



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:39 PM UTC

PDB ID : 4Z90 / pdb_00004z90
Title : ELIC bound with the anesthetic isoflurane in the resting state
Authors : Chen, Q.; Kinde, M.; Arjunan, P.; Cohen, A.; Xu, Y.; Tang, P.
Deposited on : 2015-04-09
Resolution : 3.00 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

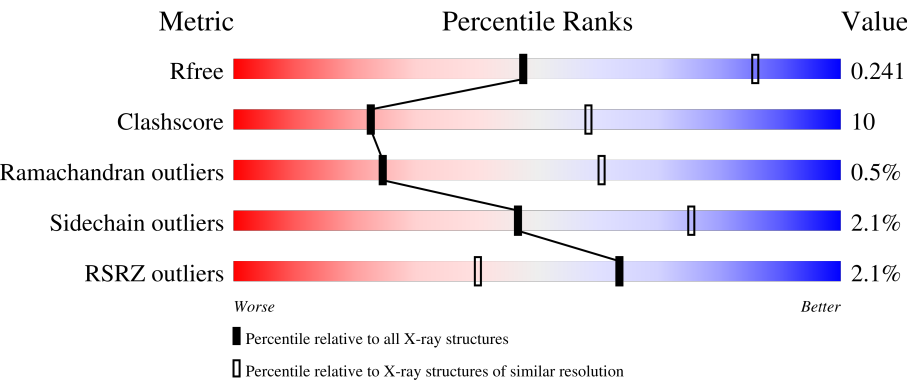
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	322	
1	B	322	
1	C	322	
1	D	322	
1	E	322	

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Mol	Chain	Length	Quality of chain
1	F	322	% 71% 24%
1	G	322	3% 76% 20%
1	H	322	2% 68% 26%
1	I	322	% 71% 24%
1	J	322	3% 67% 28%

2 Entry composition

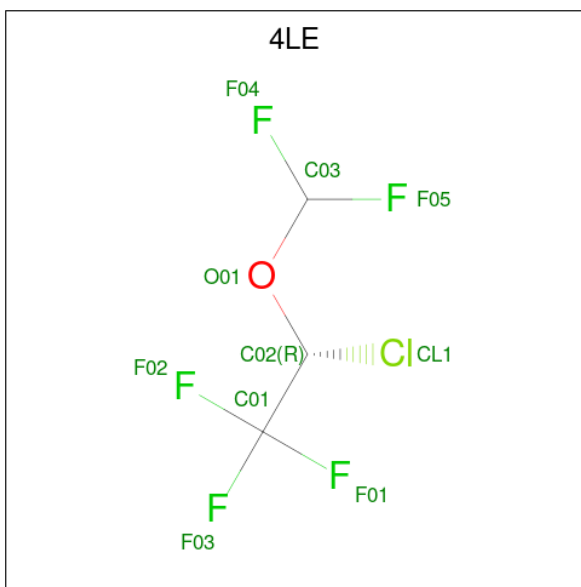
There are 4 unique types of molecules in this entry. The entry contains 25850 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Gamma-aminobutyric-acid receptor subunit beta-1.

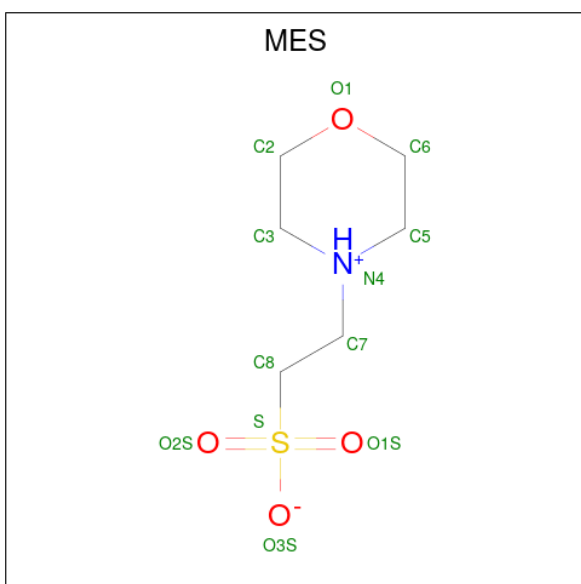
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	B	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	C	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	D	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	E	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	F	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	G	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	H	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	I	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	J	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			

- Molecule 2 is (2R)-2-chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane (CCD ID: 4LE) (formula: C₃H₂ClF₅O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	O	0	0
			10	3	1	5	1		
2	E	1	Total	C	Cl	F	O	0	0
			10	3	1	5	1		
2	F	1	Total	C	Cl	F	O	0	0
			10	3	1	5	1		
2	F	1	Total	C	Cl	F	O	0	0
			10	3	1	5	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	J	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

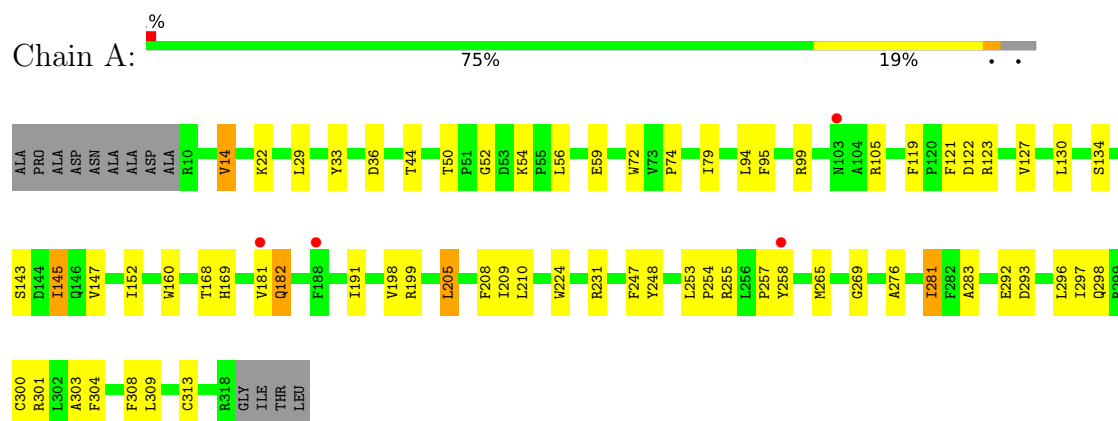
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	B	45	Total	O	0	0
			45	45		
4	C	58	Total	O	0	0
			58	58		
4	D	30	Total	O	0	0
			30	30		
4	E	48	Total	O	0	0
			48	48		
4	F	33	Total	O	0	0
			33	33		
4	G	55	Total	O	0	0
			55	55		
4	H	42	Total	O	0	0
			42	42		
4	I	43	Total	O	0	0
			43	43		
4	J	33	Total	O	0	0
			33	33		

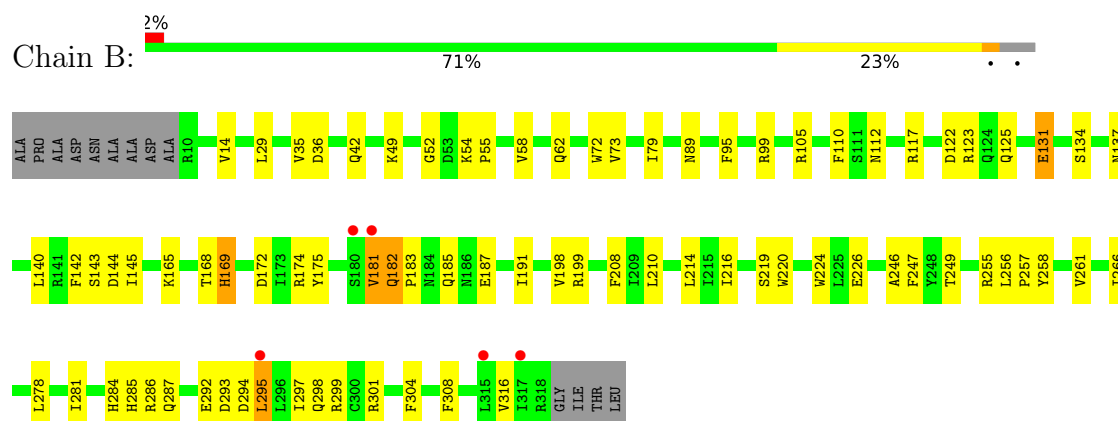
3 Residue-property plots

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.

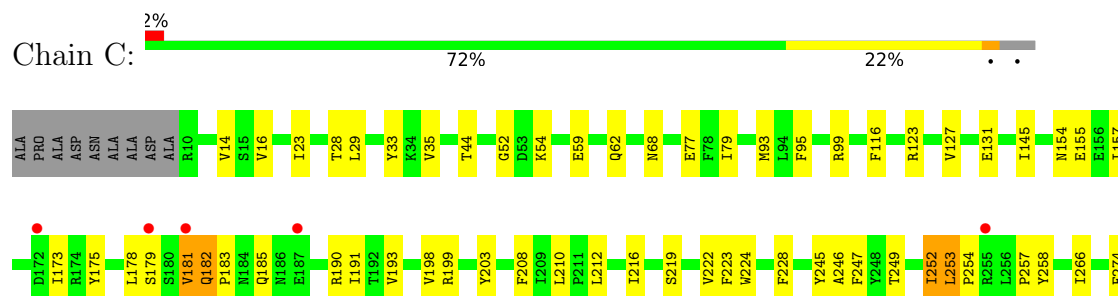
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



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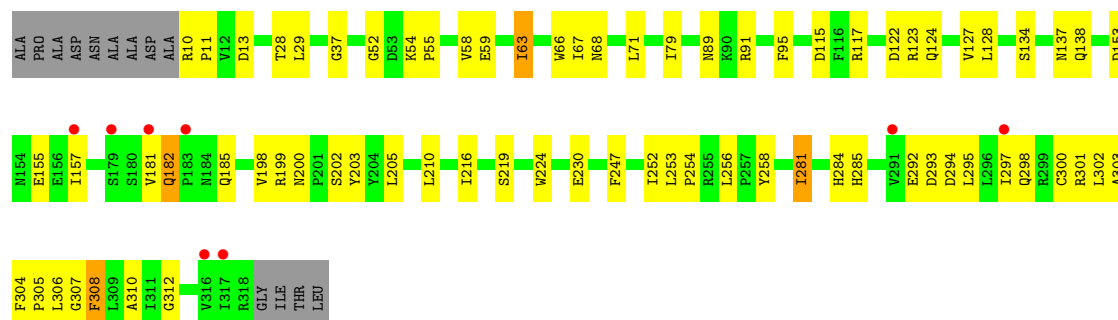
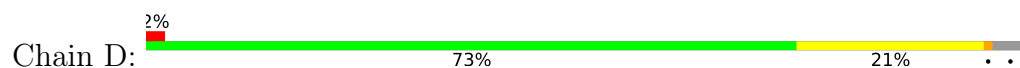


- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

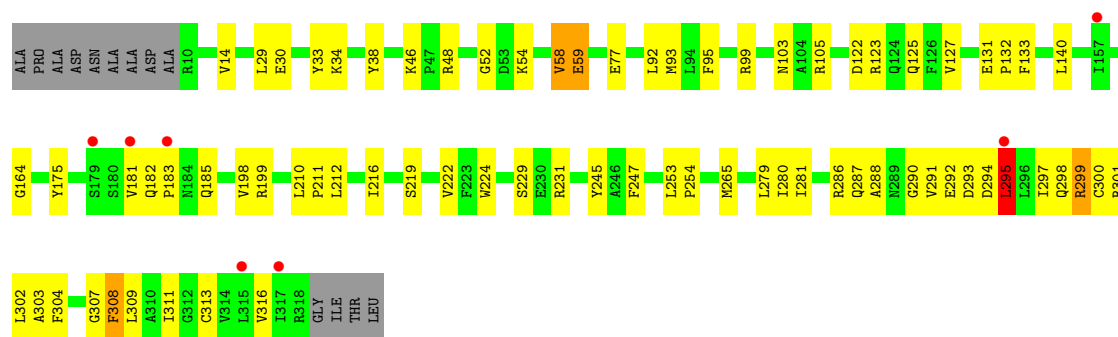
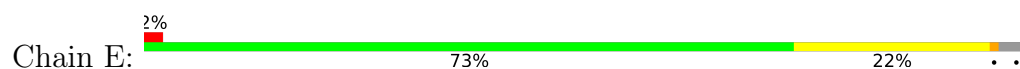




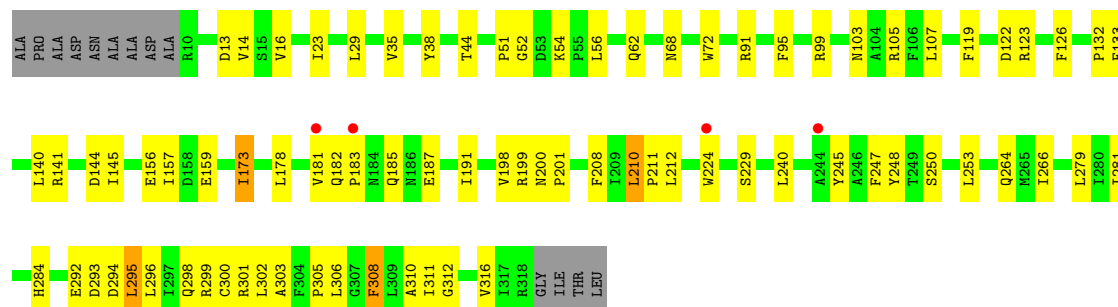
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



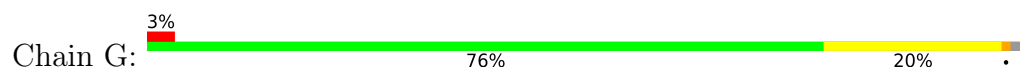
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

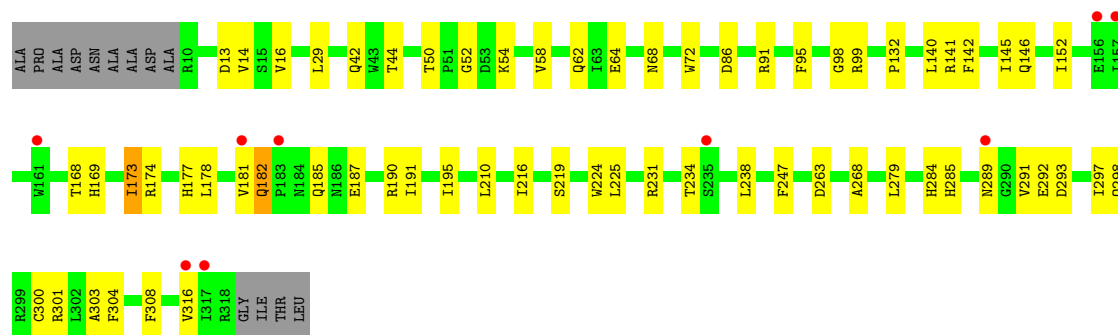


- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

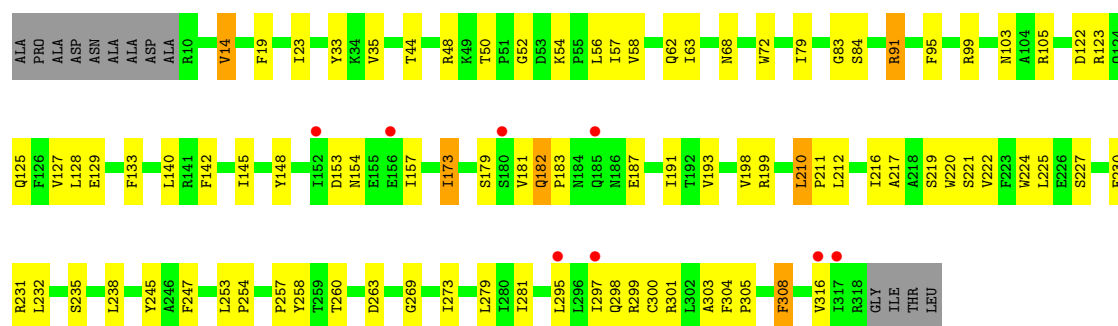


- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

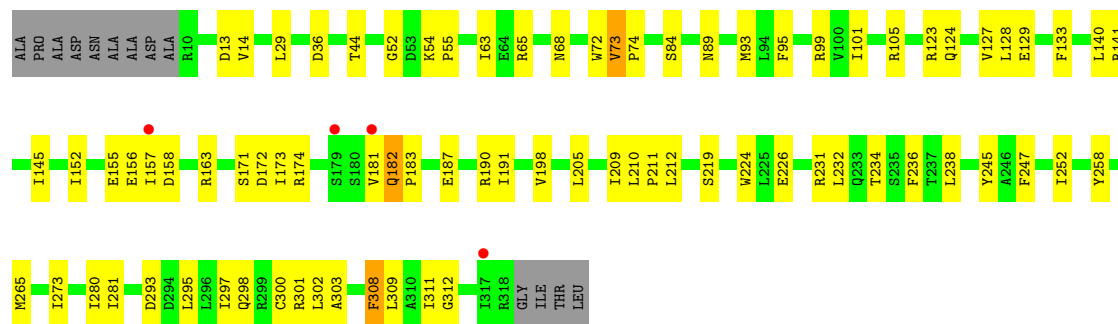




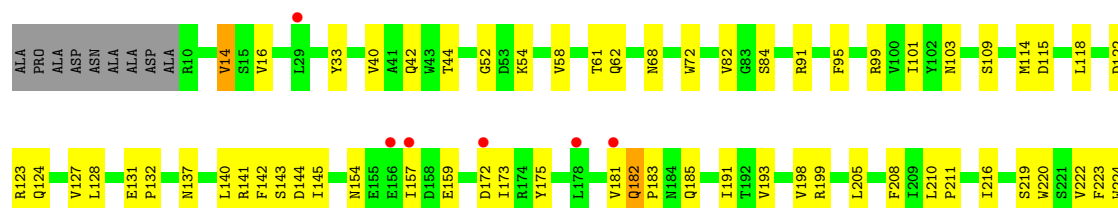
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

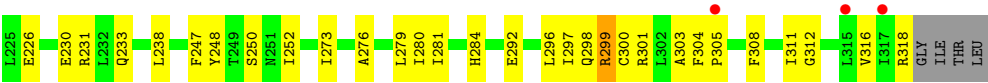


• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.85Å 267.08Å 111.13Å 90.00° 106.94° 90.00°	Depositor
Resolution (Å)	36.97 – 3.00 36.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.97-3.00) 99.8 (36.97-3.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.209 , 0.243 0.213 , 0.241	Depositor DCC
R_{free} test set	5887 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	92.7	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25850	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: MES, 4LE

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	0.79	0/2595	0.90	2/3536 (0.1%)
1	B	0.92	1/2595 (0.0%)	0.97	5/3536 (0.1%)
1	C	0.88	0/2595	0.93	4/3536 (0.1%)
1	D	1.01	0/2595	0.98	4/3536 (0.1%)
1	E	0.84	0/2595	0.91	6/3536 (0.2%)
1	F	0.74	0/2595	0.90	5/3536 (0.1%)
1	G	0.94	0/2595	0.95	4/3536 (0.1%)
1	H	0.81	0/2595	0.92	3/3536 (0.1%)
1	I	0.88	0/2595	0.96	5/3536 (0.1%)
1	J	0.72	0/2595	0.91	4/3536 (0.1%)
All	All	0.86	1/25950 (0.0%)	0.93	42/35360 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	GLU	C-O	-5.09	1.18	1.24

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	73	VAL	CA-C-N	8.60	128.36	119.76
1	I	73	VAL	C-N-CA	8.60	128.36	119.76
1	A	210	LEU	CA-C-N	-7.83	111.57	119.56
1	A	210	LEU	C-N-CA	-7.83	111.57	119.56
1	J	84	SER	CA-C-N	7.19	127.14	120.03
1	J	84	SER	C-N-CA	7.19	127.14	120.03
1	C	210	LEU	CA-C-N	-6.77	111.83	119.28
1	C	210	LEU	C-N-CA	-6.77	111.83	119.28
1	B	210	LEU	CA-C-N	-6.71	112.08	119.19
1	B	210	LEU	C-N-CA	-6.71	112.08	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	46	LYS	CA-C-N	6.50	127.97	119.84
1	E	46	LYS	C-N-CA	6.50	127.97	119.84
1	G	210	LEU	CA-C-N	-6.38	112.26	119.28
1	G	210	LEU	C-N-CA	-6.38	112.26	119.28
1	H	83	GLY	N-CA-C	-6.26	104.91	112.48
1	I	157	ILE	N-CA-C	-6.22	106.44	112.29
1	F	173	ILE	N-CA-C	6.22	116.82	108.11
1	G	190	ARG	N-CA-C	6.11	118.36	108.34
1	J	173	ILE	N-CA-C	6.02	116.79	108.12
1	D	210	LEU	CA-C-N	-5.95	113.49	119.56
1	D	210	LEU	C-N-CA	-5.95	113.49	119.56
1	H	210	LEU	CA-C-N	-5.87	113.57	119.56
1	H	210	LEU	C-N-CA	-5.87	113.57	119.56
1	J	299	ARG	N-CA-C	-5.84	105.05	111.82
1	C	228	PHE	N-CA-C	-5.76	104.60	111.69
1	D	157	ILE	N-CA-C	-5.72	106.74	112.17
1	E	299	ARG	N-CA-C	-5.64	105.28	111.82
1	E	295	LEU	N-CA-C	-5.59	105.26	111.36
1	F	299	ARG	N-CA-C	-5.47	105.47	111.82
1	B	73	VAL	CA-C-N	5.42	125.18	119.76
1	B	73	VAL	C-N-CA	5.42	125.18	119.76
1	F	210	LEU	CA-C-N	-5.38	114.13	119.56
1	F	210	LEU	C-N-CA	-5.38	114.13	119.56
1	B	169	HIS	CB-CA-C	-5.34	104.81	111.43
1	D	37	GLY	N-CA-C	5.28	118.25	110.80
1	G	98	GLY	N-CA-C	5.27	121.09	114.25
1	C	16	VAL	N-CA-C	5.17	116.02	108.53
1	I	84	SER	CA-C-N	5.12	125.02	119.85
1	I	84	SER	C-N-CA	5.12	125.02	119.85
1	E	164	GLY	N-CA-C	-5.10	107.10	111.95
1	F	16	VAL	N-CA-C	5.09	115.92	108.53
1	E	59	GLU	N-CA-C	5.05	117.72	109.59

There are no chirality outliers.

There are no planarity outliers.

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	2527	0	2503	45	0
1	B	2527	0	2503	63	0
1	C	2527	0	2503	58	0
1	D	2527	0	2503	58	1
1	E	2527	0	2503	51	0
1	F	2527	0	2503	55	0
1	G	2527	0	2503	49	1
1	H	2527	0	2503	68	0
1	I	2527	0	2503	64	0
1	J	2527	0	2503	70	0
2	A	10	0	1	0	0
2	E	10	0	1	0	0
2	F	20	0	2	2	0
3	A	24	0	24	0	0
3	B	12	0	12	0	0
3	C	12	0	12	1	0
3	D	12	0	12	0	0
3	F	12	0	12	0	0
3	G	12	0	12	1	0
3	H	12	0	12	1	0
3	I	12	0	12	0	0
3	J	12	0	12	1	0
4	A	33	0	0	8	0
4	B	45	0	0	8	0
4	C	58	0	0	11	0
4	D	30	0	0	8	0
4	E	48	0	0	11	0
4	F	33	0	0	5	0
4	G	55	0	0	12	0
4	H	42	0	0	5	0
4	I	43	0	0	8	0
4	J	33	0	0	5	0
All	All	25850	0	25154	530	1

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 10.

All (530) 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:123:ARG:CG	1:D:198:VAL:HG12	1.79	1.11
1:B:79:ILE:HD11	1:B:131:GLU:HB3	1.24	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ARG:HG2	1:D:198:VAL:CG1	1.82	1.07
1:I:123:ARG:CG	1:I:198:VAL:HG12	1.83	1.07
1:A:123:ARG:HG2	1:A:198:VAL:CG1	1.85	1.06
1:I:123:ARG:HG2	1:I:198:VAL:CG1	1.87	1.03
1:I:123:ARG:HG2	1:I:198:VAL:HG12	1.05	1.02
1:C:123:ARG:HG2	1:C:198:VAL:HG22	1.44	0.99
1:A:123:ARG:CG	1:A:198:VAL:HG12	1.93	0.98
1:H:123:ARG:HG2	1:H:198:VAL:HG22	1.46	0.97
1:D:123:ARG:HG2	1:D:198:VAL:HG12	0.98	0.95
1:B:79:ILE:HD11	1:B:131:GLU:CB	1.98	0.93
1:A:123:ARG:HG2	1:A:198:VAL:HG12	0.97	0.90
2:F:401:4LE:F05	2:F:401:4LE:CL1	2.17	0.87
1:H:257:PRO:O	4:H:501:HOH:O	1.92	0.87
1:E:30:GLU:OE1	4:E:501:HOH:O	1.95	0.85
1:B:79:ILE:CD1	1:B:131:GLU:HB3	2.06	0.84
1:C:62:GLN:NE2	1:D:68:ASN:OD1	2.12	0.83
1:G:91:ARG:NH1	4:G:503:HOH:O	2.12	0.82
1:E:123:ARG:HG2	1:E:198:VAL:HG12	1.60	0.82
1:J:16:VAL:HG11	1:J:191:ILE:CD1	2.10	0.81
1:B:187:GLU:OE2	1:I:141:ARG:NH1	2.13	0.79
1:C:190:ARG:NH2	4:C:501:HOH:O	2.14	0.79
1:H:316:VAL:HG12	1:H:316:VAL:O	1.83	0.79
1:E:293:ASP:O	4:E:502:HOH:O	2.00	0.79
1:I:232:LEU:HD22	1:I:281:ILE:HD11	1.64	0.79
1:J:118:LEU:HD21	1:J:318:ARG:HA	1.66	0.77
1:I:158:ASP:O	4:I:501:HOH:O	2.04	0.76
1:J:220:TRP:HZ2	1:J:308:PHE:HD2	1.33	0.76
1:G:132:PRO:O	4:G:501:HOH:O	2.03	0.76
1:C:131:GLU:OE1	4:C:501:HOH:O	2.05	0.74
1:H:129:GLU:OE2	4:H:502:HOH:O	2.05	0.74
1:G:231:ARG:NH2	1:G:292:GLU:OE2	2.21	0.73
1:C:79:ILE:O	4:C:502:HOH:O	2.06	0.73
1:J:44:THR:HA	1:J:99:ARG:HA	1.70	0.73
1:B:117:ARG:O	4:B:501:HOH:O	2.08	0.72
1:B:79:ILE:CD1	1:B:131:GLU:CB	2.67	0.72
1:C:284:HIS:HD2	1:C:292:GLU:HG2	1.55	0.72
1:E:48:ARG:NH1	4:E:505:HOH:O	2.23	0.72
1:A:59:GLU:OE2	4:A:501:HOH:O	2.08	0.71
1:D:284:HIS:ND1	1:D:292:GLU:OE1	2.24	0.71
1:I:155:GLU:OE1	4:I:502:HOH:O	2.07	0.71
1:E:125:GLN:OE1	4:E:503:HOH:O	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:ARG:HG2	1:F:198:VAL:HG12	1.71	0.71
1:G:42:GLN:OE1	1:H:179:SER:OG	2.07	0.71
1:G:263:ASP:OD2	4:G:502:HOH:O	2.08	0.71
1:J:284:HIS:ND1	1:J:292:GLU:OE1	2.19	0.71
1:B:168:THR:O	1:B:169:HIS:ND1	2.25	0.70
1:F:132:PRO:O	4:F:501:HOH:O	2.09	0.70
1:A:143:SER:N	4:A:503:HOH:O	2.24	0.70
1:I:226:GLU:OE2	1:J:284:HIS:NE2	2.25	0.70
1:D:13:ASP:O	4:D:501:HOH:O	2.10	0.69
1:D:181:VAL:HG22	1:D:182:GLN:H	1.57	0.69
1:A:14:VAL:N	4:A:503:HOH:O	2.25	0.68
1:H:181:VAL:HG22	1:H:182:GLN:H	1.58	0.68
1:J:123:ARG:HG2	1:J:198:VAL:HG22	1.75	0.68
1:H:216:ILE:O	1:H:219:SER:OG	2.10	0.68
1:C:127:VAL:HG23	1:C:193:VAL:O	1.93	0.68
1:D:59:GLU:OE2	4:D:503:HOH:O	2.12	0.68
1:H:99:ARG:O	4:H:503:HOH:O	2.10	0.68
1:G:177:HIS:ND1	4:G:509:HOH:O	2.27	0.67
1:E:287:GLN:NE2	1:E:293:ASP:OD1	2.27	0.67
1:D:137:ASN:OD1	4:D:502:HOH:O	2.11	0.67
1:C:203:TYR:N	4:C:507:HOH:O	2.27	0.66
1:G:181:VAL:HG22	1:G:182:GLN:H	1.60	0.66
1:H:224:TRP:CD2	1:H:301:ARG:HD2	2.30	0.66
1:J:61:THR:OG1	4:J:501:HOH:O	2.12	0.66
1:G:152:ILE:O	4:G:505:HOH:O	2.14	0.66
1:C:93:MET:SD	4:C:535:HOH:O	2.53	0.66
1:A:231:ARG:NH2	1:A:292:GLU:OE2	2.26	0.66
1:D:185:GLN:N	4:D:505:HOH:O	2.28	0.66
1:C:54:LYS:O	4:C:504:HOH:O	2.15	0.66
1:J:181:VAL:HG22	1:J:182:GLN:H	1.61	0.65
1:G:64:GLU:OE1	4:G:504:HOH:O	2.13	0.65
1:J:216:ILE:O	1:J:219:SER:OG	2.11	0.65
1:A:205:LEU:HD12	1:A:209:ILE:HG13	1.78	0.65
1:C:155:GLU:OE1	4:C:503:HOH:O	2.14	0.65
1:I:252:ILE:HD11	1:J:250:SER:HB2	1.79	0.65
1:F:145:ILE:HD13	1:F:191:ILE:HD13	1.78	0.65
1:I:224:TRP:CE2	1:I:301:ARG:HD3	2.32	0.65
1:B:226:GLU:OE2	4:B:503:HOH:O	2.14	0.64
1:G:289:ASN:HB2	1:G:291:VAL:HG12	1.79	0.64
1:C:224:TRP:CD2	1:C:301:ARG:HD2	2.33	0.64
1:E:132:PRO:HG3	1:E:140:LEU:HD22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:16:VAL:CG1	1:J:191:ILE:CD1	2.75	0.64
1:A:122:ASP:OD1	1:A:199:ARG:NH1	2.31	0.64
1:H:62:GLN:NE2	1:I:68:ASN:OD1	2.29	0.64
1:I:209:ILE:HG23	1:I:265:MET:HE1	1.79	0.64
1:J:141:ARG:NH2	4:J:506:HOH:O	2.31	0.64
1:F:44:THR:HA	1:F:99:ARG:HA	1.81	0.63
1:D:115:ASP:O	1:D:124:GLN:NE2	2.32	0.62
1:B:29:LEU:HD13	4:B:523:HOH:O	1.98	0.62
1:E:286:ARG:NH1	4:E:506:HOH:O	2.23	0.62
1:I:309:LEU:N	4:I:507:HOH:O	2.33	0.62
1:D:115:ASP:OD2	1:D:117:ARG:NH2	2.28	0.62
1:A:297:ILE:O	1:A:298:GLN:HB3	1.99	0.62
1:D:10:ARG:NH1	4:D:507:HOH:O	2.33	0.62
1:B:122:ASP:OD1	1:B:199:ARG:NH1	2.33	0.61
1:D:216:ILE:O	1:D:219:SER:HB3	2.00	0.61
1:I:308:PHE:HA	1:I:311:ILE:HG12	1.82	0.61
1:A:33:TYR:OH	1:A:127:VAL:N	2.29	0.61
1:B:168:THR:C	1:B:169:HIS:ND1	2.59	0.61
1:E:212:LEU:HD12	1:E:265:MET:HE2	1.83	0.61
1:C:59:GLU:OE2	1:D:134:SER:OG	2.13	0.61
1:C:145:ILE:HD13	1:C:191:ILE:HD13	1.81	0.61
1:G:62:GLN:NE2	1:H:68:ASN:OD1	2.29	0.61
1:H:182:GLN:HB2	1:H:183:PRO:HD3	1.82	0.60
1:F:298:GLN:HA	1:F:301:ARG:HG3	1.81	0.60
1:F:122:ASP:OD1	1:F:199:ARG:NH1	2.34	0.60
1:F:247:PHE:CD2	1:G:247:PHE:HE2	2.20	0.60
1:C:44:THR:HA	1:C:99:ARG:HA	1.83	0.59
1:J:131:GLU:OE2	1:J:175:TYR:OH	2.14	0.59
1:I:247:PHE:CD2	1:J:247:PHE:HE2	2.21	0.59
1:B:285:HIS:NE2	4:B:502:HOH:O	2.10	0.59
1:C:33:TYR:OH	1:C:127:VAL:O	2.20	0.59
1:A:44:THR:HA	1:A:99:ARG:HA	1.85	0.58
1:J:16:VAL:CG1	1:J:191:ILE:HD11	2.33	0.58
1:C:181:VAL:HG12	1:C:182:GLN:H	1.67	0.58
1:C:284:HIS:CD2	1:C:292:GLU:HG2	2.38	0.58
1:A:160:TRP:O	4:A:502:HOH:O	2.17	0.58
1:I:174:ARG:NH1	4:I:509:HOH:O	2.35	0.58
1:H:142:PHE:CD2	1:H:191:ILE:HG13	2.39	0.58
1:A:283:ALA:HB2	1:A:296:LEU:HD23	1.85	0.58
1:A:224:TRP:CE2	1:A:301:ARG:HD3	2.39	0.57
1:D:306:LEU:O	1:D:310:ALA:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:PHE:CD2	1:E:247:PHE:HE2	2.21	0.57
1:I:231:ARG:HB3	1:I:280:ILE:HD13	1.86	0.57
1:J:300:CYS:HA	1:J:303:ALA:HB3	1.85	0.57
1:C:99:ARG:O	4:C:505:HOH:O	2.16	0.57
1:F:306:LEU:O	1:F:310:ALA:N	2.37	0.57
1:H:19:PHE:CE2	1:H:148:TYR:HD2	2.22	0.57
1:C:33:TYR:OH	1:C:127:VAL:N	2.37	0.57
1:J:137:ASN:ND2	1:J:172:ASP:OD2	2.36	0.57
4:G:503:HOH:O	1:H:133:PHE:O	2.18	0.57
1:B:131:GLU:OE2	1:B:175:TYR:OH	2.14	0.57
1:I:124:GLN:OE1	4:I:504:HOH:O	2.17	0.57
1:J:16:VAL:HG11	1:J:191:ILE:HD11	1.87	0.57
1:J:279:LEU:HD23	1:J:300:CYS:SG	2.44	0.57
1:B:42:GLN:OE1	1:C:179:SER:OG	2.14	0.57
1:B:208:PHE:HE1	1:B:249:THR:HA	1.69	0.56
1:B:62:GLN:NE2	1:C:68:ASN:OD1	2.31	0.56
1:H:316:VAL:O	1:H:316:VAL:CG1	2.53	0.56
1:I:182:GLN:HB2	1:I:183:PRO:HD3	1.87	0.56
1:G:225:LEU:HB2	1:G:231:ARG:HG2	1.87	0.56
1:H:44:THR:HA	1:H:99:ARG:HA	1.87	0.56
1:I:89:ASN:ND2	4:I:503:HOH:O	2.09	0.56
1:J:16:VAL:HG23	1:J:40:VAL:O	2.06	0.56
1:B:137:ASN:ND2	1:B:172:ASP:OD2	2.38	0.56
1:A:181:VAL:HG12	1:A:182:GLN:H	1.71	0.56
1:B:123:ARG:HG2	1:B:198:VAL:HG23	1.88	0.56
1:H:33:TYR:OH	1:H:127:VAL:N	2.36	0.56
1:E:77:GLU:OE2	4:E:504:HOH:O	2.18	0.56
1:H:154:ASN:O	1:H:157:ILE:HG12	2.07	0.55
1:G:13:ASP:OD1	1:G:141:ARG:NH1	2.40	0.55
1:B:143:SER:OG	1:B:144:ASP:OD2	2.24	0.55
1:C:252:ILE:HG12	4:C:534:HOH:O	2.07	0.55
1:F:212:LEU:HD12	1:F:245:TYR:CE2	2.41	0.55
1:G:72:TRP:HH2	1:G:140:LEU:HD12	1.70	0.55
1:B:208:PHE:CD1	1:B:249:THR:HG22	2.42	0.55
1:E:183:PRO:O	1:E:185:GLN:HG2	2.07	0.55
1:H:52:GLY:C	1:H:54:LYS:H	2.15	0.55
1:D:300:CYS:HA	1:D:303:ALA:HB3	1.89	0.55
1:B:224:TRP:CE2	1:B:301:ARG:HD3	2.42	0.54
1:B:247:PHE:CD1	1:C:247:PHE:HE2	2.25	0.54
1:E:122:ASP:OD2	1:E:199:ARG:NH1	2.40	0.54
1:J:238:LEU:HB3	1:J:273:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:293:ASP:OD1	1:F:296:LEU:N	2.36	0.54
1:B:284:HIS:ND1	1:B:292:GLU:HG2	2.23	0.54
1:B:72:TRP:CH2	1:B:140:LEU:HD12	2.42	0.54
1:A:121:PHE:HZ	1:A:205:LEU:HD11	1.72	0.54
1:I:55:PRO:HB3	1:I:95:PHE:CD2	2.43	0.54
1:B:181:VAL:HG12	1:B:182:GLN:H	1.72	0.54
1:D:122:ASP:OD1	1:D:199:ARG:NH1	2.40	0.54
1:I:300:CYS:HA	1:I:303:ALA:HB3	1.90	0.54
1:E:95:PHE:HB2	1:E:99:ARG:HG3	1.90	0.53
1:H:128:LEU:HB2	1:H:193:VAL:HG22	1.90	0.53
1:A:300:CYS:HA	1:A:303:ALA:HB3	1.91	0.53
1:I:219:SER:HA	1:I:238:LEU:HD13	1.90	0.53
1:B:216:ILE:O	1:B:219:SER:OG	2.22	0.53
1:J:95:PHE:HB2	1:J:99:ARG:HG3	1.90	0.53
1:B:95:PHE:HB2	1:B:99:ARG:HG3	1.89	0.53
1:D:202:SER:OG	1:D:203:TYR:N	2.41	0.53
1:E:309:LEU:O	1:E:313:CYS:HB2	2.09	0.53
1:I:210:LEU:HB3	1:I:211:PRO:HD3	1.90	0.53
1:J:297:ILE:O	1:J:298:GLN:HB3	2.09	0.53
1:A:247:PHE:HE2	1:E:247:PHE:CD2	2.26	0.53
1:F:95:PHE:HB2	1:F:99:ARG:HG3	1.90	0.53
1:G:44:THR:HA	1:G:99:ARG:HA	1.90	0.53
1:G:279:LEU:HD23	1:G:300:CYS:SG	2.48	0.53
1:I:205:LEU:HD23	1:I:209:ILE:HG13	1.89	0.53
1:G:297:ILE:O	1:G:298:GLN:HB3	2.09	0.52
1:C:253:LEU:HB3	1:C:254:PRO:HD2	1.90	0.52
1:E:131:GLU:OE2	1:E:175:TYR:OH	2.14	0.52
1:E:297:ILE:O	1:E:298:GLN:HB3	2.08	0.52
1:E:103:ASN:ND2	4:E:515:HOH:O	2.42	0.52
1:E:216:ILE:O	1:E:219:SER:HB3	2.09	0.52
1:D:224:TRP:CE2	1:D:301:ARG:HD3	2.44	0.52
1:B:298:GLN:HA	1:B:301:ARG:HG3	1.91	0.52
1:J:115:ASP:O	1:J:124:GLN:NE2	2.41	0.52
1:H:33:TYR:OH	1:H:127:VAL:O	2.25	0.52
1:H:95:PHE:HB2	1:H:99:ARG:HG3	1.91	0.52
1:F:133:PHE:HE2	1:J:91:ARG:HB2	1.74	0.52
1:E:224:TRP:CE2	1:E:301:ARG:HD3	2.45	0.51
1:E:299:ARG:NH1	4:E:506:HOH:O	2.42	0.51
1:E:231:ARG:HB3	1:E:280:ILE:HD13	1.93	0.51
3:G:401:MES:O2S	4:G:506:HOH:O	2.18	0.51
1:G:146:GLN:N	4:G:512:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:125:GLN:N	4:H:507:HOH:O	2.28	0.51
1:H:308:PHE:C	1:H:308:PHE:CD2	2.88	0.51
1:F:308:PHE:HA	1:F:311:ILE:HG13	1.91	0.51
1:H:238:LEU:HB3	1:H:273:ILE:HD12	1.93	0.51
1:E:308:PHE:C	1:E:308:PHE:CD2	2.89	0.51
1:E:288:ALA:O	1:E:291:VAL:HG12	2.10	0.51
1:J:154:ASN:O	1:J:157:ILE:HG12	2.11	0.51
1:E:33:TYR:OH	1:E:127:VAL:N	2.38	0.51
1:A:22:LYS:NZ	4:A:510:HOH:O	2.43	0.51
1:C:298:GLN:HG3	1:C:301:ARG:NH2	2.26	0.51
1:I:152:ILE:O	4:I:505:HOH:O	2.20	0.50
1:F:91:ARG:NH1	1:F:103:ASN:HD22	2.09	0.50
1:F:302:LEU:HA	1:F:305:PRO:HG2	1.93	0.50
1:D:55:PRO:HB3	1:D:95:PHE:CD2	2.47	0.50
1:E:52:GLY:C	1:E:54:LYS:H	2.18	0.50
1:F:308:PHE:CD2	1:F:308:PHE:C	2.89	0.50
1:J:276:ALA:HB2	1:J:304:PHE:HE2	1.76	0.50
1:E:58:VAL:HG13	1:E:92:LEU:HB2	1.93	0.50
1:G:72:TRP:CH2	1:G:140:LEU:HD12	2.46	0.50
1:J:72:TRP:HH2	1:J:140:LEU:HD12	1.77	0.50
4:A:501:HOH:O	1:B:134:SER:N	2.43	0.50
1:E:224:TRP:CD2	1:E:301:ARG:HD3	2.47	0.50
1:F:279:LEU:HD23	1:F:300:CYS:SG	2.52	0.50
1:I:298:GLN:HA	1:I:301:ARG:HG3	1.93	0.50
1:J:82:VAL:N	1:J:109:SER:O	2.38	0.50
1:A:145:ILE:HG23	1:A:168:THR:HG21	1.93	0.50
1:F:51:PRO:HD2	1:F:56:LEU:HD12	1.93	0.50
1:H:212:LEU:HD13	1:H:245:TYR:CD2	2.46	0.50
1:D:298:GLN:HA	1:D:301:ARG:HG3	1.94	0.50
1:I:247:PHE:CD2	1:J:247:PHE:CE2	2.99	0.50
1:J:52:GLY:C	1:J:54:LYS:H	2.20	0.50
1:C:216:ILE:O	1:C:219:SER:OG	2.29	0.49
1:H:173:ILE:O	1:H:187:GLU:HA	2.12	0.49
1:J:91:ARG:CZ	1:J:103:ASN:HD22	2.25	0.49
1:H:50:THR:OG1	1:H:52:GLY:O	2.30	0.49
1:A:50:THR:OG1	1:A:52:GLY:O	2.30	0.49
1:G:284:HIS:O	1:G:285:HIS:HD2	1.96	0.49
1:H:247:PHE:CD2	1:I:247:PHE:HE2	2.30	0.49
3:J:401:MES:O1S	4:J:502:HOH:O	2.19	0.49
1:G:52:GLY:C	1:G:54:LYS:H	2.20	0.49
1:A:95:PHE:HB2	1:A:99:ARG:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ARG:NE	4:A:511:HOH:O	2.44	0.49
1:J:183:PRO:O	1:J:185:GLN:HG2	2.13	0.49
1:A:36:ASP:CG	1:A:105:ARG:HH21	2.20	0.49
1:G:132:PRO:CG	1:G:140:LEU:HD22	2.43	0.49
1:I:308:PHE:O	1:I:312:GLY:N	2.46	0.49
1:A:247:PHE:CD2	1:B:247:PHE:HE1	2.31	0.49
1:C:219:SER:O	1:C:222:VAL:HG23	2.12	0.49
1:G:268:ALA:HB1	1:G:308:PHE:CE1	2.48	0.49
1:J:114:MET:O	4:J:503:HOH:O	2.19	0.49
1:B:36:ASP:OD2	1:B:105:ARG:NH2	2.36	0.49
1:B:105:ARG:NH1	4:C:502:HOH:O	2.46	0.49
1:B:220:TRP:HZ2	1:B:308:PHE:CD2	2.31	0.49
1:H:219:SER:O	1:H:222:VAL:HG23	2.12	0.49
1:I:93:MET:HE3	1:I:101:ILE:HD12	1.94	0.49
1:F:308:PHE:O	1:F:312:GLY:N	2.45	0.48
1:J:140:LEU:O	4:J:504:HOH:O	2.20	0.48
1:H:122:ASP:OD1	1:H:199:ARG:NH1	2.47	0.48
1:H:219:SER:HB2	1:H:238:LEU:HD23	1.95	0.48
1:B:292:GLU:O	1:B:294:ASP:N	2.47	0.48
1:F:293:ASP:C	1:F:295:LEU:H	2.22	0.48
1:D:230:GLU:OE2	1:E:229:SER:OG	2.20	0.48
1:A:257:PRO:HG2	1:A:258:TYR:CD2	2.49	0.48
1:A:309:LEU:O	1:A:313:CYS:HB2	2.14	0.48
1:B:52:GLY:C	1:B:54:LYS:H	2.21	0.48
1:C:247:PHE:CD2	1:D:247:PHE:HE2	2.32	0.48
4:F:503:HOH:O	1:J:99:ARG:NH1	2.47	0.48
1:H:145:ILE:HD13	1:H:191:ILE:HD13	1.96	0.48
1:I:36:ASP:OD1	1:I:105:ARG:NH2	2.46	0.48
1:C:308:PHE:C	1:C:308:PHE:CD2	2.91	0.48
1:G:99:ARG:O	4:G:507:HOH:O	2.20	0.48
1:C:29:LEU:HB2	4:C:528:HOH:O	2.13	0.47
1:G:247:PHE:CD2	1:H:247:PHE:HE2	2.31	0.47
1:B:72:TRP:HH2	1:B:140:LEU:HD12	1.79	0.47
1:B:165:LYS:HG3	1:I:163:ARG:HG2	1.95	0.47
1:D:224:TRP:CG	1:E:281:ILE:HD11	2.49	0.47
1:I:36:ASP:CG	1:I:105:ARG:HH21	2.22	0.47
1:J:231:ARG:HB3	1:J:280:ILE:HD13	1.96	0.47
1:E:300:CYS:HA	1:E:303:ALA:HB3	1.96	0.47
1:F:68:ASN:OD1	1:J:62:GLN:NE2	2.32	0.47
1:F:119:PHE:CE1	1:F:253:LEU:HD22	2.49	0.47
1:A:208:PHE:CE1	1:A:248:TYR:CE2	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:ASN:O	4:D:504:HOH:O	2.20	0.47
1:H:198:VAL:HG12	1:H:199:ARG:N	2.30	0.47
1:D:138:GLN:HG3	1:D:185:GLN:NE2	2.30	0.47
1:D:202:SER:OG	4:D:504:HOH:O	2.21	0.47
1:J:132:PRO:HD3	1:J:142:PHE:CE2	2.49	0.47
1:B:224:TRP:CD2	1:B:301:ARG:HD3	2.50	0.47
1:H:298:GLN:HG3	1:H:301:ARG:NH2	2.30	0.47
1:I:52:GLY:C	1:I:54:LYS:H	2.22	0.47
1:J:72:TRP:CH2	1:J:140:LEU:HD12	2.50	0.47
1:B:55:PRO:HB3	1:B:95:PHE:CD2	2.50	0.47
1:D:10:ARG:HB3	1:D:11:PRO:HD3	1.97	0.47
1:F:62:GLN:NE2	1:G:68:ASN:OD1	2.44	0.47
1:A:224:TRP:CD2	1:A:301:ARG:HD3	2.51	0.46
1:B:112:ASN:ND2	1:B:125:GLN:O	2.48	0.46
1:I:145:ILE:HD13	1:I:191:ILE:HG21	1.97	0.46
1:A:281:ILE:HD11	1:E:224:TRP:HB2	1.97	0.46
1:F:208:PHE:HE1	1:F:248:TYR:CZ	2.33	0.46
1:I:133:PHE:N	4:I:510:HOH:O	2.48	0.46
1:I:173:ILE:O	1:I:187:GLU:HA	2.15	0.46
1:C:300:CYS:HA	1:C:303:ALA:HB3	1.98	0.46
1:E:93:MET:HB2	4:E:519:HOH:O	2.15	0.46
1:E:307:GLY:O	1:E:311:ILE:HG12	2.16	0.46
1:G:168:THR:C	1:G:169:HIS:CD2	2.93	0.46
1:D:297:ILE:O	1:D:298:GLN:HB2	2.15	0.46
1:F:72:TRP:CH2	1:F:140:LEU:HD12	2.50	0.46
1:F:250:SER:HB2	1:J:252:ILE:HD11	1.98	0.46
1:F:264:GLN:NE2	4:F:506:HOH:O	2.49	0.46
1:I:44:THR:HA	1:I:99:ARG:HA	1.97	0.46
1:I:234:THR:HG1	1:J:233:GLN:HE21	1.57	0.46
1:D:303:ALA:O	1:D:307:GLY:N	2.36	0.46
1:C:23:ILE:HG12	1:C:35:VAL:HG22	1.98	0.46
1:F:23:ILE:HG21	1:F:126:PHE:CD2	2.51	0.46
1:B:142:PHE:CD2	1:B:191:ILE:HG13	2.50	0.46
1:E:210:LEU:HB3	1:E:211:PRO:HD3	1.97	0.46
1:F:133:PHE:CE2	1:J:91:ARG:HB2	2.50	0.46
1:B:89:ASN:ND2	4:B:505:HOH:O	2.20	0.46
1:D:52:GLY:C	1:D:54:LYS:H	2.24	0.46
1:A:253:LEU:HB3	1:A:254:PRO:HD2	1.98	0.45
1:F:240:LEU:HD11	2:F:402:4LE:F01	2.06	0.45
1:F:300:CYS:HA	1:F:303:ALA:HB3	1.98	0.45
1:I:171:SER:OG	1:I:172:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:14:VAL:HG13	1:H:142:PHE:HD1	1.82	0.45
1:F:173:ILE:O	1:F:187:GLU:HA	2.17	0.45
1:H:279:LEU:HD23	1:H:300:CYS:SG	2.56	0.45
1:I:234:THR:OG1	1:J:233:GLN:NE2	2.40	0.45
1:C:183:PRO:O	1:C:185:GLN:HG2	2.16	0.45
1:D:63:ILE:O	1:D:67:ILE:HG12	2.16	0.45
1:F:144:ASP:HB2	4:F:505:HOH:O	2.17	0.45
1:F:210:LEU:HB3	1:F:211:PRO:HD3	1.99	0.45
1:G:146:GLN:HG2	4:G:512:HOH:O	2.15	0.45
1:J:308:PHE:O	1:J:312:GLY:N	2.50	0.45
1:J:220:TRP:CZ3	1:J:305:PRO:HA	2.51	0.45
1:A:72:TRP:CH2	1:A:74:PRO:HG3	2.51	0.45
1:C:282:PHE:CZ	1:C:286:ARG:HG3	2.52	0.45
1:D:253:LEU:HB3	1:D:254:PRO:HD2	1.98	0.45
1:A:52:GLY:C	1:A:54:LYS:H	2.25	0.45
1:A:119:PHE:CE1	1:A:253:LEU:HD22	2.52	0.45
1:G:234:THR:O	1:G:238:LEU:HD13	2.17	0.45
1:G:285:HIS:HA	4:G:530:HOH:O	2.16	0.45
1:H:91:ARG:NH1	1:H:103:ASN:HD22	2.15	0.45
1:B:246:ALA:HA	1:B:266:ILE:HD13	1.98	0.45
1:E:222:VAL:O	1:E:231:ARG:HG2	2.17	0.45
1:B:79:ILE:CD1	1:B:131:GLU:HB2	2.47	0.45
1:F:13:ASP:OD1	1:F:141:ARG:NH1	2.49	0.45
1:G:95:PHE:HB2	1:G:99:ARG:HG3	1.98	0.45
1:H:232:LEU:O	1:H:235:SER:OG	2.34	0.45
1:H:300:CYS:HA	1:H:303:ALA:HB3	1.99	0.45
1:J:308:PHE:HA	1:J:311:ILE:HG22	1.99	0.45
1:D:308:PHE:C	1:D:308:PHE:CD2	2.95	0.45
1:F:281:ILE:HD11	1:J:224:TRP:CG	2.52	0.45
1:H:227:SER:O	1:H:231:ARG:HG3	2.16	0.45
1:I:224:TRP:CG	1:J:281:ILE:HD11	2.52	0.45
1:C:224:TRP:CE2	1:C:301:ARG:HD2	2.52	0.44
1:C:224:TRP:CG	1:D:281:ILE:HD11	2.52	0.44
1:F:183:PRO:O	1:F:185:GLN:HG2	2.17	0.44
1:J:42:GLN:HG3	1:J:101:ILE:HG12	1.99	0.44
1:A:224:TRP:CG	1:B:281:ILE:HD11	2.53	0.44
1:B:298:GLN:HG2	1:B:301:ARG:NH2	2.32	0.44
1:E:292:GLU:O	1:E:294:ASP:N	2.50	0.44
1:F:284:HIS:NE2	1:J:226:GLU:OE2	2.40	0.44
1:J:122:ASP:OD1	1:J:199:ARG:NH1	2.51	0.44
1:C:95:PHE:HB2	1:C:99:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:ASP:C	1:E:295:LEU:H	2.24	0.44
1:F:156:GLU:HG2	1:F:157:ILE:HG23	1.99	0.44
1:C:52:GLY:C	1:C:54:LYS:H	2.26	0.44
1:J:298:GLN:HA	1:J:301:ARG:HG3	1.98	0.44
1:B:278:LEU:O	1:B:281:ILE:HG22	2.17	0.44
1:F:29:LEU:HD21	1:J:159:GLU:OE2	2.17	0.44
1:F:35:VAL:O	1:F:107:LEU:HD12	2.18	0.44
1:G:279:LEU:HD22	1:G:304:PHE:CZ	2.53	0.44
1:I:29:LEU:HA	1:I:29:LEU:HD23	1.75	0.44
1:B:145:ILE:HD13	1:B:191:ILE:HD13	1.99	0.44
1:C:154:ASN:O	1:C:157:ILE:HG12	2.17	0.44
1:C:306:LEU:O	1:C:310:ALA:N	2.50	0.44
1:D:284:HIS:O	1:D:285:HIS:HD2	2.00	0.44
1:F:224:TRP:CE2	1:F:301:ARG:HD3	2.53	0.44
1:D:89:ASN:HB2	1:E:133:PHE:CE1	2.53	0.43
1:E:212:LEU:HD23	1:E:245:TYR:CD2	2.52	0.43
1:A:265:MET:O	1:A:269:GLY:N	2.47	0.43
1:B:255:ARG:O	1:B:256:LEU:HD12	2.18	0.43
1:D:292:GLU:O	1:D:294:ASP:N	2.51	0.43
1:H:304:PHE:HB2	1:H:305:PRO:HD3	2.00	0.43
1:J:296:LEU:O	1:J:299:ARG:HB2	2.18	0.43
1:C:208:PHE:CD1	1:C:249:THR:HG22	2.52	0.43
1:H:298:GLN:HA	1:H:301:ARG:HG3	1.99	0.43
1:G:132:PRO:HG3	1:G:140:LEU:HD22	2.00	0.43
1:I:238:LEU:HB3	1:I:273:ILE:HD13	2.00	0.43
1:B:36:ASP:CG	1:B:105:ARG:HH21	2.23	0.43
1:B:286:ARG:HD3	1:B:287:GLN:HG3	2.00	0.43
1:D:123:ARG:CD	1:D:198:VAL:HG12	2.46	0.43
1:H:48:ARG:NH1	4:H:503:HOH:O	2.51	0.43
1:J:14:VAL:HG11	1:J:140:LEU:HD21	2.00	0.43
1:H:297:ILE:O	1:H:298:GLN:HB3	2.19	0.43
1:D:293:ASP:OD1	1:D:295:LEU:HB3	2.19	0.43
1:B:49:LYS:HA	4:B:514:HOH:O	2.18	0.43
1:F:247:PHE:HE2	1:J:247:PHE:CD2	2.37	0.43
1:G:173:ILE:O	1:G:187:GLU:HA	2.19	0.43
1:I:156:GLU:OE1	1:I:156:GLU:N	2.52	0.43
1:A:276:ALA:HB2	1:A:304:PHE:HE2	1.82	0.43
1:B:257:PRO:HG2	1:B:258:TYR:CD2	2.54	0.43
1:D:127:VAL:C	1:D:128:LEU:HD12	2.44	0.43
1:D:205:LEU:HD23	1:D:205:LEU:HA	1.65	0.43
1:H:23:ILE:HG12	1:H:35:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:210:LEU:HB3	1:J:211:PRO:HD3	1.99	0.43
1:B:214:LEU:HD23	1:B:214:LEU:HA	1.78	0.42
1:D:28:THR:HG21	1:D:254:PRO:HB2	2.01	0.42
1:D:252:ILE:HD13	4:D:509:HOH:O	2.18	0.42
1:D:302:LEU:HD23	1:D:302:LEU:HA	1.85	0.42
1:G:224:TRP:CE2	1:G:301:ARG:HD3	2.54	0.42
1:I:298:GLN:HG2	1:I:301:ARG:CZ	2.49	0.42
1:J:33:TYR:OH	1:J:127:VAL:N	2.41	0.42
1:C:297:ILE:O	1:C:298:GLN:HB3	2.19	0.42
1:D:153:ASP:C	1:D:155:GLU:H	2.27	0.42
1:G:300:CYS:HA	1:G:303:ALA:HB3	2.01	0.42
1:H:128:LEU:HB2	1:H:193:VAL:CG2	2.49	0.42
1:H:253:LEU:HB3	1:H:254:PRO:HD2	2.01	0.42
1:I:308:PHE:C	1:I:308:PHE:CD2	2.97	0.42
1:B:261:VAL:HG23	4:B:501:HOH:O	2.19	0.42
1:D:304:PHE:HB2	1:D:305:PRO:HD3	2.01	0.42
1:F:52:GLY:C	1:F:54:LYS:H	2.27	0.42
1:H:153:ASP:OD1	1:H:154:ASN:N	2.52	0.42
1:I:293:ASP:OD1	1:I:295:LEU:HB3	2.19	0.42
1:B:183:PRO:O	1:B:185:GLN:HG2	2.18	0.42
1:H:225:LEU:HD12	1:I:232:LEU:HD23	2.00	0.42
1:I:123:ARG:CG	1:I:198:VAL:CG1	2.71	0.42
1:C:257:PRO:HG2	1:C:258:TYR:CD2	2.55	0.42
1:J:143:SER:OG	1:J:144:ASP:OD2	2.32	0.42
1:A:253:LEU:HD13	4:A:521:HOH:O	2.20	0.42
1:C:224:TRP:HB2	1:D:281:ILE:HD11	2.01	0.42
1:H:72:TRP:CH2	1:H:140:LEU:HD12	2.54	0.42
1:B:35:VAL:HB	1:B:110:PHE:CE1	2.54	0.42
1:C:224:TRP:CB	1:D:281:ILE:HD11	2.49	0.42
1:J:208:PHE:HE1	1:J:248:TYR:CZ	2.38	0.42
1:A:56:LEU:HB3	1:A:94:LEU:HB2	2.02	0.42
1:A:168:THR:HG22	1:A:169:HIS:N	2.34	0.42
1:B:214:LEU:HD22	1:C:274:PHE:CG	2.55	0.42
1:D:256:LEU:HD13	1:D:258:TYR:HE1	1.85	0.42
1:H:105:ARG:HH11	1:H:105:ARG:HD3	1.69	0.42
1:H:224:TRP:CE2	1:H:301:ARG:HB3	2.54	0.42
1:H:269:GLY:O	1:H:273:ILE:HG12	2.19	0.42
1:A:308:PHE:CD1	1:A:308:PHE:C	2.97	0.42
1:B:174:ARG:HH22	1:I:13:ASP:CG	2.28	0.42
1:G:142:PHE:CD2	1:G:191:ILE:HG13	2.55	0.42
1:F:229:SER:OG	1:J:230:GLU:OE2	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.55	0.41
3:H:401:MES:H51	3:H:401:MES:H81	1.81	0.41
1:I:72:TRP:HH2	1:I:140:LEU:HD12	1.84	0.41
1:A:29:LEU:HA	1:A:29:LEU:HD23	1.84	0.41
1:A:134:SER:OG	1:E:59:GLU:OE2	2.28	0.41
1:B:224:TRP:HB2	1:C:281:ILE:HD11	2.01	0.41
1:E:38:TYR:CZ	1:E:105:ARG:HD2	2.55	0.41
1:F:185:GLN:NE2	4:F:502:HOH:O	2.15	0.41
1:F:200:ASN:HA	1:F:201:PRO:HD3	1.86	0.41
1:F:292:GLU:O	1:F:294:ASP:N	2.54	0.41
1:H:225:LEU:CD1	1:I:232:LEU:HD23	2.50	0.41
1:J:205:LEU:HD23	1:J:205:LEU:HA	1.88	0.41
1:A:130:LEU:HB3	1:A:191:ILE:HB	2.02	0.41
1:C:288:ALA:O	1:C:291:VAL:HG12	2.19	0.41
1:G:16:VAL:O	1:G:145:ILE:HD12	2.20	0.41
1:I:127:VAL:O	1:I:128:LEU:HD12	2.20	0.41
1:B:297:ILE:O	1:B:298:GLN:HB2	2.21	0.41
1:B:298:GLN:HG2	1:B:301:ARG:CZ	2.50	0.41
1:C:212:LEU:HB2	1:C:245:TYR:CE2	2.56	0.41
1:E:302:LEU:HD23	1:E:302:LEU:HA	1.88	0.41
1:F:178:LEU:HD23	1:F:178:LEU:HA	1.88	0.41
1:H:260:THR:H	1:H:263:ASP:HB2	1.86	0.41
1:I:95:PHE:HB2	1:I:99:ARG:HG3	2.03	0.41
1:C:175:TYR:HB2	1:C:178:LEU:HD11	2.03	0.41
1:D:127:VAL:O	1:D:128:LEU:HD12	2.20	0.41
1:G:168:THR:O	1:G:169:HIS:CD2	2.74	0.41
1:C:247:PHE:CD2	1:D:247:PHE:CE2	3.08	0.41
1:G:216:ILE:O	1:G:219:SER:HB3	2.21	0.41
1:G:224:TRP:CG	1:H:281:ILE:HD11	2.55	0.41
1:I:65:ARG:HH21	1:J:68:ASN:CG	2.29	0.41
1:I:123:ARG:CD	1:I:198:VAL:HG12	2.47	0.41
1:J:220:TRP:C	1:J:222:VAL:H	2.28	0.41
1:E:253:LEU:HB3	1:E:254:PRO:HD2	2.03	0.41
1:H:210:LEU:HB3	1:H:211:PRO:HD3	2.03	0.41
3:C:401:MES:H51	3:C:401:MES:H81	1.88	0.41
1:E:279:LEU:HD22	1:E:304:PHE:HE1	1.86	0.41
1:E:288:ALA:C	1:E:290:GLY:H	2.29	0.41
1:F:159:GLU:OE2	1:G:29:LEU:HD21	2.21	0.41
1:F:250:SER:CB	1:J:252:ILE:HD11	2.50	0.41
1:C:28:THR:HG22	1:C:116:PHE:CZ	2.55	0.41
1:C:246:ALA:HA	1:C:266:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:ASP:C	1:E:295:LEU:N	2.79	0.41
1:F:132:PRO:CG	1:F:140:LEU:HD22	2.51	0.41
1:G:86:ASP:OD1	1:H:84:SER:OG	2.35	0.41
1:J:128:LEU:HB2	1:J:193:VAL:HB	2.02	0.41
1:J:145:ILE:HD13	1:J:191:ILE:HD13	2.03	0.41
1:J:223:PHE:HE2	1:J:304:PHE:CD2	2.39	0.41
1:E:34:LYS:NZ	4:E:520:HOH:O	2.53	0.41
1:F:293:ASP:C	1:F:295:LEU:N	2.78	0.41
1:G:298:GLN:HA	1:G:301:ARG:HG3	2.03	0.41
1:E:297:ILE:HG13	4:E:502:HOH:O	2.21	0.40
1:G:268:ALA:HB1	1:G:308:PHE:HE1	1.85	0.40
1:D:123:ARG:CG	1:D:198:VAL:CG1	2.66	0.40
1:H:224:TRP:CE2	1:H:301:ARG:HD2	2.56	0.40
1:H:297:ILE:C	1:H:299:ARG:H	2.30	0.40
1:I:212:LEU:HD12	1:I:245:TYR:CE2	2.56	0.40
1:G:178:LEU:HA	1:G:178:LEU:HD23	1.79	0.40
1:G:181:VAL:CG1	1:G:185:GLN:HG3	2.51	0.40
1:H:182:GLN:HB2	1:H:183:PRO:CD	2.49	0.40
1:I:297:ILE:HG22	1:I:298:GLN:N	2.36	0.40
1:C:302:LEU:O	1:C:302:LEU:HD23	2.21	0.40
1:D:66:TRP:HB3	1:D:71:LEU:HD23	2.03	0.40
1:D:91:ARG:HB2	1:E:133:PHE:HE2	1.87	0.40
1:F:38:TYR:CZ	1:F:105:ARG:HD2	2.57	0.40
1:G:50:THR:OG1	1:G:52:GLY:O	2.38	0.40
1:H:225:LEU:HD23	1:H:230:GLU:HB3	2.03	0.40
1:B:295:LEU:O	1:B:299:ARG:HD3	2.22	0.40
4:B:505:HOH:O	1:C:77:GLU:OE2	2.22	0.40
1:C:198:VAL:HG12	1:C:199:ARG:N	2.35	0.40
1:C:223:PHE:HB2	1:C:301:ARG:HG2	2.04	0.40
1:D:308:PHE:O	1:D:312:GLY:N	2.55	0.40
1:F:212:LEU:HD11	1:F:266:ILE:HG12	2.04	0.40
1:H:56:LEU:HD12	1:H:57:ILE:H	1.87	0.40
1:H:221:SER:OG	1:I:236:PHE:HZ	2.03	0.40
1:I:72:TRP:CH2	1:I:74:PRO:HG3	2.57	0.40
1:I:129:GLU:OE2	1:I:190:ARG:NH1	2.54	0.40
1:I:140:LEU:C	1:I:140:LEU:HD23	2.46	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:ASP:OD2	1:G:174:ARG:NH2[2_556]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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	307/322 (95%)	283 (92%)	22 (7%)	2 (1%)	18	53
1	B	307/322 (95%)	282 (92%)	23 (8%)	2 (1%)	18	53
1	C	307/322 (95%)	282 (92%)	24 (8%)	1 (0%)	36	70
1	D	307/322 (95%)	284 (92%)	22 (7%)	1 (0%)	36	70
1	E	307/322 (95%)	281 (92%)	24 (8%)	2 (1%)	18	53
1	F	307/322 (95%)	283 (92%)	22 (7%)	2 (1%)	18	53
1	G	307/322 (95%)	282 (92%)	23 (8%)	2 (1%)	18	53
1	H	307/322 (95%)	282 (92%)	24 (8%)	1 (0%)	36	70
1	I	307/322 (95%)	286 (93%)	19 (6%)	2 (1%)	18	53
1	J	307/322 (95%)	282 (92%)	24 (8%)	1 (0%)	36	70
All	All	3070/3220 (95%)	2827 (92%)	227 (7%)	16 (0%)	24	60

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	182	GLN
1	C	182	GLN
1	E	182	GLN
1	F	182	GLN
1	H	182	GLN
1	J	182	GLN
1	A	293	ASP
1	D	182	GLN
1	F	181	VAL

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Mol	Chain	Res	Type
1	G	182	GLN
1	I	181	VAL
1	A	182	GLN
1	B	182	GLN
1	E	181	VAL
1	B	293	ASP
1	G	293	ASP

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	277/284 (98%)	270 (98%)	7 (2%)	42	72
1	B	277/284 (98%)	271 (98%)	6 (2%)	45	74
1	C	277/284 (98%)	270 (98%)	7 (2%)	42	72
1	D	277/284 (98%)	271 (98%)	6 (2%)	45	74
1	E	277/284 (98%)	271 (98%)	6 (2%)	45	74
1	F	277/284 (98%)	273 (99%)	4 (1%)	59	80
1	G	277/284 (98%)	272 (98%)	5 (2%)	51	77
1	H	277/284 (98%)	268 (97%)	9 (3%)	34	67
1	I	277/284 (98%)	271 (98%)	6 (2%)	45	74
1	J	277/284 (98%)	274 (99%)	3 (1%)	65	83
All	All	2770/2840 (98%)	2711 (98%)	59 (2%)	47	75

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	79	ILE
1	A	145	ILE
1	A	147	VAL
1	A	152	ILE
1	A	205	LEU

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Mol	Chain	Res	Type
1	A	281	ILE
1	B	14	VAL
1	B	58	VAL
1	B	181	VAL
1	B	295	LEU
1	B	304	PHE
1	B	316	VAL
1	C	14	VAL
1	C	173	ILE
1	C	181	VAL
1	C	252	ILE
1	C	253	LEU
1	C	308	PHE
1	C	316	VAL
1	D	29	LEU
1	D	58	VAL
1	D	63	ILE
1	D	79	ILE
1	D	281	ILE
1	D	308	PHE
1	E	14	VAL
1	E	29	LEU
1	E	58	VAL
1	E	295	LEU
1	E	308	PHE
1	E	316	VAL
1	F	14	VAL
1	F	295	LEU
1	F	308	PHE
1	F	316	VAL
1	G	14	VAL
1	G	58	VAL
1	G	173	ILE
1	G	195	ILE
1	G	316	VAL
1	H	14	VAL
1	H	58	VAL
1	H	63	ILE
1	H	79	ILE
1	H	91	ARG
1	H	173	ILE
1	H	258	TYR

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Mol	Chain	Res	Type
1	H	295	LEU
1	H	308	PHE
1	I	14	VAL
1	I	63	ILE
1	I	73	VAL
1	I	258	TYR
1	I	302	LEU
1	I	308	PHE
1	J	14	VAL
1	J	58	VAL
1	J	316	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	233	GLN
1	A	251	ASN
1	B	139	GLN
1	B	184	ASN
1	B	251	ASN
1	B	264	GLN
1	B	298	GLN
1	C	169	HIS
1	C	185	GLN
1	C	251	ASN
1	D	69	ASN
1	D	125	GLN
1	D	169	HIS
1	D	185	GLN
1	D	251	ASN
1	D	285	HIS
1	E	177	HIS
1	E	233	GLN
1	E	251	ASN
1	F	103	ASN
1	F	169	HIS
1	F	251	ASN
1	G	169	HIS
1	G	177	HIS
1	G	251	ASN
1	G	285	HIS

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Mol	Chain	Res	Type
1	H	103	ASN
1	H	125	GLN
1	H	251	ASN
1	I	103	ASN
1	I	169	HIS
1	I	251	ASN
1	J	103	ASN
1	J	139	GLN
1	J	251	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
3	MES	C	401	-	12,12,12	2.31	1 (8%)	15,16,16	2.50	6 (40%)
3	MES	G	401	-	12,12,12	2.31	1 (8%)	15,16,16	2.17	7 (46%)
3	MES	B	401	-	12,12,12	2.41	1 (8%)	15,16,16	2.17	5 (33%)
3	MES	A	402	-	12,12,12	2.38	1 (8%)	15,16,16	2.45	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	4LE	F	401	-	6,9,9	0.37	0	8,13,13	1.68	2 (25%)
2	4LE	A	401	-	6,9,9	0.67	0	8,13,13	1.94	3 (37%)
3	MES	H	401	-	12,12,12	2.32	1 (8%)	15,16,16	2.44	7 (46%)
3	MES	D	401	-	12,12,12	2.18	1 (8%)	15,16,16	2.38	6 (40%)
3	MES	F	403	-	12,12,12	2.26	1 (8%)	15,16,16	2.40	7 (46%)
3	MES	I	401	-	12,12,12	2.25	1 (8%)	15,16,16	2.04	6 (40%)
2	4LE	E	401	-	6,9,9	0.39	0	8,13,13	1.40	2 (25%)
3	MES	A	403	-	12,12,12	2.37	1 (8%)	15,16,16	1.85	4 (26%)
3	MES	J	401	-	12,12,12	2.30	1 (8%)	15,16,16	2.19	7 (46%)
2	4LE	F	402	-	6,9,9	0.50	0	8,13,13	1.29	0

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
3	MES	C	401	-	-	5/6/14/14	0/1/1/1
3	MES	G	401	-	-	3/6/14/14	0/1/1/1
3	MES	B	401	-	-	4/6/14/14	0/1/1/1
3	MES	A	402	-	-	3/6/14/14	0/1/1/1
2	4LE	F	401	-	-	5/8/10/10	-
2	4LE	A	401	-	-	3/8/10/10	-
3	MES	H	401	-	-	4/6/14/14	0/1/1/1
3	MES	D	401	-	-	1/6/14/14	0/1/1/1
3	MES	F	403	-	-	1/6/14/14	0/1/1/1
3	MES	I	401	-	-	2/6/14/14	0/1/1/1
2	4LE	E	401	-	-	3/8/10/10	-
3	MES	A	403	-	-	3/6/14/14	0/1/1/1
3	MES	J	401	-	-	5/6/14/14	0/1/1/1
2	4LE	F	402	-	-	4/8/10/10	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	MES	C8-S	-8.16	1.66	1.77
3	A	403	MES	C8-S	-7.98	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	MES	C8-S	-7.96	1.66	1.77
3	H	401	MES	C8-S	-7.81	1.66	1.77
3	C	401	MES	C8-S	-7.79	1.66	1.77
3	G	401	MES	C8-S	-7.76	1.66	1.77
3	J	401	MES	C8-S	-7.71	1.66	1.77
3	F	403	MES	C8-S	-7.55	1.67	1.77
3	I	401	MES	C8-S	-7.53	1.67	1.77
3	D	401	MES	C8-S	-7.29	1.67	1.77

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	MES	C5-N4-C3	5.57	120.84	108.84
3	H	401	MES	C5-N4-C3	5.49	120.67	108.84
3	C	401	MES	C5-N4-C3	5.39	120.45	108.84
3	F	403	MES	C5-N4-C3	5.32	120.31	108.84
3	D	401	MES	C5-N4-C3	5.31	120.28	108.84
3	B	401	MES	C5-N4-C3	5.30	120.25	108.84
3	J	401	MES	C5-N4-C3	4.84	119.26	108.84
3	A	403	MES	C5-N4-C3	4.53	118.61	108.84
3	I	401	MES	C5-N4-C3	4.44	118.42	108.84
3	G	401	MES	C5-N4-C3	4.30	118.10	108.84
3	C	401	MES	O1S-S-C8	4.05	112.85	106.73
3	A	402	MES	C6-C5-N4	-3.57	104.69	110.12
3	D	401	MES	C7-N4-C5	3.42	120.36	111.24
3	F	403	MES	C7-N4-C5	3.33	120.12	111.24
3	G	401	MES	C6-C5-N4	-3.31	105.09	110.12
3	D	401	MES	O2S-S-C8	3.31	111.72	106.73
3	H	401	MES	C7-N4-C5	3.30	120.02	111.24
3	C	401	MES	C7-N4-C5	3.26	119.93	111.24
3	J	401	MES	C6-C5-N4	-3.23	105.20	110.12
3	A	402	MES	C7-N4-C5	3.22	119.82	111.24
3	C	401	MES	C7-N4-C3	3.14	119.62	111.24
3	F	403	MES	C7-N4-C3	3.06	119.40	111.24
3	A	402	MES	C7-N4-C3	3.04	119.34	111.24
3	D	401	MES	C7-N4-C3	3.03	119.32	111.24
3	D	401	MES	O1S-S-C8	3.02	111.29	106.73
3	C	401	MES	C6-C5-N4	-3.00	105.56	110.12
3	H	401	MES	O1S-S-C8	2.97	111.21	106.73
3	H	401	MES	C7-N4-C3	2.97	119.14	111.24
2	A	401	4LE	O01-C02-C01	-2.95	104.86	108.15
2	A	401	4LE	F03-C01-F02	2.92	113.22	106.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	401	MES	C6-C5-N4	-2.92	105.68	110.12
3	F	403	MES	C6-C5-N4	-2.89	105.73	110.12
3	G	401	MES	O2S-S-C8	2.83	111.00	106.73
2	F	401	4LE	O01-C02-C01	2.80	111.27	108.15
3	I	401	MES	O1S-S-C8	2.71	110.82	106.73
3	F	403	MES	C2-C3-N4	-2.68	106.05	110.12
3	G	401	MES	C7-N4-C5	2.68	118.38	111.24
3	H	401	MES	C2-C3-N4	-2.62	106.13	110.12
3	J	401	MES	C7-N4-C3	2.61	118.19	111.24
3	A	403	MES	O1S-S-C8	2.59	110.64	106.73
3	A	402	MES	C2-C3-N4	-2.58	106.19	110.12
3	G	401	MES	C7-N4-C3	2.58	118.11	111.24
3	B	401	MES	O3S-S-C8	2.52	110.94	106.00
3	C	401	MES	C2-C3-N4	-2.49	106.33	110.12
3	B	401	MES	C7-N4-C5	2.48	117.86	111.24
2	E	401	4LE	F01-C01-C02	-2.44	106.16	111.81
3	J	401	MES	C2-C3-N4	-2.43	106.42	110.12
3	J	401	MES	C7-N4-C5	2.41	117.67	111.24
3	I	401	MES	C6-C5-N4	-2.41	106.46	110.12
3	I	401	MES	C7-N4-C5	2.40	117.62	111.24
3	F	403	MES	O3S-S-C8	2.37	110.64	106.00
3	B	401	MES	C7-N4-C3	2.31	117.39	111.24
2	F	401	4LE	F02-C01-C02	-2.31	106.46	111.81
3	F	403	MES	O1S-S-C8	2.28	110.17	106.73
3	I	401	MES	C7-N4-C3	2.25	117.25	111.24
3	G	401	MES	O3S-S-C8	2.20	110.32	106.00
3	G	401	MES	C2-C3-N4	-2.19	106.80	110.12
3	A	402	MES	O1S-S-C8	2.18	110.02	106.73
2	A	401	4LE	F01-C01-C02	-2.18	106.77	111.81
3	A	403	MES	C6-C5-N4	-2.15	106.85	110.12
3	A	403	MES	C7-N4-C5	2.14	116.95	111.24
3	I	401	MES	O3S-S-C8	2.13	110.18	106.00
2	E	401	4LE	F03-C01-F02	2.13	111.51	106.87
3	J	401	MES	O3S-S-C8	2.12	110.15	106.00
3	J	401	MES	O1S-S-C8	2.11	109.92	106.73
3	D	401	MES	C6-C5-N4	-2.11	106.92	110.12
3	H	401	MES	O3S-S-C8	2.04	110.00	106.00
3	B	401	MES	C6-C5-N4	-2.00	107.07	110.12

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	4LE	F03-C01-C02-O01
2	E	401	4LE	F01-C01-C02-O01
2	E	401	4LE	F02-C01-C02-O01
2	E	401	4LE	F03-C01-C02-O01
2	F	401	4LE	F01-C01-C02-O01
2	F	401	4LE	F02-C01-C02-O01
2	F	401	4LE	F03-C01-C02-O01
2	F	401	4LE	F04-C03-O01-C02
2	F	401	4LE	F05-C03-O01-C02
2	F	402	4LE	F02-C01-C02-O01
2	F	402	4LE	F05-C03-O01-C02
3	A	402	MES	C8-C7-N4-C5
3	A	403	MES	C7-C8-S-O1S
3	A	403	MES	C7-C8-S-O2S
3	C	401	MES	N4-C7-C8-S
3	H	401	MES	C7-C8-S-O1S
3	I	401	MES	C8-C7-N4-C3
3	J	401	MES	C7-C8-S-O2S
3	J	401	MES	C7-C8-S-O3S
2	A	401	4LE	F01-C01-C02-O01
2	A	401	4LE	F02-C01-C02-O01
2	F	402	4LE	F01-C01-C02-O01
2	F	402	4LE	F03-C01-C02-O01
3	B	401	MES	C7-C8-S-O3S
3	H	401	MES	C7-C8-S-O3S
3	A	403	MES	C7-C8-S-O3S
3	A	402	MES	C8-C7-N4-C3
3	C	401	MES	C8-C7-N4-C3
3	D	401	MES	C8-C7-N4-C3
3	F	403	MES	C8-C7-N4-C3
3	G	401	MES	C8-C7-N4-C5
3	H	401	MES	C8-C7-N4-C3
3	I	401	MES	C8-C7-N4-C5
3	J	401	MES	C8-C7-N4-C3
3	C	401	MES	C7-C8-S-O3S
3	A	402	MES	C7-C8-S-O1S
3	B	401	MES	C7-C8-S-O1S
3	B	401	MES	C7-C8-S-O2S
3	C	401	MES	C7-C8-S-O1S
3	C	401	MES	C7-C8-S-O2S
3	H	401	MES	C7-C8-S-O2S
3	J	401	MES	C7-C8-S-O1S
3	B	401	MES	N4-C7-C8-S

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Mol	Chain	Res	Type	Atoms
3	G	401	MES	N4-C7-C8-S
3	G	401	MES	C8-C7-N4-C3
3	J	401	MES	C8-C7-N4-C5

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	MES	1	0
3	G	401	MES	1	0
2	F	401	4LE	1	0
3	H	401	MES	1	0
3	J	401	MES	1	0
2	F	402	4LE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	309/322 (95%)	-0.12	4 (1%) 75 53	62, 93, 151, 241	0
1	B	309/322 (95%)	-0.20	5 (1%) 70 47	55, 80, 175, 227	0
1	C	309/322 (95%)	-0.12	8 (2%) 57 34	53, 83, 179, 228	0
1	D	309/322 (95%)	-0.18	8 (2%) 57 34	51, 78, 171, 249	0
1	E	309/322 (95%)	-0.07	7 (2%) 61 38	58, 89, 169, 236	0
1	F	309/322 (95%)	-0.04	4 (1%) 75 53	59, 98, 166, 264	0
1	G	309/322 (95%)	-0.14	9 (2%) 53 31	54, 81, 149, 231	0
1	H	309/322 (95%)	-0.11	8 (2%) 57 34	59, 88, 175, 256	0
1	I	309/322 (95%)	-0.04	4 (1%) 75 53	58, 86, 175, 236	0
1	J	309/322 (95%)	0.11	9 (2%) 53 31	63, 98, 190, 244	0
All	All	3090/3220 (95%)	-0.09	66 (2%) 63 40	51, 88, 174, 264	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	317	ILE	4.1
1	E	157	ILE	4.1
1	B	181	VAL	3.6
1	G	317	ILE	3.6
1	F	181	VAL	3.5
1	H	317	ILE	3.5
1	G	157	ILE	3.4
1	G	316	VAL	3.3
1	C	172	ASP	3.2
1	J	315	LEU	3.2
1	D	179	SER	3.2
1	A	181	VAL	3.1
1	J	305	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	179	SER	3.0
1	J	172	ASP	3.0
1	J	156	GLU	3.0
1	I	179	SER	3.0
1	C	181	VAL	2.9
1	D	317	ILE	2.9
1	E	317	ILE	2.8
1	F	183	PRO	2.8
1	A	258	TYR	2.8
1	H	156	GLU	2.7
1	C	291	VAL	2.7
1	A	188	PHE	2.6
1	G	181	VAL	2.6
1	H	185	GLN	2.5
1	I	157	ILE	2.5
1	C	255	ARG	2.5
1	D	181	VAL	2.5
1	E	181	VAL	2.5
1	E	315	LEU	2.5
1	G	183	PRO	2.4
1	J	29	LEU	2.4
1	G	289	ASN	2.4
1	C	187	GLU	2.3
1	J	317	ILE	2.3
1	I	181	VAL	2.3
1	D	183	PRO	2.3
1	G	161	TRP	2.3
1	F	244	ALA	2.3
1	D	157	ILE	2.2
1	H	295	LEU	2.2
1	B	295	LEU	2.2
1	C	317	ILE	2.2
1	D	297	ILE	2.2
1	I	317	ILE	2.2
1	B	315	LEU	2.2
1	H	180	SER	2.2
1	G	156	GLU	2.2
1	J	181	VAL	2.1
1	G	235	SER	2.1
1	J	157	ILE	2.1
1	A	103	ASN	2.1
1	C	315	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	295	LEU	2.1
1	B	180	SER	2.1
1	D	316	VAL	2.1
1	H	152	ILE	2.1
1	D	291	VAL	2.1
1	H	316	VAL	2.1
1	E	183	PRO	2.1
1	J	178	LEU	2.0
1	C	179	SER	2.0
1	F	224	TRP	2.0
1	H	297	ILE	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 oligosaccharides 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
3	MES	F	403	12/12	0.63	0.19	117,127,146,150	0
3	MES	J	401	12/12	0.64	0.15	146,154,166,168	0
3	MES	C	401	12/12	0.73	0.15	109,123,138,142	0
3	MES	D	401	12/12	0.74	0.16	115,125,128,128	0
3	MES	A	403	12/12	0.75	0.17	127,135,140,142	0
3	MES	A	402	12/12	0.76	0.13	106,120,174,174	0
3	MES	G	401	12/12	0.77	0.13	108,117,138,140	0
3	MES	I	401	12/12	0.79	0.12	125,131,157,160	0
3	MES	H	401	12/12	0.82	0.13	116,122,150,150	0
3	MES	B	401	12/12	0.84	0.10	108,116,132,136	0
2	4LE	A	401	10/10	0.87	0.21	116,119,131,140	0
2	4LE	F	402	10/10	0.89	0.18	109,117,122,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	4LE	E	401	10/10	0.95	0.11	109,119,146,148	0
2	4LE	F	401	10/10	0.96	0.09	119,120,127,146	0

6.5 Other polymers [i](#)

There are no such residues in this entry.