



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:00 PM EDT

PDB ID : 3EOB / pdb_00003eob
Title : Crystal structure the Fab fragment of Efalizumab in complex with LFA-1 I domain, Form II
Authors : Li, S.; Ding, J.
Deposited on : 2008-09-26
Resolution : 3.60 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
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

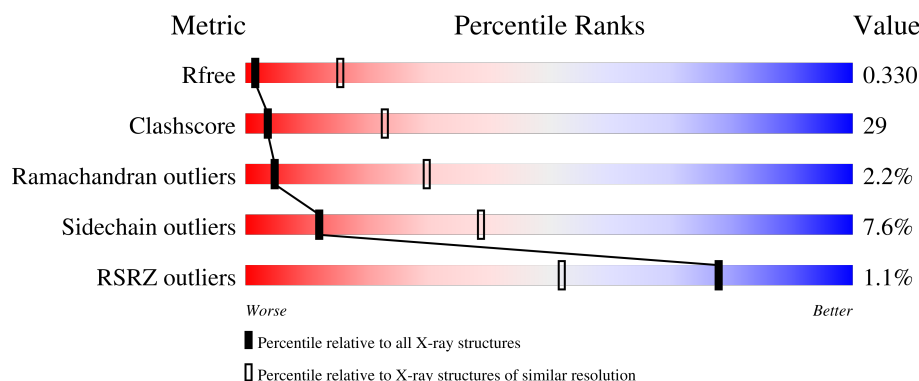
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 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	214	2% 53% 41% 6%
1	L	214	2% 45% 46% 7%
2	B	220	2% 51% 41% 5%
2	H	220	45% 46% 5%
3	I	181	2% 44% 45% 10%

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Mol	Chain	Length	Quality of chain
3	J	181	% 41% 47% 10% ••

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9454 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 Efalizumab Fab fragment, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1647	1030	276	335	6			
1	A	214	Total	C	N	O	S	0	0	0
			1647	1030	276	335	6			

- Molecule 2 is a protein called Efalizumab Fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1641	1043	273	318	7			
2	B	215	Total	C	N	O	S	0	0	0
			1641	1043	273	318	7			

- Molecule 3 is a protein called Integrin alpha-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	179	Total	C	N	O	S	0	0	0
			1438	929	231	274	4			
3	J	179	Total	C	N	O	S	0	0	0
			1438	929	231	274	4			

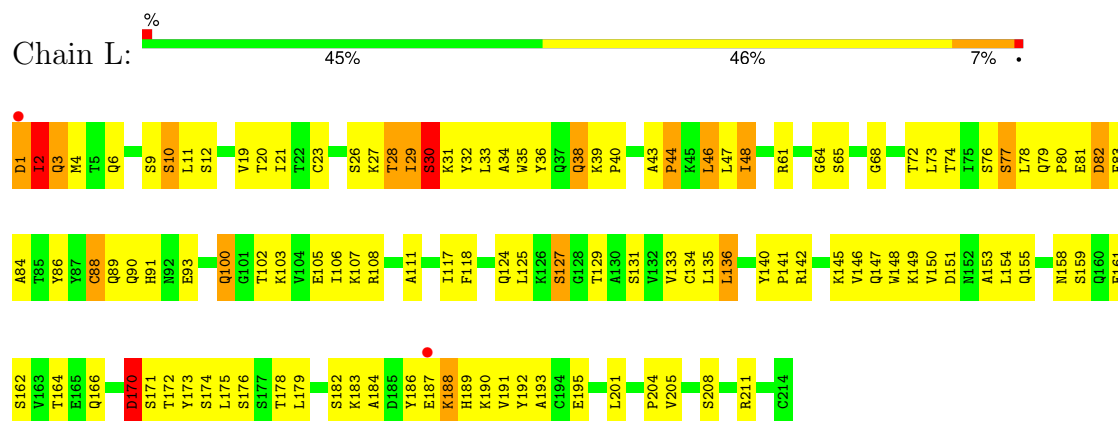
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	1	Total	Zn	0	0
			1	1		
4	J	1	Total	Zn	0	0
			1	1		

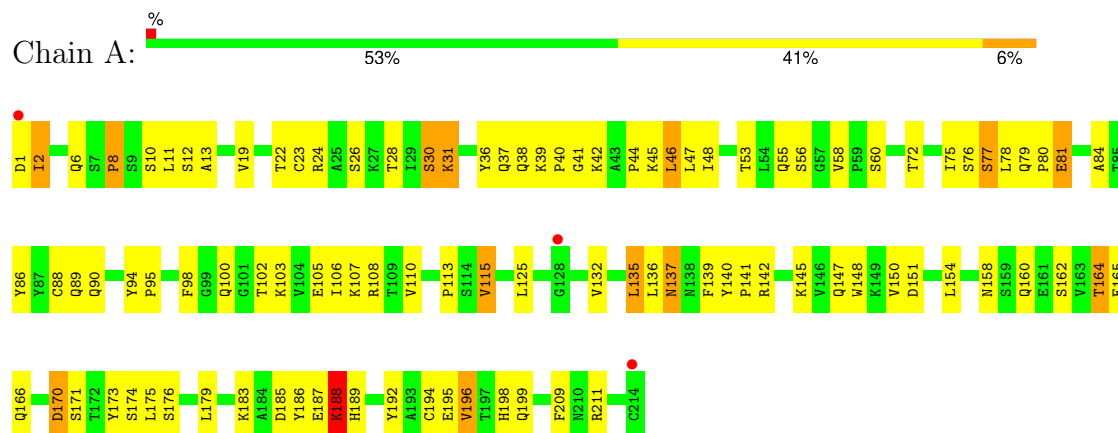
3 Residue-property plots

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: Efalizumab Fab fragment, light chain

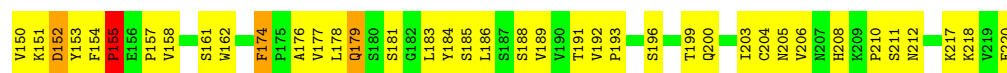


• Molecule 1: Efalizumab Fab fragment, light chain

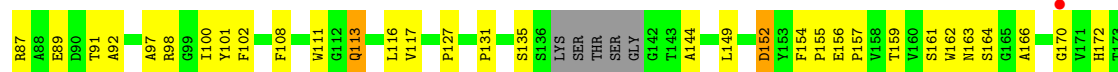


• Molecule 2: Efalizumab Fab fragment, heavy chain

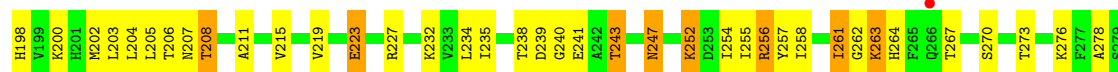
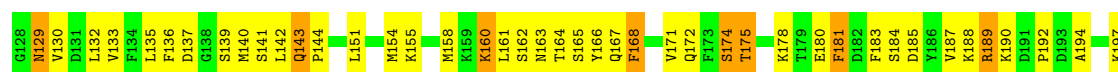
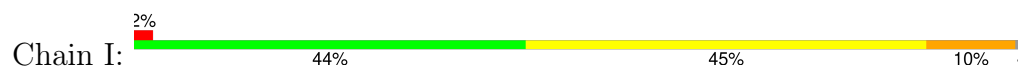




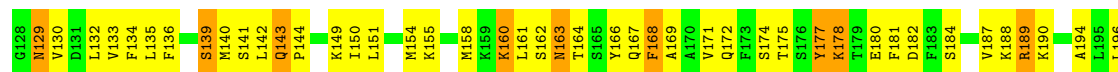
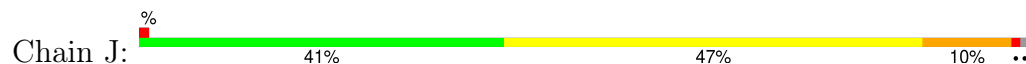
• Molecule 2: Efalizumab Fab fragment, heavy chain



• Molecule 3: Integrin alpha-L



• Molecule 3: Integrin alpha-L



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	111.10Å 111.10Å 470.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.60 50.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-3.60) 97.7 (50.00-3.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.57Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.267 , 0.333 0.267 , 0.330	Depositor DCC
R_{free} test set	1031 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	99.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 86.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9454	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 2.89% 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: ZN

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	0.62	0/1682	1.07	7/2280 (0.3%)
1	L	0.58	0/1682	1.09	9/2280 (0.4%)
2	B	0.64	0/1684	1.09	9/2291 (0.4%)
2	H	0.66	0/1684	1.15	11/2291 (0.5%)
3	I	0.72	2/1465 (0.1%)	1.21	15/1970 (0.8%)
3	J	0.77	0/1465	1.23	16/1970 (0.8%)
All	All	0.67	2/9662 (0.0%)	1.14	67/13082 (0.5%)

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	H	0	1
3	I	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	141	SER	CA-CB	-7.18	1.41	1.53
3	I	238	THR	CA-CB	5.03	1.61	1.53

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	141	SER	CA-CB-OG	-10.81	89.47	111.10
2	H	61	ASN	N-CA-C	-10.27	92.71	109.96
3	I	168	PHE	N-CA-C	8.79	121.87	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	102	PHE	N-CA-C	8.57	120.24	111.07
2	B	61	ASN	N-CA-C	-8.23	94.13	108.20
2	H	57	GLU	N-CA-C	-7.75	99.00	110.23
2	H	102	PHE	N-CA-C	7.72	119.33	111.07
3	J	261	ILE	N-CA-C	7.71	119.00	107.75
3	J	168	PHE	N-CA-C	7.36	121.76	110.36
2	B	54	SER	N-CA-C	7.34	120.21	111.33
3	J	285	PHE	N-CA-C	7.19	121.64	113.02
2	B	52	HIS	CA-C-N	7.07	128.68	119.84
2	B	52	HIS	C-N-CA	7.07	128.68	119.84
3	I	303	GLN	N-CA-C	-6.98	104.80	113.38
3	I	285	PHE	N-CA-C	6.79	121.40	113.18
1	L	183	LYS	N-CA-C	-6.75	104.77	112.87
3	I	232	LYS	N-CA-C	6.72	118.83	109.15
2	H	133	ALA	CA-C-N	6.62	126.53	119.85
2	H	133	ALA	C-N-CA	6.62	126.53	119.85
1	A	31	LYS	N-CA-C	-6.31	105.62	113.38
2	H	174	PHE	N-CA-C	6.24	118.69	110.08
2	B	215	VAL	N-CA-C	6.21	117.06	107.99
3	J	260	GLY	CA-C-N	-5.96	115.18	123.10
3	J	260	GLY	C-N-CA	-5.96	115.18	123.10
1	L	170	ASP	N-CA-C	5.91	119.75	112.54
3	I	299	PHE	N-CA-C	-5.90	104.54	110.97
3	J	296	LYS	N-CA-C	-5.89	104.44	111.69
2	B	44	GLY	N-CA-C	5.88	120.12	112.25
3	J	273	THR	N-CA-C	-5.85	104.98	111.36
1	A	115	VAL	N-CA-C	5.81	117.36	108.71
3	I	223	GLU	N-CA-C	-5.80	104.55	111.69
3	I	175	THR	N-CA-C	-5.79	105.88	113.12
3	I	301	GLU	N-CA-C	-5.76	106.29	113.38
1	A	2	ILE	N-CA-C	-5.76	97.37	109.34
3	I	208	THR	N-CA-C	5.72	117.52	111.28
2	B	135	SER	N-CA-C	5.72	118.65	110.24
3	I	256	ARG	N-CA-C	5.65	118.17	109.07
3	I	141	SER	N-CA-C	-5.63	106.45	113.15
1	L	30	SER	CB-CA-C	-5.62	109.10	115.79
1	A	196	VAL	N-CA-C	5.61	116.48	107.73
1	L	127	SER	N-CA-C	-5.53	107.07	113.88
3	I	296	LYS	N-CA-C	-5.39	105.40	111.28
3	J	139	SER	CA-CB-OG	-5.35	100.41	111.10
3	I	183	PHE	N-CA-C	5.32	117.77	111.33
1	A	135	LEU	N-CA-C	5.30	117.72	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	LYS	N-CA-C	-5.30	106.98	113.50
3	I	185	ASP	N-CA-C	-5.30	105.59	111.36
3	J	214	TYR	N-CA-C	-5.29	105.43	111.14
3	J	217	THR	N-CA-C	5.25	119.69	113.28
1	L	38	GLN	N-CA-C	5.23	117.19	107.99
1	L	86	TYR	N-CA-C	5.18	116.75	108.41
2	H	174	PHE	CA-C-N	5.18	125.19	119.90
2	H	174	PHE	C-N-CA	5.18	125.19	119.90
3	J	202	MET	N-CA-C	5.17	116.92	111.28
2	B	10	GLY	N-CA-C	5.16	117.16	110.45
1	L	48	ILE	N-CA-C	5.15	115.33	108.11
3	J	262	GLY	CA-C-N	5.15	131.38	121.54
3	J	262	GLY	C-N-CA	5.15	131.38	121.54
2	H	151	LYS	N-CA-C	5.13	118.11	110.52
3	J	241	GLU	N-CA-C	-5.12	104.12	110.41
3	J	256	ARG	N-CA-C	5.10	117.93	109.46
2	H	96	CYS	N-CA-C	-5.09	100.60	108.90
1	L	118	PHE	CA-C-N	5.07	125.60	120.38
1	L	118	PHE	C-N-CA	5.07	125.60	120.38
3	J	163	ASN	N-CA-C	-5.05	106.42	112.58
1	A	75	ILE	CB-CA-C	-5.03	104.92	111.81
2	H	99	GLY	N-CA-C	5.02	118.58	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	103	TYR	Sidechain
3	I	261	ILE	Peptide

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	1647	0	1608	73	1
1	L	1647	0	1608	110	0
2	B	1641	0	1591	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1641	0	1591	104	0
3	I	1438	0	1449	94	0
3	J	1438	0	1449	107	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
All	All	9454	0	9296	547	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 29.

All (547) 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:A:115:VAL:HG21	1:A:196:VAL:HG21	1.38	1.05
1:L:1:ASP:O	1:L:2:ILE:HG13	1.59	1.03
1:L:175:LEU:HD23	1:L:176:SER:N	1.78	0.97
3:J:143:GLN:HG3	3:J:144:PRO:HD2	1.49	0.94
1:L:80:PRO:HA	1:L:106:ILE:HD13	1.50	0.94
2:H:51:ILE:HD12	2:H:58:THR:HG22	1.50	0.90
3:I:262:GLY:C	3:I:263:LYS:HG2	1.96	0.90
1:L:12:SER:HB3	1:L:107:LYS:HG3	1.53	0.90
2:B:113:GLN:H	2:B:113:GLN:HE21	1.19	0.89
3:I:254:ILE:O	3:I:256:ARG:HD3	1.75	0.87
3:J:302:LEU:HD23	3:J:305:LYS:HD2	1.53	0.87
3:I:264:HIS:HE2	3:J:241:GLU:CD	1.83	0.87
1:A:187:GLU:HA	1:A:211:ARG:NE	1.90	0.86
2:H:51:ILE:HD12	2:H:58:THR:CG2	2.05	0.85
2:B:57:GLU:OE1	3:J:197:LYS:NZ	2.11	0.84
3:J:178:LYS:HD3	3:J:180:GLU:OE2	1.81	0.81
1:L:142:ARG:HD2	1:L:173:TYR:CE2	2.15	0.81
1:L:46:LEU:HD22	1:L:47:LEU:N	1.96	0.80
1:L:193:ALA:HA	1:L:208:SER:HB3	1.62	0.80
3:J:172:GLN:OE1	3:J:202:MET:HG3	1.83	0.79
2:H:22:CYS:HB3	2:H:79:LEU:HB3	1.62	0.79
1:L:147:GLN:HB3	1:L:195:GLU:HB3	1.62	0.79
2:H:113:GLN:H	2:H:113:GLN:NE2	1.81	0.77
2:H:57:GLU:OE1	3:I:198:HIS:NE2	2.18	0.76
3:I:160:LYS:HE2	3:I:303:GLN:HG2	1.68	0.75
3:I:171:VAL:HG21	3:I:219:VAL:HG21	1.69	0.75
3:I:262:GLY:C	3:I:263:LYS:CG	2.59	0.75
3:J:239:ASP:C	3:J:239:ASP:OD1	2.26	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:76:SER:O	1:L:77:SER:HB2	1.87	0.75
3:J:162:SER:O	3:J:163:ASN:HB3	1.87	0.74
3:I:215:VAL:HG11	3:I:234:LEU:HD13	1.70	0.73
1:L:1:ASP:O	1:L:2:ILE:CG1	2.35	0.73
3:I:298:LEU:O	3:I:298:LEU:HD23	1.89	0.73
1:A:12:SER:HA	1:A:105:GLU:O	1.87	0.73
3:J:151:LEU:HD23	3:J:154:MET:HE2	1.69	0.73
2:H:35:ASN:OD1	2:H:50:MET:HB3	1.90	0.72
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.70	0.72
3:I:243:THR:HG22	3:J:205:LEU:HD22	1.71	0.71
1:L:33:LEU:HD21	1:L:88:CYS:SG	2.30	0.71
2:B:113:GLN:H	2:B:113:GLN:NE2	1.89	0.71
2:H:56:SER:O	2:H:58:THR:HG23	1.89	0.71
1:A:115:VAL:CG2	1:A:196:VAL:HG21	2.17	0.71
3:J:252:LYS:HE3	3:J:252:LYS:HA	1.73	0.71
2:H:51:ILE:HG13	2:H:52:HIS:N	2.05	0.70
3:I:302:LEU:HD23	3:I:305:LYS:HD2	1.72	0.70
1:A:22:THR:HG22	1:A:72:THR:OG1	1.92	0.69
2:B:51:ILE:HD12	2:B:58:THR:CG2	2.22	0.69
1:L:175:LEU:HD23	1:L:176:SER:H	1.55	0.69
1:L:46:LEU:HD22	1:L:47:LEU:H	1.57	0.69
1:L:20:THR:HG22	1:L:74:THR:HG23	1.75	0.68
1:L:80:PRO:HA	1:L:106:ILE:CD1	2.24	0.68
2:B:201:THR:HG23	2:B:218:LYS:HE3	1.75	0.68
3:I:160:LYS:HE2	3:I:303:GLN:HE21	1.59	0.67
2:B:203:ILE:HG12	2:B:218:LYS:CB	2.25	0.67
3:J:167:GLN:HG2	3:J:227:ARG:NH2	2.09	0.67
1:L:147:GLN:NE2	1:L:154:LEU:HD23	2.09	0.67
3:I:289:LEU:HD22	3:I:294:LYS:HG2	1.76	0.67
2:B:34:MET:HB3	2:B:79:LEU:HD22	1.77	0.67
3:J:298:LEU:HD23	3:J:298:LEU:O	1.95	0.67
1:A:98:PHE:HZ	2:B:108:PHE:HE1	1.41	0.66
3:I:223:GLU:N	3:I:223:GLU:OE2	2.29	0.66
2:H:131:PRO:HD3	2:H:217:LYS:HE2	1.78	0.66
1:L:103:LYS:H	1:L:103:LYS:HD2	1.61	0.65
2:H:34:MET:HE3	2:H:79:LEU:HD22	1.78	0.65
2:B:162:TRP:HZ2	2:B:188:SER:O	1.78	0.65
1:L:79:GLN:HB3	1:L:80:PRO:HD2	1.79	0.65
2:B:51:ILE:HB	2:B:58:THR:HG22	1.78	0.65
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.77	0.65
1:A:189:HIS:O	1:A:211:ARG:NH1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:HD21	2:B:172:HIS:CD2	2.15	0.65
2:H:186:LEU:HD12	2:H:186:LEU:C	2.21	0.64
2:B:101:TYR:CE2	3:J:198:HIS:HA	2.32	0.64
2:H:30:THR:HA	2:H:53:PRO:HB2	1.80	0.64
3:J:233:VAL:HG12	3:J:234:LEU:N	2.13	0.64
2:H:29:PHE:HB2	2:H:77:ASN:ND2	2.13	0.63
2:H:176:ALA:HA	2:H:186:LEU:HB3	1.80	0.63
2:B:131:PRO:HD3	2:B:217:LYS:HE2	1.79	0.63
1:A:6:GLN:NE2	1:A:102:THR:HG23	2.14	0.63
3:J:132:LEU:C	3:J:132:LEU:HD23	2.24	0.63
1:L:36:TYR:CD2	1:L:46:LEU:HA	2.33	0.63
2:B:29:PHE:HB2	2:B:77:ASN:ND2	2.13	0.63
1:L:149:LYS:HE2	1:L:154:LEU:HD11	1.81	0.63
3:J:150:ILE:O	3:J:154:MET:HG3	1.99	0.63
1:A:6:GLN:HE21	1:A:102:THR:HG23	1.64	0.62
1:A:151:ASP:OD2	1:A:189:HIS:HB3	1.98	0.62
1:L:36:TYR:HD2	1:L:46:LEU:HA	1.64	0.62
3:J:133:VAL:HG22	3:J:169:ALA:HB3	1.80	0.62
2:B:56:SER:O	2:B:58:THR:HG23	1.99	0.62
2:B:69:THR:HB	2:B:82:GLN:HB3	1.81	0.62
2:B:203:ILE:HG12	2:B:218:LYS:HA	1.81	0.62
2:H:20:LEU:HD22	2:H:115:THR:HG21	1.81	0.62
3:I:235:ILE:HD13	3:I:257:TYR:HB2	1.80	0.62
1:A:150:VAL:HG13	1:A:192:TYR:CE2	2.34	0.62
2:H:101:TYR:HE2	3:I:198:HIS:HA	1.64	0.62
1:L:151:ASP:OD2	1:L:189:HIS:HB3	2.00	0.61
3:I:239:ASP:OD1	3:I:239:ASP:C	2.41	0.61
1:L:182:SER:C	1:L:184:ALA:H	2.08	0.61
3:I:189:ARG:O	3:I:190:LYS:HB2	1.99	0.61
2:B:67:ARG:NH2	2:B:87:ARG:HH12	1.99	0.61
1:L:3:GLN:H	1:L:26:SER:HB2	1.65	0.61
1:L:28:THR:HA	1:L:68:GLY:O	2.01	0.60
3:I:188:LYS:HG2	3:I:189:ARG:HD2	1.83	0.60
2:B:83:MET:HE2	2:B:86:LEU:HD21	1.83	0.60
3:I:143:GLN:HG3	3:I:144:PRO:HD2	1.84	0.60
2:B:41:PRO:O	2:B:43:LYS:HG3	2.02	0.60
2:B:164:SER:H	2:B:205:ASN:HD21	1.50	0.60
1:L:124:GLN:HG2	1:L:129:THR:O	2.02	0.60
1:L:188:LYS:HB2	1:L:188:LYS:NZ	2.17	0.60
3:J:301:GLU:O	3:J:305:LYS:HG3	2.02	0.60
2:H:101:TYR:CE2	3:I:198:HIS:HA	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:20:LEU:HD12	2:H:81:LEU:HD23	1.83	0.59
2:H:113:GLN:H	2:H:113:GLN:HE21	1.50	0.59
1:L:134:CYS:HB2	1:L:148:TRP:CZ2	2.37	0.59
1:A:79:GLN:HB3	1:A:80:PRO:HD2	1.85	0.59
1:A:189:HIS:HB2	1:A:192:TYR:OH	2.03	0.59
3:J:140:MET:HA	3:J:203:LEU:HD23	1.85	0.59
2:H:94:TYR:O	2:H:115:THR:HG22	2.01	0.59
3:I:172:GLN:OE1	3:I:202:MET:HG3	2.02	0.59
2:H:145:ALA:HB2	2:H:191:THR:HG22	1.84	0.59
2:H:179:GLN:OE1	2:H:185:SER:HB2	2.01	0.59
2:B:203:ILE:HG23	2:B:217:LYS:C	2.27	0.59
1:L:182:SER:C	1:L:184:ALA:N	2.60	0.59
1:A:185:ASP:O	1:A:189:HIS:ND1	2.34	0.59
2:H:91:THR:HG23	2:H:118:THR:HA	1.85	0.59
1:A:132:VAL:HB	1:A:179:LEU:HB3	1.84	0.58
3:I:261:ILE:HG21	3:I:292:PHE:CD2	2.39	0.58
1:L:149:LYS:HA	1:L:153:ALA:O	2.02	0.58
1:L:140:TYR:HA	1:L:141:PRO:O	2.04	0.58
1:L:158:ASN:O	1:L:179:LEU:HD12	2.03	0.58
3:I:175:THR:OG1	3:I:205:LEU:HD12	2.04	0.58
1:L:34:ALA:HA	1:L:48:ILE:O	2.04	0.58
2:H:103:TYR:CE2	3:I:203:LEU:HD11	2.38	0.57
1:A:106:ILE:H	1:A:166:GLN:HE22	1.53	0.57
2:H:83:MET:HE2	2:H:86:LEU:HD21	1.87	0.57
1:A:113:PRO:HD3	1:A:198:HIS:ND1	2.20	0.57
1:L:9:SER:O	1:L:10:SER:HB3	2.05	0.57
3:I:247:ASN:HD22	3:I:247:ASN:C	2.12	0.57
1:L:186:TYR:HA	1:L:192:TYR:OH	2.05	0.57
3:I:261:ILE:HG21	3:I:292:PHE:CE2	2.40	0.56
1:L:23:CYS:HB2	1:L:35:TRP:CH2	2.40	0.56
3:J:300:THR:HG22	3:J:303:GLN:OE1	2.05	0.56
1:L:4:MET:HE2	1:L:33:LEU:HD11	1.86	0.56
2:B:87:ARG:CG	2:B:89:GLU:HG2	2.35	0.56
3:J:232:LYS:HD3	3:J:232:LYS:H	1.69	0.56
1:L:164:THR:HG22	1:L:174:SER:H	1.71	0.56
3:J:252:LYS:HA	3:J:252:LYS:CE	2.34	0.56
2:H:154:PHE:CG	2:H:155:PRO:HA	2.40	0.56
3:I:161:LEU:O	3:I:164:THR:CG2	2.54	0.56
1:A:162:SER:HB2	1:A:176:SER:HB3	1.86	0.56
2:B:101:TYR:HE2	3:J:198:HIS:HA	1.70	0.56
3:I:136:PHE:CZ	3:I:172:GLN:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:178:LEU:HD13	2:H:184:TYR:CE2	2.41	0.56
3:I:264:HIS:NE2	3:J:241:GLU:OE1	2.37	0.56
1:A:108:ARG:NH2	1:A:170:ASP:O	2.39	0.56
1:L:103:LYS:HD2	1:L:103:LYS:N	2.21	0.56
2:H:147:GLY:HA3	2:H:189:VAL:HG12	1.88	0.55
1:A:55:GLN:O	1:A:58:VAL:HG23	2.06	0.55
3:J:132:LEU:HD23	3:J:133:VAL:N	2.21	0.55
3:J:247:ASN:C	3:J:247:ASN:HD22	2.13	0.55
2:H:134:PRO:HD2	2:H:220:GLU:HG3	1.87	0.55
3:I:129:ASN:ND2	3:I:129:ASN:H	2.04	0.55
2:B:113:GLN:HE21	2:B:113:GLN:N	1.97	0.55
1:L:2:ILE:O	1:L:2:ILE:HG22	2.05	0.55
2:B:3:GLN:HE21	2:B:3:GLN:HA	1.72	0.55
3:I:280:LYS:HA	3:I:281:PRO:C	2.31	0.55
1:A:103:LYS:H	1:A:103:LYS:HD2	1.71	0.55
1:A:183:LYS:HG2	1:A:187:GLU:OE2	2.06	0.55
2:H:8:GLY:O	2:H:18:LEU:HD11	2.05	0.55
3:J:302:LEU:HA	3:J:305:LYS:HD2	1.88	0.55
2:H:51:ILE:HD11	2:H:56:SER:HA	1.88	0.55
3:I:252:LYS:HE3	3:I:252:LYS:HA	1.89	0.55
2:B:152:ASP:HB3	2:B:183:LEU:HD13	1.89	0.55
2:B:87:ARG:HG3	2:B:89:GLU:HG2	1.89	0.55
2:B:178:LEU:HD13	2:B:184:TYR:CZ	2.42	0.54
3:J:140:MET:HA	3:J:203:LEU:CD2	2.37	0.54
1:A:189:HIS:O	1:A:211:ARG:HD3	2.08	0.54
2:B:57:GLU:OE2	3:J:198:HIS:CE1	2.60	0.54
2:H:40:ALA:O	2:H:41:PRO:C	2.49	0.54
2:B:186:LEU:O	2:B:186:LEU:HD12	2.07	0.54
3:I:270:SER:O	3:I:273:THR:OG1	2.23	0.54
1:A:39:LYS:HD3	1:A:84:ALA:HB2	1.89	0.54
2:B:159:THR:OG1	2:B:207:ASN:HB3	2.08	0.54
3:I:188:LYS:HE2	3:I:189:ARG:CZ	2.37	0.54
2:B:67:ARG:NH2	2:B:87:ARG:NH1	2.56	0.54
2:B:67:ARG:HH21	2:B:87:ARG:HH12	1.55	0.54
2:B:41:PRO:HD3	2:B:91:THR:O	2.08	0.54
2:H:132:LEU:HB2	2:H:147:GLY:H	1.72	0.53
2:H:178:LEU:HD13	2:H:184:TYR:CZ	2.43	0.53
1:A:209:PHE:CD1	1:A:209:PHE:C	2.86	0.53
3:J:135:LEU:HD13	3:J:215:VAL:CG2	2.37	0.53
3:J:136:PHE:HD1	3:J:136:PHE:H	1.55	0.53
1:A:160:GLN:HB3	2:B:177:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:PRO:HD2	2:B:213:THR:HG21	1.90	0.53
3:J:151:LEU:O	3:J:155:LYS:HG3	2.08	0.53
2:B:33:TRP:CE3	2:B:50:MET:HE3	2.43	0.53
2:B:203:ILE:HG12	2:B:218:LYS:CA	2.39	0.53
3:J:164:THR:HG23	3:J:166:TYR:H	1.72	0.53
2:H:6:GLU:OE1	2:H:112:GLY:HA3	2.08	0.53
3:I:243:THR:HG22	3:J:205:LEU:CD2	2.39	0.53
1:A:154:LEU:H	1:A:154:LEU:HD12	1.74	0.53
2:B:161:SER:O	2:B:205:ASN:ND2	2.40	0.53
2:H:154:PHE:CD1	2:H:155:PRO:HA	2.44	0.53
3:I:255:ILE:CG2	3:I:285:PHE:HE2	2.21	0.53
1:L:89:GLN:HG2	1:L:90:GLN:N	2.24	0.53
2:H:57:GLU:CD	3:I:198:HIS:HE2	2.16	0.53
2:H:152:ASP:HB3	2:H:183:LEU:HD13	1.91	0.53
3:I:167:GLN:O	3:I:167:GLN:HG3	2.08	0.53
3:I:197:LYS:HZ3	3:I:198:HIS:HE2	1.58	0.52
3:J:168:PHE:N	3:J:168:PHE:CD1	2.76	0.52
3:I:189:ARG:HD2	3:I:189:ARG:N	2.23	0.52
1:A:76:SER:O	1:A:77:SER:HB2	2.08	0.52
1:A:115:VAL:HA	1:A:135:LEU:O	2.10	0.52
2:B:154:PHE:HB2	2:B:183:LEU:HD23	1.90	0.52
2:H:55:ASP:O	2:H:56:SER:HB2	2.09	0.52
2:H:196:SER:HB2	2:H:200:GLN:HG3	1.90	0.52
3:I:178:LYS:HE3	3:I:180:GLU:OE1	2.09	0.52
1:L:187:GLU:HA	1:L:211:ARG:NE	2.23	0.52
2:H:39:GLN:C	2:H:92:ALA:HB1	2.34	0.52
2:B:39:GLN:C	2:B:92:ALA:HB1	2.35	0.52
3:J:233:VAL:CG1	3:J:234:LEU:N	2.72	0.52
1:L:187:GLU:HA	1:L:211:ARG:CD	2.40	0.52
2:H:68:PHE:CE2	2:H:83:MET:HG2	2.44	0.52
2:B:33:TRP:CZ3	2:B:50:MET:HE3	2.44	0.52
1:L:184:ALA:O	1:L:188:LYS:NZ	2.42	0.52
1:A:150:VAL:O	1:A:151:ASP:HB2	2.10	0.52
2:H:72:VAL:HG22	2:H:73:ASP:N	2.25	0.52
1:A:142:ARG:HB2	1:A:173:TYR:CE1	2.45	0.52
3:J:149:LYS:HD2	3:J:292:PHE:HB3	1.92	0.52
3:J:161:LEU:O	3:J:164:THR:HG22	2.09	0.52
3:J:172:GLN:CD	3:J:202:MET:HG3	2.34	0.52
3:J:262:GLY:O	3:J:264:HIS:N	2.40	0.52
2:H:132:LEU:HB2	2:H:147:GLY:C	2.35	0.52
2:B:55:ASP:OD1	3:J:197:LYS:HE3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:139:SER:OG	3:J:142:LEU:HD23	2.09	0.52
3:I:132:LEU:HD23	3:I:133:VAL:N	2.25	0.52
3:J:247:ASN:C	3:J:247:ASN:ND2	2.68	0.52
1:L:106:ILE:H	1:L:166:GLN:HE22	1.56	0.51
3:I:161:LEU:O	3:I:164:THR:HG22	2.09	0.51
3:I:164:THR:OG1	3:I:165:SER:N	2.42	0.51
1:L:21:ILE:O	1:L:72:THR:HG23	2.10	0.51
1:L:135:LEU:C	1:L:136:LEU:HD23	2.35	0.51
1:L:193:ALA:CA	1:L:208:SER:HB3	2.35	0.51
1:L:186:TYR:C	1:L:188:LYS:H	2.16	0.51
2:H:83:MET:HE2	2:H:86:LEU:CD2	2.40	0.51
3:I:291:THR:HB	3:I:293:GLU:OE1	2.10	0.51
2:B:203:ILE:HG12	2:B:218:LYS:HB2	1.91	0.51
2:B:219:VAL:O	2:B:220:GLU:HB2	2.09	0.51
1:L:149:LYS:HE2	1:L:154:LEU:CD1	2.40	0.51
2:H:208:HIS:CD2	2:H:210:PRO:HD2	2.46	0.51
2:H:72:VAL:HG22	2:H:73:ASP:H	1.74	0.51
1:A:48:ILE:HA	1:A:53:THR:O	2.10	0.51
1:A:113:PRO:HA	1:A:139:PHE:HB3	1.93	0.51
2:B:149:LEU:HD12	2:B:187:SER:HB3	1.92	0.51
1:L:46:LEU:CD2	1:L:47:LEU:H	2.21	0.51
3:I:241:GLU:OE1	3:J:264:HIS:NE2	2.43	0.51
3:I:137:ASP:CG	3:I:139:SER:HG	2.19	0.51
2:B:51:ILE:HD12	2:B:58:THR:HG22	1.92	0.51
2:B:62:GLN:HG3	2:B:63:LYS:N	2.26	0.50
1:L:11:LEU:HD12	1:L:11:LEU:C	2.36	0.50
1:L:193:ALA:HA	1:L:208:SER:CB	2.39	0.50
3:J:188:LYS:HD3	3:J:189:ARG:HD2	1.92	0.50
1:L:201:LEU:HD13	1:L:205:VAL:HG23	1.93	0.50
3:J:188:LYS:HD3	3:J:189:ARG:CD	2.41	0.50
3:I:174:SER:HA	3:I:205:LEU:O	2.12	0.50
1:A:148:TRP:CZ3	1:A:194:CYS:HB2	2.46	0.50
1:L:150:VAL:HG22	1:L:192:TYR:CE2	2.46	0.50
3:J:149:LYS:HE2	3:J:293:GLU:HG3	1.92	0.50
1:L:150:VAL:HB	1:L:155:GLN:OE1	2.12	0.50
2:B:176:ALA:HA	2:B:186:LEU:HB3	1.93	0.50
1:L:21:ILE:HD12	1:L:73:LEU:HD23	1.94	0.50
3:I:162:SER:O	3:I:163:ASN:HB3	2.11	0.50
2:B:163:ASN:O	2:B:166:ALA:HB3	2.12	0.50
3:I:235:ILE:CD1	3:I:257:TYR:HB2	2.41	0.49
3:J:175:THR:HA	3:J:207:ASN:ND2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:38:GLN:HE21	1:L:44:PRO:HD3	1.77	0.49
2:H:60:TYR:CE2	2:H:70:ILE:HG13	2.47	0.49
3:J:262:GLY:C	3:J:264:HIS:H	2.20	0.49
3:J:302:LEU:HD23	3:J:305:LYS:CD	2.34	0.49
1:L:175:LEU:HD23	1:L:176:SER:C	2.37	0.49
2:B:178:LEU:HD13	2:B:184:TYR:CE2	2.47	0.49
1:L:170:ASP:O	1:L:171:SER:HB2	2.12	0.49
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.48	0.49
2:H:158:VAL:CG2	2:H:186:LEU:HD21	2.43	0.49
3:I:188:LYS:HE2	3:I:189:ARG:NH1	2.28	0.49
2:B:8:GLY:O	2:B:18:LEU:HD11	2.13	0.49
3:I:151:LEU:HA	3:I:154:MET:HE2	1.95	0.49
3:I:263:LYS:NZ	3:I:291:THR:HG22	2.28	0.49
2:B:57:GLU:CD	3:J:198:HIS:HE2	2.21	0.49
2:H:57:GLU:CD	3:I:198:HIS:NE2	2.72	0.48
3:I:135:LEU:HD11	3:I:211:ALA:HB1	1.95	0.48
3:I:160:LYS:CE	3:I:303:GLN:HG2	2.40	0.48
1:A:186:TYR:C	1:A:188:LYS:H	2.22	0.48
2:B:40:ALA:O	2:B:41:PRO:C	2.55	0.48
3:J:184:SER:O	3:J:187:VAL:HG22	2.12	0.48
3:I:171:VAL:CG2	3:I:219:VAL:HG21	2.41	0.48
1:A:13:ALA:HB3	1:A:78:LEU:HD22	1.96	0.48
1:L:12:SER:HA	1:L:105:GLU:O	2.14	0.48
1:A:110:VAL:HG13	1:A:140:TYR:O	2.13	0.48
2:B:209:LYS:HB2	2:B:210:PRO:HD3	1.95	0.48
1:L:140:TYR:HA	1:L:141:PRO:C	2.38	0.48
3:I:129:ASN:HB2	3:I:227:ARG:CZ	2.44	0.48
2:H:36:TRP:CE2	2:H:81:LEU:HB2	2.49	0.48
2:H:203:ILE:HG23	2:H:217:LYS:C	2.39	0.48
2:B:55:ASP:OD1	3:J:194:ALA:HB1	2.14	0.48
2:B:203:ILE:HA	2:B:218:LYS:HA	1.96	0.48
1:L:38:GLN:HE22	2:H:39:GLN:HE22	1.61	0.47
2:H:132:LEU:HB2	2:H:147:GLY:CA	2.45	0.47
3:J:160:LYS:HE2	3:J:303:GLN:HG2	1.96	0.47
1:L:146:VAL:HA	1:L:195:GLU:O	2.15	0.47
3:I:160:LYS:HB2	3:I:160:LYS:NZ	2.29	0.47
1:A:140:TYR:HA	1:A:141:PRO:O	2.15	0.47
1:A:170:ASP:O	1:A:171:SER:HB2	2.14	0.47
3:J:256:ARG:NH2	3:J:278:ALA:O	2.47	0.47
3:I:129:ASN:HB2	3:I:227:ARG:NH2	2.30	0.47
3:I:180:GLU:O	3:I:181:PHE:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:GLU:OE1	3:J:198:HIS:NE2	2.36	0.47
3:J:196:LEU:O	3:J:199:VAL:HG23	2.14	0.47
1:A:6:GLN:NE2	1:A:86:TYR:O	2.40	0.47
3:J:234:LEU:HD23	3:J:256:ARG:HG2	1.95	0.47
2:H:179:GLN:HG2	2:H:183:LEU:O	2.15	0.47
1:A:106:ILE:HG22	1:A:107:LYS:N	2.27	0.47
1:L:61:ARG:HG2	1:L:61:ARG:NH2	2.30	0.47
1:L:161:GLU:HB3	1:L:175:LEU:HD21	1.95	0.47
2:H:91:THR:HG23	2:H:117:VAL:O	2.14	0.47
3:I:151:LEU:O	3:I:155:LYS:HG3	2.15	0.47
1:A:164:THR:HG23	1:A:165:GLU:O	2.15	0.47
2:B:186:LEU:HD12	2:B:186:LEU:C	2.40	0.47
2:B:156:GLU:HB3	2:B:157:PRO:HA	1.97	0.47
1:L:131:SER:HA	1:L:179:LEU:O	2.15	0.47
2:H:162:TRP:CZ3	2:H:204:CYS:HB3	2.50	0.47
2:B:51:ILE:HG13	2:B:52:HIS:N	2.30	0.47
2:B:196:SER:HB2	2:B:200:GLN:CG	2.45	0.47
3:J:162:SER:O	3:J:163:ASN:CB	2.55	0.47
3:J:261:ILE:HD13	3:J:295:LEU:HD11	1.97	0.47
1:L:83:PHE:O	1:L:84:ALA:HB2	2.15	0.47
3:I:258:ILE:HG22	3:I:278:ALA:HB2	1.95	0.47
2:B:61:ASN:O	2:B:62:GLN:C	2.57	0.47
3:J:236:ILE:O	3:J:259:ILE:N	2.47	0.47
1:L:27:LYS:O	1:L:28:THR:C	2.58	0.46
2:H:51:ILE:HG13	2:H:52:HIS:H	1.80	0.46
2:H:153:TYR:C	2:H:153:TYR:CD1	2.93	0.46
2:H:192:VAL:HB	2:H:193:PRO:CD	2.45	0.46
3:J:158:MET:HE1	3:J:181:PHE:HZ	1.80	0.46
2:B:61:ASN:O	2:B:63:LYS:N	2.48	0.46
3:J:261:ILE:O	3:J:262:GLY:O	2.34	0.46
1:L:64:GLY:O	1:L:65:SER:HB3	2.16	0.46
1:A:186:TYR:CZ	1:A:211:ARG:HG3	2.50	0.46
1:L:150:VAL:HG22	1:L:192:TYR:CD2	2.51	0.46
1:L:33:LEU:HD12	1:L:90:GLN:HA	1.98	0.46
1:A:11:LEU:C	1:A:11:LEU:HD12	2.40	0.46
2:B:113:GLN:NE2	2:B:113:GLN:N	2.60	0.46
3:J:189:ARG:NH2	3:J:189:ARG:HG3	2.31	0.46
2:H:51:ILE:HD11	2:H:56:SER:CA	2.46	0.46
1:A:158:ASN:HD21	1:A:179:LEU:HD11	1.81	0.46
2:H:132:LEU:HB2	2:H:147:GLY:N	2.31	0.46
3:I:243:THR:CG2	3:J:205:LEU:HD22	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:ARG:HD2	2:B:89:GLU:HG2	1.96	0.46
3:J:158:MET:HE1	3:J:181:PHE:CZ	2.51	0.46
1:A:11:LEU:HD21	1:A:19:VAL:HG13	1.98	0.46
3:J:133:VAL:CG1	3:J:134:PHE:N	2.78	0.46
2:H:69:THR:HB	2:H:82:GLN:HB3	1.98	0.45
2:H:203:ILE:HG23	2:H:218:LYS:CA	2.46	0.45
1:L:188:LYS:HB2	1:L:188:LYS:HZ2	1.79	0.45
2:H:63:LYS:HE3	2:H:63:LYS:HB2	1.84	0.45
2:H:98:ARG:NH1	2:H:110:TYR:CD2	2.84	0.45
2:H:55:ASP:O	2:H:56:SER:CB	2.65	0.45
2:H:60:TYR:HE2	2:H:70:ILE:HG13	1.82	0.45
3:I:252:LYS:HA	3:I:252:LYS:CE	2.46	0.45
3:J:271:GLN:NE2	3:J:288:ILE:HD13	2.32	0.45
1:L:107:LYS:HA	1:L:140:TYR:OH	2.16	0.45
1:L:190:LYS:HA	1:L:211:ARG:HB2	1.98	0.45
3:J:236:ILE:HB	3:J:258:ILE:HA	1.98	0.45
2:H:196:SER:HB2	2:H:200:GLN:CG	2.46	0.45
2:B:27:TYR:CE1	2:B:98:ARG:HD2	2.51	0.45
2:B:144:ALA:CB	2:B:197:LEU:HD11	2.46	0.45
1:A:89:GLN:HG2	1:A:90:GLN:N	2.31	0.45
2:B:87:ARG:CD	2:B:89:GLU:HG2	2.47	0.45
3:J:132:LEU:C	3:J:132:LEU:CD2	2.89	0.45
1:L:151:ASP:OD1	1:L:191:VAL:HB	2.17	0.45
2:H:127:PRO:HB2	2:H:150:VAL:HG13	1.99	0.45
3:J:296:LYS:O	3:J:299:PHE:HB3	2.17	0.45
2:B:57:GLU:HB2	3:J:197:LYS:HE2	1.97	0.45
2:B:176:ALA:HB2	2:B:186:LEU:HD23	1.99	0.45
2:B:179:GLN:HG3	2:B:181:SER:OG	2.17	0.45
1:A:199:GLN:O	1:A:199:GLN:HG2	2.17	0.45
3:J:164:THR:HG23	3:J:166:TYR:HB2	1.99	0.45
3:J:252:LYS:HE3	3:J:252:LYS:CA	2.46	0.45
1:L:125:LEU:C	1:L:127:SER:H	2.25	0.44
2:H:57:GLU:OE2	3:I:198:HIS:CE1	2.70	0.44
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.99	0.44
2:H:127:PRO:HB3	2:H:153:TYR:HB3	2.00	0.44
2:B:67:ARG:NE	2:B:87:ARG:HH22	2.15	0.44
3:J:135:LEU:HD13	3:J:215:VAL:HG21	2.00	0.44
1:L:30:SER:HB3	1:L:31:LYS:H	1.52	0.44
1:L:164:THR:HG22	1:L:174:SER:N	2.31	0.44
1:A:76:SER:O	1:A:77:SER:CB	2.65	0.44
3:J:271:GLN:HG2	3:J:288:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:29:ILE:O	1:L:30:SER:C	2.58	0.44
1:L:76:SER:O	1:L:77:SER:CB	2.63	0.44
1:A:11:LEU:HD21	1:A:19:VAL:CG1	2.47	0.44
1:A:89:GLN:HB2	1:A:98:PHE:CD2	2.53	0.44
2:B:195:SER:C	2:B:197:LEU:H	2.26	0.44
2:H:68:PHE:CE2	2:H:83:MET:HE3	2.52	0.44
3:J:133:VAL:HG12	3:J:134:PHE:N	2.32	0.44
1:L:19:VAL:HG12	1:L:20:THR:N	2.33	0.44
2:H:67:ARG:HD2	2:H:84:ASN:O	2.18	0.44
3:J:234:LEU:HD23	3:J:256:ARG:CG	2.48	0.44
1:L:61:ARG:HG2	1:L:61:ARG:HH21	1.83	0.44
3:I:129:ASN:ND2	3:I:129:ASN:N	2.66	0.44
3:I:255:ILE:HG23	3:I:285:PHE:CE2	2.53	0.44
1:A:98:PHE:CZ	2:B:108:PHE:HE1	2.30	0.44
3:J:129:ASN:N	3:J:129:ASN:HD22	2.15	0.44
1:L:27:LYS:O	1:L:28:THR:O	2.36	0.44
2:H:33:TRP:CZ3	2:H:50:MET:HE3	2.53	0.44
3:I:129:ASN:N	3:I:129:ASN:HD22	2.16	0.44
1:A:39:LYS:NZ	1:A:81:GLU:O	2.47	0.44
3:J:188:LYS:O	3:J:188:LYS:HG2	2.18	0.44
2:H:22:CYS:N	2:H:79:LEU:O	2.50	0.43
3:I:204:LEU:HB3	3:I:205:LEU:H	1.59	0.43
1:A:115:VAL:HG22	1:A:136:LEU:CD2	2.48	0.43
3:J:213:ASN:HD21	3:J:248:ILE:HA	1.83	0.43
3:J:288:ILE:O	3:J:288:ILE:HG13	2.18	0.43
2:H:87:ARG:HG3	2:H:89:GLU:CG	2.49	0.43
3:I:136:PHE:H	3:I:136:PHE:HD1	1.64	0.43
3:I:306:ILE:C	3:I:306:ILE:HD12	2.43	0.43
3:J:136:PHE:CZ	3:J:172:GLN:HB2	2.53	0.43
3:J:274:LEU:O	3:J:275:HIS:C	2.60	0.43
1:L:2:ILE:HG21	1:L:90:GLN:HG2	2.00	0.43
1:L:133:VAL:HG22	1:L:178:THR:HG23	2.00	0.43
2:H:3:GLN:HE21	2:H:3:GLN:HB3	1.55	0.43
2:H:98:ARG:NH1	2:H:110:TYR:HD2	2.17	0.43
2:H:132:LEU:HB2	2:H:147:GLY:O	2.18	0.43
3:I:263:LYS:HZ3	3:I:291:THR:HG22	1.83	0.43
1:A:38:GLN:HE21	1:A:44:PRO:HD3	1.83	0.43
3:J:291:THR:HB	3:J:293:GLU:OE1	2.17	0.43
1:L:100:GLN:HE21	1:L:100:GLN:HB3	1.60	0.43
3:I:298:LEU:HD23	3:I:298:LEU:C	2.41	0.43
1:L:108:ARG:HH21	1:L:172:THR:HG23	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:175:LEU:HD23	1:L:176:SER:CA	2.46	0.43
2:H:203:ILE:HG23	2:H:218:LYS:N	2.33	0.43
2:B:190:VAL:O	2:B:190:VAL:HG13	2.18	0.43
2:H:211:SER:O	2:H:212:ASN:C	2.61	0.43
3:I:164:THR:HG23	3:I:166:TYR:HB2	1.99	0.43
2:B:36:TRP:CE2	2:B:81:LEU:HB2	2.54	0.43
2:B:68:PHE:CE2	2:B:83:MET:HG2	2.54	0.43
2:H:181:SER:OG	2:H:183:LEU:HD12	2.18	0.43
1:A:148:TRP:CE2	1:A:179:LEU:HB2	2.53	0.43
3:J:239:ASP:OD1	3:J:239:ASP:N	2.50	0.43
1:L:103:LYS:H	1:L:103:LYS:CD	2.29	0.43
2:H:162:TRP:HZ2	2:H:188:SER:O	2.02	0.43
3:I:234:LEU:HD23	3:I:256:ARG:HG2	2.00	0.43
1:A:154:LEU:HD12	1:A:154:LEU:N	2.32	0.43
3:J:233:VAL:CG1	3:J:234:LEU:H	2.31	0.43
1:L:3:GLN:N	1:L:26:SER:HB2	2.33	0.43
1:A:40:PRO:C	1:A:42:LYS:H	2.26	0.43
3:J:224:LEU:HD12	3:J:224:LEU:N	2.34	0.43
1:L:46:LEU:CD2	1:L:47:LEU:N	2.73	0.42
2:B:116:LEU:HD23	2:B:117:VAL:N	2.34	0.42
1:L:111:ALA:HB3	1:L:140:TYR:N	2.34	0.42
1:A:8:PRO:O	1:A:102:THR:HB	2.18	0.42
2:B:29:PHE:C	2:B:31:GLY:H	2.27	0.42
2:B:131:PRO:HD3	2:B:217:LYS:CE	2.47	0.42
1:L:184:ALA:O	1:L:188:LYS:HB2	2.19	0.42
2:H:161:SER:OG	2:H:205:ASN:ND2	2.47	0.42
3:J:142:LEU:HD22	3:J:239:ASP:OD2	2.20	0.42
3:I:190:LYS:O	3:I:192:PRO:HD3	2.20	0.42
3:I:206:THR:O	3:I:208:THR:N	2.52	0.42
1:A:94:TYR:HB3	1:A:95:PRO:HA	2.02	0.42
2:B:5:VAL:HG12	2:B:6:GLU:N	2.34	0.42
2:B:30:THR:HA	2:B:53:PRO:HB2	2.01	0.42
2:B:205:ASN:OD1	2:B:216:ASP:OD1	2.37	0.42
2:H:101:TYR:O	3:I:200:LYS:NZ	2.43	0.42
3:I:194:ALA:O	3:I:197:LYS:HG2	2.18	0.42
2:B:170:GLY:O	2:B:190:VAL:HA	2.19	0.42
3:J:171:VAL:HG21	3:J:219:VAL:HG21	2.02	0.42
3:J:188:LYS:HE2	3:J:189:ARG:CZ	2.49	0.42
3:J:233:VAL:HG12	3:J:234:LEU:H	1.83	0.42
1:A:103:LYS:HD2	1:A:103:LYS:N	2.34	0.42
3:J:285:PHE:N	3:J:285:PHE:CD1	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:32:TYR:HD2	1:L:91:HIS:CE1	2.37	0.42
2:H:57:GLU:OE2	3:I:198:HIS:NE2	2.52	0.42
2:H:64:PHE:O	2:H:68:PHE:HB2	2.19	0.42
3:J:253:ASP:N	3:J:253:ASP:OD2	2.51	0.42
3:I:158:MET:HG2	3:I:168:PHE:CD1	2.55	0.42
1:A:147:GLN:HB3	1:A:195:GLU:HB3	2.01	0.42
2:B:195:SER:O	2:B:197:LEU:N	2.53	0.42
3:J:298:LEU:HD23	3:J:298:LEU:C	2.44	0.42
2:B:97:ALA:HB1	2:B:108:PHE:HB3	2.02	0.42
3:I:294:LYS:HA	3:I:297:ASP:OD1	2.19	0.42
3:J:143:GLN:CG	3:J:144:PRO:HD2	2.35	0.42
3:J:178:LYS:HB2	3:J:202:MET:CE	2.50	0.41
1:L:102:THR:O	1:L:102:THR:OG1	2.37	0.41
2:H:73:ASP:OD2	2:H:75:SER:HB3	2.19	0.41
3:I:151:LEU:HD23	3:I:154:MET:CE	2.50	0.41
1:A:28:THR:O	1:A:28:THR:HG23	2.20	0.41
3:J:299:PHE:O	3:J:302:LEU:N	2.51	0.41
1:L:6:GLN:HG3	1:L:23:CYS:SG	2.60	0.41
1:L:79:GLN:HB2	1:L:82:ASP:OD1	2.19	0.41
1:L:192:TYR:O	1:L:208:SER:HB2	2.19	0.41
2:H:186:LEU:C	2:H:186:LEU:CD1	2.88	0.41
3:I:184:SER:HA	3:I:187:VAL:HG12	2.02	0.41
1:A:36:TYR:HA	1:A:45:LYS:O	2.21	0.41
3:J:177:TYR:OH	3:J:210:GLY:HA3	2.19	0.41
1:L:162:SER:HB3	2:H:174:PHE:HB3	2.03	0.41
2:H:6:GLU:HG3	2:H:113:GLN:OE1	2.21	0.41
2:H:51:ILE:CD1	2:H:58:THR:HG22	2.35	0.41
1:A:55:GLN:O	1:A:56:SER:C	2.62	0.41
3:J:182:ASP:HB2	3:J:224:LEU:HB3	2.01	0.41
3:J:222:GLU:HA	3:J:226:ALA:H	1.84	0.41
1:L:124:GLN:HB2	2:H:130:PHE:CD2	2.56	0.41
1:L:158:ASN:OD1	1:L:158:ASN:N	2.54	0.41
3:I:158:MET:HG2	3:I:168:PHE:CE1	2.56	0.41
1:A:140:TYR:HA	1:A:141:PRO:C	2.45	0.41
3:J:196:LEU:C	3:J:199:VAL:HG23	2.46	0.41
3:J:281:PRO:O	3:J:282:ALA:C	2.64	0.41
2:H:4:LEU:HD23	2:H:4:LEU:HA	1.92	0.41
3:I:129:ASN:H	3:I:129:ASN:HD22	1.68	0.41
1:L:39:LYS:O	1:L:40:PRO:C	2.62	0.41
1:L:43:ALA:HB2	2:H:112:GLY:O	2.20	0.41
1:L:80:PRO:HG2	1:L:81:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:199:THR:HG23	2:H:200:GLN:HG2	2.03	0.41
3:I:160:LYS:CE	3:I:303:GLN:HE21	2.32	0.41
3:I:160:LYS:CD	3:I:303:GLN:HG2	2.51	0.41
3:I:241:GLU:CD	3:J:264:HIS:HE2	2.29	0.41
3:I:243:THR:HG22	3:I:243:THR:O	2.21	0.41
1:A:46:LEU:HG	2:B:108:PHE:O	2.21	0.41
1:A:90:GLN:OE1	1:A:90:GLN:O	2.39	0.41
2:B:108:PHE:HB2	2:B:111:TRP:NE1	2.36	0.41
2:B:177:VAL:O	2:B:177:VAL:HG13	2.20	0.41
3:J:206:THR:O	3:J:206:THR:HG22	2.21	0.41
1:L:2:ILE:HD11	1:L:93:GLU:OE2	2.21	0.41
1:L:11:LEU:HD12	1:L:11:LEU:O	2.20	0.41
1:L:134:CYS:HB2	1:L:148:TRP:CH2	2.55	0.41
2:H:87:ARG:HG3	2:H:89:GLU:HG3	2.03	0.41
2:B:154:PHE:HA	2:B:155:PRO:HA	1.76	0.41
1:A:30:SER:HB3	1:A:31:LYS:H	1.36	0.40
3:J:174:SER:OG	3:J:205:LEU:O	2.34	0.40
1:L:12:SER:HB2	1:L:107:LYS:HZ3	1.86	0.40
1:L:175:LEU:CD2	1:L:176:SER:N	2.66	0.40
2:H:129:VAL:CG2	2:H:206:VAL:HG21	2.52	0.40
2:H:196:SER:O	2:H:199:THR:HG22	2.22	0.40
3:I:239:ASP:OD1	3:I:240:GLY:N	2.55	0.40
3:I:273:THR:O	3:I:276:LYS:HG2	2.22	0.40
2:H:68:PHE:CD2	2:H:83:MET:HG2	2.57	0.40
2:H:129:VAL:HG21	2:H:206:VAL:HG21	2.04	0.40
1:A:24:ARG:HE	1:A:24:ARG:HB2	1.29	0.40
1:A:174:SER:C	2:B:174:PHE:HE2	2.30	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:A:1:ASP:OD2	1:A:1:ASP:OD2[9_554]	2.06	0.14

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	212/214 (99%)	193 (91%)	17 (8%)	2 (1%)	14	46
1	L	212/214 (99%)	182 (86%)	22 (10%)	8 (4%)	2	21
2	B	211/220 (96%)	183 (87%)	22 (10%)	6 (3%)	4	26
2	H	211/220 (96%)	191 (90%)	16 (8%)	4 (2%)	6	33
3	I	177/181 (98%)	157 (89%)	16 (9%)	4 (2%)	5	30
3	J	177/181 (98%)	158 (89%)	16 (9%)	3 (2%)	7	35
All	All	1200/1230 (98%)	1064 (89%)	109 (9%)	27 (2%)	5	30

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	2	ILE
1	L	28	THR
2	H	152	ASP
2	B	152	ASP
2	B	196	SER
3	J	262	GLY
3	J	263	LYS
1	L	77	SER
3	I	207	ASN
1	A	77	SER
2	B	62	GLN
1	L	10	SER
1	L	78	LEU
2	H	104	GLY
1	L	82	ASP
3	I	174	SER
3	I	181	PHE
3	I	267	THR
1	A	41	GLY
2	B	28	SER
2	B	41	PRO
3	J	190	LYS
2	H	41	PRO
2	B	210	PRO
1	L	29	ILE
1	L	204	PRO

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Mol	Chain	Res	Type
2	H	155	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	189/189 (100%)	171 (90%)	18 (10%)	8	32
1	L	189/189 (100%)	175 (93%)	14 (7%)	13	39
2	B	182/186 (98%)	176 (97%)	6 (3%)	33	58
2	H	182/186 (98%)	167 (92%)	15 (8%)	10	36
3	I	159/161 (99%)	147 (92%)	12 (8%)	12	39
3	J	159/161 (99%)	143 (90%)	16 (10%)	7	30
All	All	1060/1072 (99%)	979 (92%)	81 (8%)	12	39

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	2	ILE
1	L	3	GLN
1	L	30	SER
1	L	44	PRO
1	L	46	LEU
1	L	88	CYS
1	L	100	GLN
1	L	117	ILE
1	L	136	LEU
1	L	145	LYS
1	L	159	SER
1	L	170	ASP
1	L	188	LYS
2	H	3	GLN
2	H	6	GLU
2	H	19	ARG

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Mol	Chain	Res	Type
2	H	25	SER
2	H	51	ILE
2	H	53	PRO
2	H	106	THR
2	H	113	GLN
2	H	116	LEU
2	H	118	THR
2	H	128	SER
2	H	155	PRO
2	H	157	PRO
2	H	177	VAL
2	H	179	GLN
3	I	129	ASN
3	I	130	VAL
3	I	140	MET
3	I	142	LEU
3	I	143	GLN
3	I	160	LYS
3	I	189	ARG
3	I	243	THR
3	I	247	ASN
3	I	252	LYS
3	I	263	LYS
3	I	288	ILE
1	A	2	ILE
1	A	8	PRO
1	A	10	SER
1	A	23	CYS
1	A	26	SER
1	A	30	SER
1	A	46	LEU
1	A	60	SER
1	A	81	GLU
1	A	88	CYS
1	A	100	GLN
1	A	125	LEU
1	A	137	ASN
1	A	145	LYS
1	A	164	THR
1	A	170	ASP
1	A	175	LEU
1	A	188	LYS

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Mol	Chain	Res	Type
2	B	3	GLN
2	B	6	GLU
2	B	51	ILE
2	B	100	ILE
2	B	113	GLN
2	B	199	THR
3	J	129	ASN
3	J	130	VAL
3	J	141	SER
3	J	143	GLN
3	J	160	LYS
3	J	177	TYR
3	J	178	LYS
3	J	189	ARG
3	J	243	THR
3	J	245	SER
3	J	247	ASN
3	J	252	LYS
3	J	263	LYS
3	J	272	GLU
3	J	279	SER
3	J	288	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	89	GLN
1	L	100	GLN
1	L	124	GLN
1	L	137	ASN
1	L	152	ASN
1	L	166	GLN
1	L	198	HIS
2	H	3	GLN
2	H	39	GLN
2	H	77	ASN
2	H	172	HIS
2	H	200	GLN
2	H	205	ASN
3	I	129	ASN
3	I	143	GLN
3	I	167	GLN

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Mol	Chain	Res	Type
3	I	247	ASN
3	I	266	GLN
1	A	3	GLN
1	A	6	GLN
1	A	38	GLN
1	A	89	GLN
1	A	100	GLN
1	A	137	ASN
1	A	138	ASN
1	A	147	GLN
1	A	152	ASN
1	A	155	GLN
1	A	166	GLN
1	A	199	GLN
2	B	3	GLN
2	B	39	GLN
2	B	77	ASN
2	B	113	GLN
2	B	205	ASN
3	J	129	ASN
3	J	143	GLN
3	J	207	ASN
3	J	247	ASN
3	J	266	GLN
3	J	271	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	214/214 (100%)	0.12	3 (1%) 73 46	54, 102, 134, 155	0
1	L	214/214 (100%)	-0.08	2 (0%) 81 56	72, 101, 129, 144	0
2	B	215/220 (97%)	0.09	4 (1%) 66 39	52, 104, 132, 159	0
2	H	215/220 (97%)	-0.15	0 100 100	53, 95, 121, 136	0
3	I	179/181 (98%)	-0.13	3 (1%) 69 41	26, 91, 122, 137	0
3	J	179/181 (98%)	-0.10	1 (0%) 85 64	26, 86, 118, 137	0
All	All	1216/1230 (98%)	-0.04	13 (1%) 78 52	26, 96, 130, 159	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ASP	4.2
2	B	170	GLY	2.9
3	I	306	ILE	2.8
2	B	219	VAL	2.7
1	A	128	GLY	2.5
1	A	214	CYS	2.4
1	L	1	ASP	2.4
2	B	47	TRP	2.3
3	I	266	GLN	2.2
1	L	187	GLU	2.2
3	J	269	GLU	2.2
2	B	210	PRO	2.2
3	I	305	LYS	2.1

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($\text{\AA}^2$)	Q<0.9
4	ZN	I	1	1/1	0.96	0.12	99,99,99,99	0
4	ZN	J	2	1/1	0.97	0.10	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.