	-	0/0/0/0	0/0/0/0
6	778	D	381	3	-	0/14/27/27	0/4/4/4
7	MES	D	382	-	-	0/6/14/14	0/1/1/1
5	SO4	F	380	-	-	0/0/0/0	0/0/0/0
6	778	F	381	3	-	0/14/27/27	0/4/4/4
7	MES	F	382	-	-	0/6/14/14	0/1/1/1
5	SO4	H	380	-	-	0/0/0/0	0/0/0/0
6	778	H	381	3	-	0/14/27/27	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MES	H	382	-	-	0/6/14/14	0/1/1/1
5	SO4	J	380	-	-	0/0/0/0	0/0/0/0
6	778	J	381	3	-	0/14/27/27	0/4/4/4
7	MES	J	382	-	-	0/6/14/14	0/1/1/1
5	SO4	L	380	-	-	0/0/0/0	0/0/0/0
6	778	L	381	3	-	0/14/27/27	0/4/4/4
7	MES	L	382	-	-	0/6/14/14	0/1/1/1

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	382	MES	C8-S	-24.16	1.41	1.77
7	D	382	MES	C8-S	-23.63	1.42	1.77
7	H	382	MES	C8-S	-23.52	1.42	1.77
7	J	382	MES	C8-S	-23.27	1.42	1.77
7	B	381	MES	C8-S	-22.80	1.43	1.77
7	F	382	MES	C8-S	-22.33	1.44	1.77
6	B	380	778	C34-C35	-5.31	1.31	1.44
6	F	381	778	C34-C35	-5.29	1.31	1.44
6	D	381	778	C34-C35	-5.19	1.32	1.44
6	H	381	778	C34-C35	-5.11	1.32	1.44
6	J	381	778	C34-C35	-5.01	1.32	1.44
7	L	382	MES	C7-C8	-4.98	1.36	1.52
6	L	381	778	C34-C35	-4.96	1.32	1.44
7	H	382	MES	C7-C8	-4.85	1.37	1.52
7	D	382	MES	C7-C8	-4.79	1.37	1.52
7	B	381	MES	C7-C8	-4.77	1.37	1.52
7	J	382	MES	C7-C8	-4.70	1.37	1.52
7	F	382	MES	C7-C8	-4.59	1.38	1.52
7	L	382	MES	C7-N4	-3.57	1.39	1.47
7	D	382	MES	C7-N4	-3.34	1.39	1.47
7	H	382	MES	C7-N4	-3.28	1.39	1.47
7	J	382	MES	C7-N4	-3.22	1.40	1.47
7	B	381	MES	C7-N4	-3.13	1.40	1.47
7	L	382	MES	C3-C2	-2.81	1.39	1.50
7	J	382	MES	C3-C2	-2.76	1.39	1.50
7	D	382	MES	C3-C2	-2.71	1.39	1.50
7	F	382	MES	C3-C2	-2.70	1.39	1.50
7	F	382	MES	C7-N4	-2.69	1.41	1.47
7	B	381	MES	C3-C2	-2.67	1.39	1.50
7	H	382	MES	C3-C2	-2.65	1.39	1.50
7	L	382	MES	C5-C6	-2.57	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	382	MES	C5-C6	-2.49	1.40	1.50
7	D	382	MES	C5-C6	-2.47	1.40	1.50
7	H	382	MES	C5-C6	-2.45	1.40	1.50
7	F	382	MES	C5-C6	-2.42	1.40	1.50
7	B	381	MES	C5-C6	-2.42	1.40	1.50
7	L	382	MES	C5-N4	-2.16	1.41	1.47
6	B	380	778	C16-C25	2.01	1.56	1.51
6	F	381	778	C20-C14	2.03	1.43	1.39
6	F	381	778	C33-C29	2.05	1.42	1.38
6	D	381	778	C33-C29	2.05	1.42	1.38
6	J	381	778	C17-N18	2.06	1.38	1.34
6	L	381	778	C20-C14	2.06	1.43	1.39
6	D	381	778	C4-N1	2.09	1.48	1.46
6	H	381	778	C28-C25	2.09	1.43	1.38
6	F	381	778	C4-N1	2.09	1.48	1.46
6	D	381	778	C27-C30	2.10	1.42	1.38
6	F	381	778	C27-C30	2.13	1.43	1.38
6	F	381	778	C17-N18	2.13	1.39	1.34
6	H	381	778	C27-C30	2.18	1.43	1.38
6	J	381	778	C20-C14	2.22	1.43	1.39
6	H	381	778	C33-C29	2.22	1.42	1.38
6	B	380	778	C27-C30	2.23	1.43	1.38
6	J	381	778	C33-C34	2.24	1.44	1.39
6	L	381	778	C17-N18	2.26	1.39	1.34
6	D	381	778	C17-N18	2.28	1.39	1.34
6	D	381	778	C27-C21	2.30	1.43	1.38
6	H	381	778	C20-C14	2.31	1.43	1.39
6	L	381	778	C33-C34	2.32	1.44	1.39
6	B	380	778	C33-C29	2.33	1.42	1.38
6	D	381	778	C33-C34	2.34	1.44	1.39
6	F	381	778	C29-C25	2.35	1.43	1.38
6	L	381	778	C29-C25	2.35	1.43	1.38
6	J	381	778	C28-C25	2.37	1.43	1.38
6	D	381	778	C20-C14	2.39	1.44	1.39
6	H	381	778	C27-C21	2.41	1.43	1.38
6	B	380	778	C33-C34	2.41	1.44	1.39
6	F	381	778	C20-C26	2.41	1.42	1.38
6	J	381	778	C29-C25	2.44	1.43	1.38
6	B	380	778	C17-N18	2.45	1.39	1.34
6	F	381	778	C28-C25	2.47	1.44	1.38
6	L	381	778	C32-C28	2.48	1.43	1.38
6	H	381	778	C17-N18	2.54	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	380	778	C20-C14	2.54	1.44	1.39
6	L	381	778	C28-C25	2.55	1.44	1.38
6	B	380	778	C27-C21	2.57	1.43	1.38
6	B	380	778	C29-C25	2.59	1.44	1.38
6	D	381	778	C29-C25	2.59	1.44	1.38
6	H	381	778	C29-C25	2.61	1.44	1.38
6	J	381	778	C32-C28	2.62	1.43	1.38
6	H	381	778	C32-C28	2.64	1.43	1.38
6	D	381	778	C20-C26	2.65	1.42	1.38
6	D	381	778	C28-C25	2.65	1.44	1.38
6	B	380	778	C28-C25	2.70	1.44	1.38
6	L	381	778	C27-C21	2.70	1.44	1.38
6	D	381	778	C32-C28	2.72	1.43	1.38
6	H	381	778	C30-C26	2.72	1.43	1.38
6	F	381	778	C27-C21	2.77	1.44	1.38
6	J	381	778	C27-C21	2.78	1.44	1.38
6	B	380	778	C20-C26	2.80	1.42	1.38
6	B	380	778	C30-C26	2.85	1.43	1.38
6	F	381	778	C32-C28	2.85	1.43	1.38
6	J	381	778	C20-C26	2.88	1.43	1.38
6	H	381	778	C20-C26	2.91	1.43	1.38
6	J	381	778	C4-C8	2.92	1.56	1.51
6	F	381	778	C30-C26	2.96	1.43	1.38
6	B	380	778	C32-C28	2.97	1.44	1.38
6	L	381	778	C20-C26	3.03	1.43	1.38
6	L	381	778	C4-N1	3.07	1.49	1.46
6	D	381	778	C30-C26	3.11	1.44	1.38
6	H	381	778	C4-C8	3.16	1.57	1.51
6	L	381	778	C30-C26	3.17	1.44	1.38
6	D	381	778	C21-C14	3.17	1.45	1.39
6	J	381	778	C12-N18	3.18	1.45	1.35
6	H	381	778	C21-C14	3.19	1.45	1.39
6	B	380	778	C21-C14	3.20	1.45	1.39
6	D	381	778	C4-C8	3.21	1.57	1.51
6	H	381	778	C12-N18	3.23	1.45	1.35
6	L	381	778	C12-N18	3.24	1.45	1.35
6	J	381	778	C30-C26	3.26	1.44	1.38
6	D	381	778	C12-N18	3.27	1.45	1.35
6	B	380	778	C12-N18	3.33	1.45	1.35
6	J	381	778	C21-C14	3.34	1.46	1.39
6	F	381	778	C12-N18	3.38	1.46	1.35
6	L	381	778	C21-C14	3.41	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	381	778	C21-C14	3.50	1.46	1.39
6	L	381	778	C4-C8	3.55	1.58	1.51
6	B	380	778	C4-C8	3.71	1.58	1.51
6	F	381	778	C4-C8	3.72	1.58	1.51
6	L	381	778	C8-N9	4.36	1.43	1.36
6	D	381	778	C8-N9	4.53	1.44	1.36
6	H	381	778	C8-N9	4.54	1.44	1.36
6	B	380	778	C8-N9	4.58	1.44	1.36
6	J	381	778	C8-N9	4.62	1.44	1.36
6	F	381	778	C8-N9	4.90	1.44	1.36
7	D	382	MES	O3S-S	10.04	1.81	1.47
7	J	382	MES	O3S-S	10.12	1.81	1.47
7	L	382	MES	O3S-S	10.20	1.81	1.47
7	F	382	MES	O3S-S	10.25	1.82	1.47
7	H	382	MES	O3S-S	10.30	1.82	1.47
7	B	381	MES	O3S-S	10.34	1.82	1.47
7	H	382	MES	O1S-S	12.57	1.81	1.45
7	L	382	MES	O1S-S	12.58	1.81	1.45
7	B	381	MES	O1S-S	12.59	1.81	1.45
7	J	382	MES	O1S-S	12.61	1.81	1.45
7	D	382	MES	O2S-S	12.63	1.82	1.45
7	D	382	MES	O1S-S	12.70	1.82	1.45
7	H	382	MES	O2S-S	12.72	1.82	1.45
7	L	382	MES	O2S-S	12.80	1.82	1.45
7	B	381	MES	O2S-S	12.85	1.82	1.45
7	F	382	MES	O2S-S	12.85	1.82	1.45
7	J	382	MES	O2S-S	12.86	1.82	1.45
7	F	382	MES	O1S-S	12.96	1.83	1.45

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	381	778	C3-N1-C4	-5.19	103.68	110.61
6	H	381	778	C3-N1-C4	-5.16	103.72	110.61
6	B	380	778	C3-N1-C4	-5.12	103.77	110.61
6	L	381	778	C3-N1-C4	-5.07	103.84	110.61
6	J	381	778	C3-N1-C4	-4.96	103.98	110.61
6	F	381	778	C3-N1-C4	-4.82	104.17	110.61
6	H	381	778	C5-C2-N1	-4.68	101.17	110.63
6	D	381	778	C5-C2-N1	-4.55	101.42	110.63
6	B	380	778	C5-C2-N1	-4.45	101.64	110.63
6	J	381	778	C5-C2-N1	-4.42	101.68	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	381	778	C5-C2-N1	-4.32	101.88	110.63
6	L	381	778	C5-C2-N1	-4.27	101.99	110.63
7	J	382	MES	O3S-S-O2S	-2.76	105.05	111.37
7	L	382	MES	O3S-S-O2S	-2.68	105.22	111.37
7	D	382	MES	O3S-S-O2S	-2.58	105.46	111.37
7	B	381	MES	O3S-S-O2S	-2.57	105.48	111.37
7	F	382	MES	O3S-S-O1S	-2.56	105.50	111.37
6	F	381	778	C16-N11-C17	-2.52	122.68	125.67
6	H	381	778	C16-N11-C17	-2.45	122.75	125.67
7	F	382	MES	O2S-S-O1S	-2.44	105.41	113.86
6	B	380	778	C16-N11-C17	-2.43	122.78	125.67
7	L	382	MES	O2S-S-O1S	-2.39	105.56	113.86
6	J	381	778	C16-N11-C17	-2.39	122.83	125.67
7	F	382	MES	O3S-S-O2S	-2.39	105.90	111.37
7	B	381	MES	O2S-S-O1S	-2.38	105.62	113.86
7	B	381	MES	O3S-S-O1S	-2.35	105.99	111.37
6	L	381	778	C16-N11-C17	-2.33	122.89	125.67
7	L	382	MES	O3S-S-O1S	-2.33	106.02	111.37
7	H	382	MES	O3S-S-O2S	-2.30	106.09	111.37
7	D	382	MES	O2S-S-O1S	-2.29	105.92	113.86
7	H	382	MES	O2S-S-O1S	-2.26	106.02	113.86
7	J	382	MES	O2S-S-O1S	-2.26	106.02	113.86
7	J	382	MES	O3S-S-O1S	-2.25	106.22	111.37
6	D	381	778	C16-N11-C17	-2.22	123.03	125.67
6	D	381	778	C7-C12-N18	-2.16	104.78	108.80
7	L	382	MES	O1-C2-C3	-2.16	106.99	111.83
7	H	382	MES	O3S-S-O1S	-2.15	106.44	111.37
6	F	381	778	C20-C14-N9	-2.14	117.30	119.93
7	J	382	MES	O1-C2-C3	-2.12	107.08	111.83
6	H	381	778	C7-C12-N18	-2.10	104.89	108.80
7	F	382	MES	O1-C2-C3	-2.10	107.14	111.83
6	F	381	778	C7-C12-N18	-2.08	104.93	108.80
7	D	382	MES	O1-C2-C3	-2.08	107.18	111.83
7	D	382	MES	O3S-S-O1S	-2.07	106.61	111.37
6	B	380	778	C7-C12-N18	-2.01	105.05	108.80
6	J	381	778	C7-C12-N18	-2.01	105.06	108.80
6	H	381	778	C21-C14-N9	2.34	123.72	120.17
6	D	381	778	C21-C14-N9	2.45	123.89	120.17
6	B	380	778	C21-C14-N9	2.45	123.89	120.17
6	J	381	778	C21-C14-N9	2.61	124.13	120.17
6	L	381	778	C21-C14-N9	2.61	124.13	120.17
6	F	381	778	C21-C14-N9	2.86	124.51	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	381	778	C4-N1-C2	3.44	114.31	110.01
6	D	381	778	C4-N1-C2	3.47	114.36	110.01
6	L	381	778	C4-N1-C2	3.60	114.51	110.01
6	B	380	778	C4-N1-C2	3.62	114.55	110.01
6	J	381	778	C4-N1-C2	3.65	114.57	110.01
6	H	381	778	C4-N1-C2	3.69	114.63	110.01
6	L	381	778	C14-N9-C8	4.07	125.90	119.97
6	D	381	778	C14-N9-C8	4.10	125.94	119.97
6	H	381	778	C14-N9-C8	4.13	125.98	119.97
6	B	380	778	C14-N9-C8	4.15	126.01	119.97
6	F	381	778	C14-N9-C8	4.19	126.07	119.97
6	D	381	778	C3-N1-C2	4.26	120.10	111.08
6	J	381	778	C3-N1-C2	4.29	120.15	111.08
6	H	381	778	C3-N1-C2	4.33	120.25	111.08
6	L	381	778	C3-N1-C2	4.34	120.27	111.08
6	J	381	778	C14-N9-C8	4.35	126.31	119.97
6	B	380	778	C3-N1-C2	4.40	120.40	111.08
6	F	381	778	C3-N1-C2	4.48	120.57	111.08
7	H	382	MES	O2S-S-C8	4.65	110.78	106.79
7	L	382	MES	O2S-S-C8	4.93	111.03	106.79
6	H	381	778	C2-C5-N9	5.03	119.73	110.69
6	B	380	778	C2-C5-N9	5.08	119.82	110.69
7	D	382	MES	O1S-S-C8	5.14	111.21	106.79
6	J	381	778	C2-C5-N9	5.16	119.96	110.69
6	D	381	778	C2-C5-N9	5.25	120.12	110.69
6	F	381	778	C2-C5-N9	5.26	120.14	110.69
7	B	381	MES	O2S-S-C8	5.49	111.51	106.79
6	L	381	778	C2-C5-N9	5.54	120.66	110.69
7	D	382	MES	O2S-S-C8	5.62	111.62	106.79
7	J	382	MES	O2S-S-C8	5.67	111.66	106.79
7	J	382	MES	O1S-S-C8	5.68	111.67	106.79
7	H	382	MES	O1S-S-C8	5.80	111.77	106.79
7	L	382	MES	O1S-S-C8	5.97	111.92	106.79
7	F	382	MES	O2S-S-C8	6.00	111.95	106.79
7	B	381	MES	O1S-S-C8	6.32	112.22	106.79
7	F	382	MES	O3S-S-C8	6.94	114.59	106.06
7	F	382	MES	O1S-S-C8	6.96	112.77	106.79
7	H	382	MES	O3S-S-C8	7.39	115.15	106.06
7	B	381	MES	O3S-S-C8	7.53	115.31	106.06
7	D	382	MES	O3S-S-C8	7.59	115.39	106.06
7	J	382	MES	O3S-S-C8	7.70	115.53	106.06
7	L	382	MES	O3S-S-C8	8.33	116.31	106.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	382	MES	2	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	314/377 (83%)	0.01	12 (3%) 41 44	41, 63, 97, 108	0
1	C	314/377 (83%)	-0.03	10 (3%) 48 52	41, 59, 87, 108	0
1	E	314/377 (83%)	0.02	10 (3%) 48 52	44, 63, 91, 106	0
1	G	314/377 (83%)	0.14	18 (5%) 24 26	41, 64, 94, 110	0
1	I	314/377 (83%)	-0.10	7 (2%) 62 65	34, 57, 87, 96	0
1	K	314/377 (83%)	-0.25	3 (0%) 82 84	31, 47, 72, 87	0
2	B	346/377 (91%)	0.09	12 (3%) 44 48	42, 57, 82, 102	0
2	D	346/377 (91%)	0.07	7 (2%) 65 68	35, 51, 77, 91	0
2	F	346/377 (91%)	0.02	10 (2%) 52 56	36, 51, 77, 101	0
2	H	346/377 (91%)	0.55	29 (8%) 12 12	40, 71, 97, 114	0
2	J	346/377 (91%)	0.15	17 (4%) 30 33	35, 55, 84, 104	0
2	L	346/377 (91%)	0.03	9 (2%) 56 60	29, 44, 71, 95	0
All	All	3960/4524 (87%)	0.06	144 (3%) 43 47	29, 57, 88, 114	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	304	ARG	6.3
1	C	306	HIS	5.9
1	G	306	HIS	5.9
2	H	305	LEU	5.9
1	G	55	PHE	5.5
1	C	55	PHE	5.1
2	H	108	SER	4.9
1	I	306	HIS	4.4
2	B	363	THR	4.4
2	H	361	TRP	4.3
1	C	305	SER	4.2

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Mol	Chain	Res	Type	RSRZ
2	H	363	THR	4.0
1	E	306	HIS	3.9
2	J	108	SER	3.9
2	H	112	GLY	3.8
1	A	333	ILE	3.8
2	L	363	THR	3.7
2	H	306	VAL	3.7
2	F	112	GLY	3.6
1	C	333	ILE	3.5
2	H	85	GLU	3.4
2	H	86	ASP	3.3
1	A	334	LEU	3.3
2	D	305	LEU	3.3
2	H	110	ASN	3.3
1	A	304	PRO	3.3
1	E	368	SER	3.2
1	G	329	ASN	3.2
2	B	362	LYS	3.2
1	G	305	SER	3.1
1	G	368	SER	3.1
2	F	363	THR	3.1
2	H	107	PRO	3.1
2	H	109	LYS	3.1
1	I	305	SER	3.0
2	H	307	GLY	2.9
2	B	86	ASP	2.9
1	A	338	LEU	2.9
2	L	49	THR	2.9
1	G	75	ILE	2.9
2	B	112	GLY	2.9
2	J	112	GLY	2.9
2	J	363	THR	2.8
2	D	363	THR	2.8
1	E	331	GLU	2.8
2	J	90	LEU	2.8
2	J	86	ASP	2.8
1	G	333	ILE	2.7
2	H	123	ALA	2.7
1	C	330	LYS	2.7
1	K	306	HIS	2.7
1	C	304	PRO	2.7
2	H	84	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	88	SER	2.7
1	A	306	HIS	2.7
2	J	111	PRO	2.7
2	B	304	ARG	2.6
2	L	84	THR	2.6
2	F	88	SER	2.6
1	C	329	ASN	2.6
2	F	305	LEU	2.6
1	C	332	ASP	2.6
1	E	330	LYS	2.6
1	A	335	ASN	2.6
2	J	84	THR	2.6
1	A	367	HIS	2.6
2	B	316	HIS	2.6
2	H	316	HIS	2.6
2	J	360	SER	2.5
1	C	336	LYS	2.5
1	A	368	SER	2.5
2	H	114	ALA	2.5
2	H	362	LYS	2.5
2	H	111	PRO	2.5
2	J	85	GLU	2.5
2	B	65	ASP	2.5
1	E	334	LEU	2.5
1	I	368	SER	2.5
2	J	46	SER	2.4
1	G	56	LEU	2.4
2	D	110	ASN	2.4
2	B	111	PRO	2.4
2	H	45	THR	2.3
1	C	331	GLU	2.3
2	L	85	GLU	2.3
2	D	304	ARG	2.3
2	J	49	THR	2.3
1	G	367	HIS	2.3
2	D	316	HIS	2.3
1	G	304	PRO	2.3
2	J	87	ARG	2.3
2	J	114	ALA	2.3
2	L	110	ASN	2.3
2	H	19	ASP	2.3
2	L	50	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	18	LEU	2.3
1	E	328	ASP	2.2
2	H	314	ASP	2.2
1	G	365	SER	2.2
2	J	314	ASP	2.2
1	I	327	CYS	2.2
1	I	329	ASN	2.2
2	H	65	ASP	2.2
2	L	86	ASP	2.2
1	I	55	PHE	2.2
2	F	113	THR	2.2
1	E	304	PRO	2.2
2	B	305	LEU	2.2
1	G	330	LYS	2.2
2	L	113	THR	2.2
1	A	329	ASN	2.2
1	A	337	ALA	2.2
2	J	123	ALA	2.2
2	H	30	GLN	2.1
2	D	114	ALA	2.1
1	K	305	SER	2.1
2	F	65	ASP	2.1
1	A	330	LYS	2.1
2	F	123	ALA	2.1
2	B	127	THR	2.1
2	J	113	THR	2.1
1	G	195	GLN	2.1
1	G	326	GLN	2.1
1	G	85	SER	2.1
1	G	78	VAL	2.1
1	I	84	PRO	2.1
2	H	225	CYS	2.1
1	G	327	CYS	2.1
2	D	90	LEU	2.1
1	E	329	ASN	2.1
1	G	303	GLN	2.1
1	K	326	GLN	2.1
2	B	306	VAL	2.1
2	F	316	HIS	2.1
2	B	90	LEU	2.1
2	F	18	LEU	2.1
1	E	325	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	326	GLN	2.1
2	F	86	ASP	2.0
2	H	35	VAL	2.0
2	H	113	THR	2.0
2	J	124	MET	2.0
1	A	305	SER	2.0
2	H	308	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
7	MES	F	382	12/12	0.95	0.31	5.66	72,73,85,86	0
7	MES	J	382	12/12	0.94	0.38	5.54	70,72,81,81	0
4	CL	C	378	1/1	0.98	0.21	3.86	61,61,61,61	0
7	MES	L	382	12/12	0.94	0.36	3.19	69,71,76,77	0
7	MES	B	381	12/12	0.94	0.30	2.92	69,71,81,83	0
7	MES	D	382	12/12	0.95	0.28	2.76	71,72,78,78	0
6	778	L	381	29/29	0.91	0.26	2.03	27,33,36,39	0
6	778	B	380	29/29	0.91	0.25	2.00	39,46,53,56	0
4	CL	K	378	1/1	0.98	0.14	1.82	67,67,67,67	0
6	778	J	381	29/29	0.89	0.25	1.72	29,39,42,42	0
6	778	F	381	29/29	0.91	0.24	1.65	36,45,52,52	0
4	CL	G	378	1/1	0.96	0.16	1.49	61,61,61,61	0
7	MES	H	382	12/12	0.93	0.26	1.43	74,75,84,84	0
6	778	D	381	29/29	0.92	0.24	1.38	35,45,47,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CL	F	379	1/1	0.99	0.17	1.36	53,53,53,53	0
5	SO4	L	380	5/5	0.99	0.19	1.35	41,44,45,47	0
4	CL	I	378	1/1	0.96	0.19	1.08	75,75,75,75	0
5	SO4	F	380	5/5	0.99	0.19	0.99	53,54,58,58	0
5	SO4	B	379	5/5	0.99	0.18	0.79	56,56,58,59	0
6	778	H	381	29/29	0.92	0.24	0.75	42,48,51,54	0
5	SO4	J	380	5/5	0.99	0.16	0.38	45,45,47,48	0
5	SO4	D	380	5/5	0.99	0.16	0.33	51,52,54,55	0
3	ZN	D	378	1/1	1.00	0.15	0.30	43,43,43,43	0
4	CL	D	379	1/1	0.98	0.15	0.12	52,52,52,52	0
3	ZN	L	378	1/1	1.00	0.16	-0.44	35,35,35,35	0
5	SO4	H	380	5/5	0.99	0.14	-0.47	60,61,62,62	0
3	ZN	J	378	1/1	1.00	0.15	-0.70	39,39,39,39	0
3	ZN	B	378	1/1	1.00	0.14	-0.90	45,45,45,45	0
3	ZN	F	378	1/1	1.00	0.14	-0.96	45,45,45,45	0
4	CL	L	379	1/1	0.99	0.12	-1.26	53,53,53,53	0
3	ZN	H	378	1/1	0.99	0.11	-1.81	55,55,55,55	0
4	CL	J	379	1/1	0.98	0.11	-2.00	63,63,63,63	0
4	CL	H	379	1/1	0.96	0.10	-2.47	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.