Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:28 am BST

PDB ID	:	3EOB
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 following versions of software and data (see references ⓘ) were used in the production of this report:

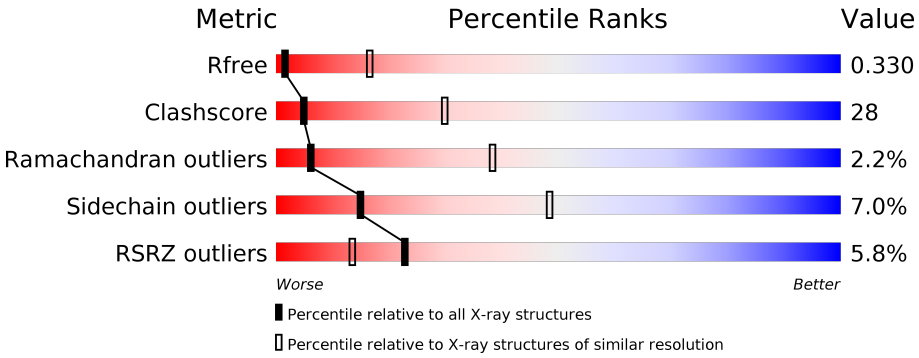
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	214	11% 55% 41% ·
1	L	214	2% 50% 43% 7%
2	B	220	15% 56% 37% 5% ·
2	H	220	2% 49% 44% 5% ·
3	I	181	2% 51% 40% 8% ·
3	J	181	2% 47% 46% 6% ·

2 Entry composition

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 (three-letter code: ZN) (formula: Zn).

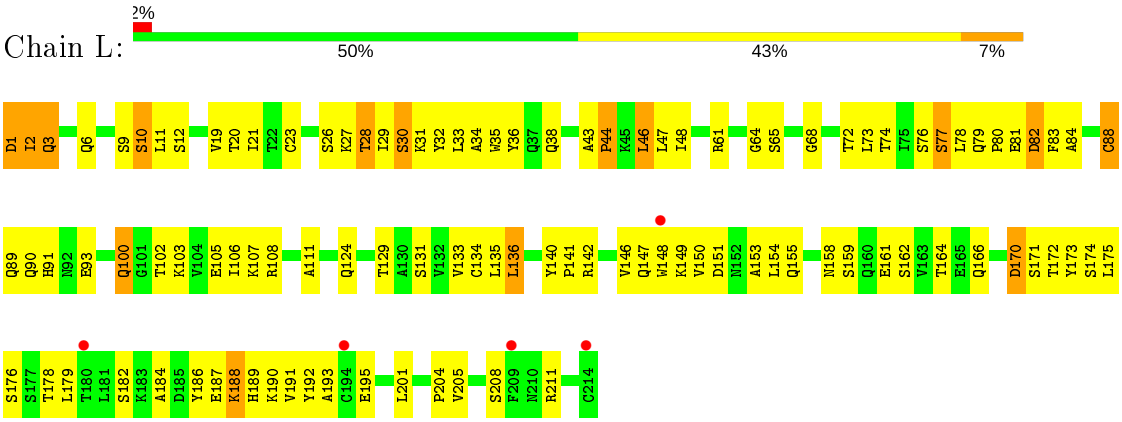
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

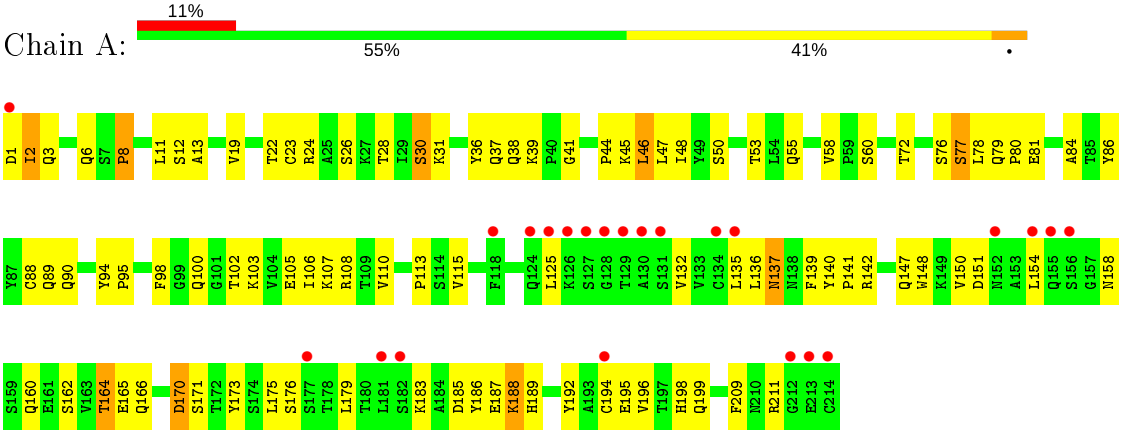
- Molecule 1: Efalizumab Fab fragment, light chain

Chain L:



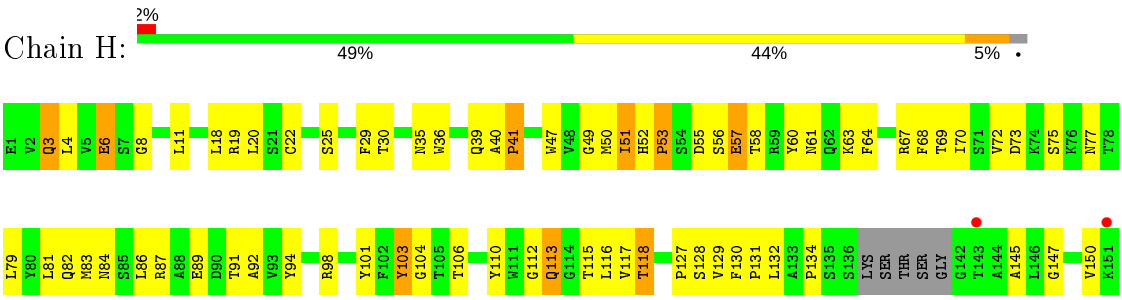
- Molecule 1: Efalizumab Fab fragment, light chain

Chain A:

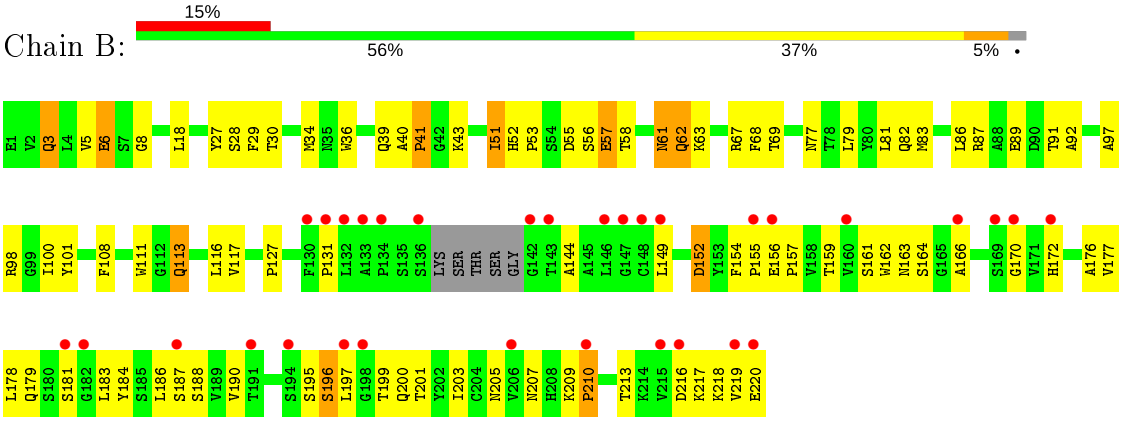


- Molecule 2: Efalizumab Fab fragment, heavy chain

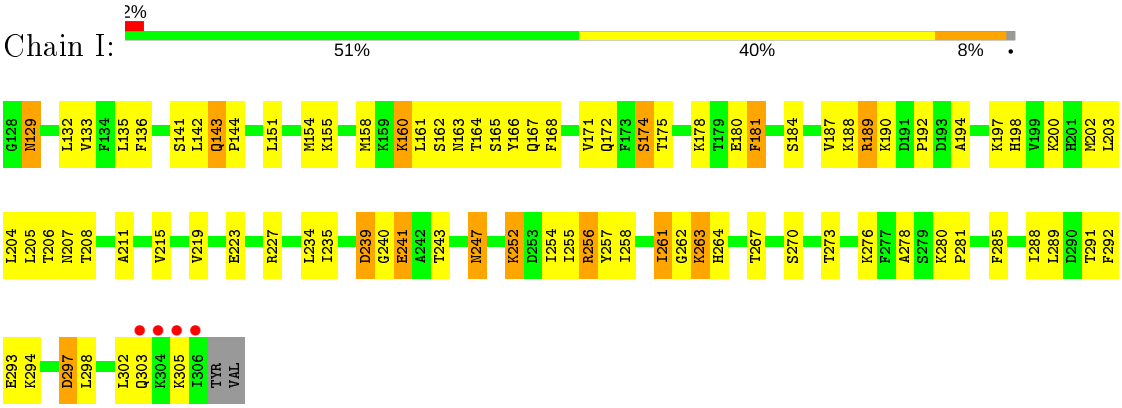
Chain H:



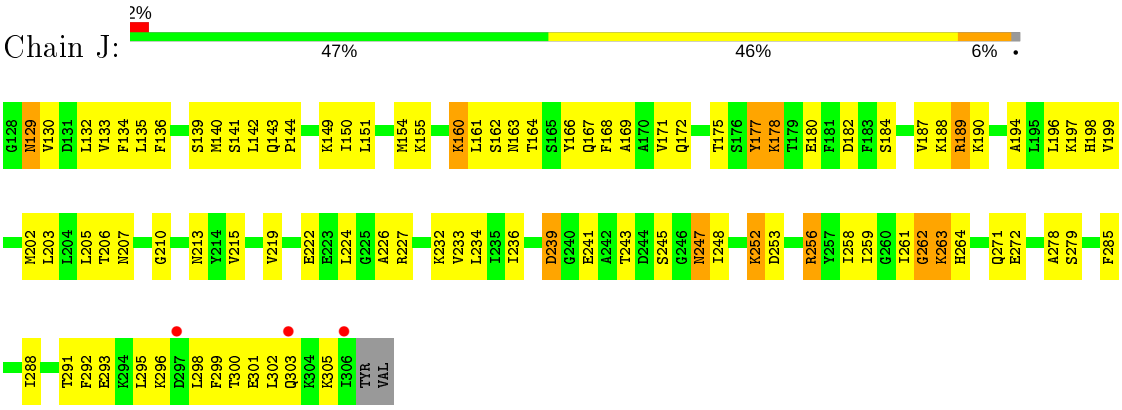
• Molecule 2: Efalizumab Fab fragment, heavy chain



• Molecule 3: Integrin alpha-L



• Molecule 3: Integrin alpha-L



4 Data and refinement statistics (i)

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 47.84 – 3.60	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-3.60) 97.8 (47.84-3.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [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 , 85.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.48	0/1682	0.73	2/2280 (0.1%)
1	L	0.45	0/1682	0.73	0/2280
2	B	0.54	2/1684 (0.1%)	0.75	1/2291 (0.0%)
2	H	0.58	2/1684 (0.1%)	0.78	2/2291 (0.1%)
3	I	0.63	3/1465 (0.2%)	0.83	4/1970 (0.2%)
3	J	0.60	0/1465	0.85	1/1970 (0.1%)
All	All	0.55	7/9662 (0.1%)	0.78	10/13082 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1
3	I	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	241	GLU	CG-CD	7.92	1.63	1.51
3	I	141	SER	CA-CB	-7.37	1.41	1.52
2	H	57	GLU	CB-CG	7.21	1.65	1.52
2	H	57	GLU	CG-CD	6.78	1.62	1.51
2	B	57	GLU	CB-CG	6.61	1.64	1.52
2	B	57	GLU	CG-CD	6.13	1.61	1.51
3	I	241	GLU	CB-CG	5.46	1.62	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	239	ASP	CB-CG-OD1	-9.41	109.83	118.30
3	I	141	SER	CA-CB-OG	-8.05	89.47	111.20
3	I	239	ASP	CB-CG-OD1	-7.86	111.22	118.30
2	H	61	ASN	N-CA-C	-6.77	92.71	111.00
2	B	61	ASN	N-CA-C	-6.25	94.13	111.00
3	I	239	ASP	CB-CG-OD2	5.38	123.15	118.30
2	H	11	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	2	ILE	CG1-CB-CG2	-5.20	99.96	111.40
3	I	141	SER	N-CA-CB	-5.13	102.81	110.50
1	A	2	ILE	N-CA-C	-5.05	97.37	111.00

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1647	0	1608	69	1
1	L	1647	0	1608	105	0
2	B	1641	0	1591	88	0
2	H	1641	0	1591	99	0
3	I	1438	0	1449	90	0
3	J	1438	0	1449	97	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
All	All	9454	0	9296	516	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 28.

All (516) 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
1:L:12:SER:HB3	1:L:107:LYS:HG3	1.53	0.90
2:B:113:GLN:HE21	2:B:113:GLN:H	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
1:A:187:GLU:HA	1:A:211:ARG:NE	1.90	0.86
3:I:262:GLY:C	3:I:263:LYS:HG2	1.96	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:I:264:HIS:HE2	3:J:241:GLU:CD	1.83	0.82
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:NE2	2:H:113:GLN:H	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
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
1:A:12:SER:HA	1:A:105:GLU:O	1.87	0.73
3:I:298:LEU:HD23	3:I:298:LEU:O	1.89	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:NE2	2:B:113:GLN:H	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:HA	3:J:252:LYS:HE3	1.73	0.71
2:H:51:ILE:HG13	2:H:52:HIS:N	2.05	0.70
3:I:262:GLY:C	3:I:263:LYS:CG	2.59	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:239:ASP:OD1	3:J:239:ASP:C	2.26	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
3:I:289:LEU:HD22	3:I:294:LYS:HG2	1.76	0.67
1:L:147:GLN:NE2	1:L:154:LEU:HD23	2.09	0.67
2:B:34:MET:HB3	2:B:79:LEU:HD22	1.77	0.67
3:J:298:LEU:O	3:J:298:LEU:HD23	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:HD2	1:L:103:LYS:H	1.61	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
1:A:137:ASN:HD21	2:B:172:HIS:CD2	2.15	0.65
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:B:131:PRO:HD3	2:B:217:LYS:HE2	1.79	0.63
2:H:176:ALA:HA	2:H:186:LEU:HB3	1.80	0.63
2:H:29:PHE:HB2	2:H:77:ASN:ND2	2.13	0.63
1:A:6:GLN:NE2	1:A:102:THR:HG23	2.14	0.63
2:B:29:PHE:HB2	2:B:77:ASN:ND2	2.13	0.63
1:L:36:TYR:CD2	1:L:46:LEU:HA	2.33	0.63
3:J:150:ILE:O	3:J:154:MET:HG3	1.99	0.63
1:L:149:LYS:HE2	1:L:154:LEU:HD11	1.81	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
3:J:133:VAL:HG22	3:J:169:ALA:HB3	1.80	0.62
1:L:36:TYR:HD2	1:L:46:LEU:HA	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:ILE:HG12	2:B:218:LYS:HA	1.81	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: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
3:I:189:ARG:O	3:I:190:LYS:HB2	1.99	0.61
1:L:151:ASP:OD2	1:L:189:HIS:HB3	2.00	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
3:I:143:GLN:HG3	3:I:144:PRO:HD2	1.84	0.60
2:B:164:SER:H	2:B:205:ASN:HD21	1.50	0.60
2:B:41:PRO:O	2:B:43:LYS:HG3	2.02	0.60
3:J:301:GLU:O	3:J:305:LYS:HG3	2.02	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
2:H:101:TYR:CE2	3:I:198:HIS:HA	2.37	0.60
2:H:113:GLN:H	2:H:113:GLN:HE21	1.50	0.59
2:H:20:LEU:HD12	2:H:81:LEU:HD23	1.83	0.59
1:A:79:GLN:HB3	1:A:80:PRO:HD2	1.85	0.59
1:L:134:CYS:HB2	1:L:148:TRP:CZ2	2.37	0.59
1:A:189:HIS:HB2	1:A:192:TYR:OH	2.03	0.59
2:H:186:LEU:C	2:H:186:LEU:HD12	2.21	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
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
3:J:132:LEU:HD23	3:J:132:LEU:C	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:239:ASP:OD1	3:I:239:ASP:C	2.41	0.57
1:L:182:SER:C	1:L:184:ALA:H	2.08	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
3:J:300:THR:HG22	3:J:303:GLN:OE1	2.05	0.56
1:L:23:CYS:HB2	1:L:35:TRP:CH2	2.40	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
3:J:252:LYS:HA	3:J:252:LYS:CE	2.34	0.56
1:L:164:THR:HG22	1:L:174:SER:H	1.71	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
1:A:108:ARG:NH2	1:A:170:ASP:O	2.39	0.56
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:L:103:LYS:N	1:L:103:LYS:HD2	2.21	0.56
1:A:55:GLN:O	1:A:58:VAL:HG23	2.06	0.55
2:H:147:GLY:HA3	2:H:189:VAL:HG12	1.88	0.55
3:J:132:LEU:HD23	3:J:133:VAL:N	2.21	0.55
2:B:113:GLN:HE21	2:B:113:GLN:N	1.97	0.55
2:H:134:PRO:HD2	2:H:220:GLU:HG3	1.87	0.55
3:I:129:ASN:H	3:I:129:ASN:ND2	2.04	0.55
2:B:3:GLN:HA	2:B:3:GLN:HE21	1.72	0.55
1:L:2:ILE:HG22	1:L:2:ILE:O	2.05	0.55
1:A:103:LYS:HD2	1:A:103:LYS:H	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:B:152:ASP:HB3	2:B:183:LEU:HD13	1.89	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: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
2:B:203:ILE:HG23	2:B:217:LYS:C	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:182:SER:C	1:L:184:ALA:N	2.60	0.54
2:B:57:GLU:OE2	3:J:198:HIS:CE1	2.60	0.54
2:B:186:LEU:HD12	2:B:186:LEU:O	2.07	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:HH21	2:B:87:ARG:HH12	1.55	0.54
2:B:67:ARG:NH2	2:B:87:ARG:NH1	2.56	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
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
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: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
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
3:I:243:THR:HG22	3:J:205:LEU:CD2	2.39	0.53
3:I:270:SER:O	3:I:273:THR:OG1	2.23	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
2:H:152:ASP:HB3	2:H:183:LEU:HD13	1.91	0.53
3:I:167:GLN:HG3	3:I:167:GLN:O	2.08	0.53
1:L:89:GLN:HG2	1:L:90:GLN:N	2.24	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
1:A:115:VAL:HA	1:A:135:LEU:O	2.10	0.52
1:A:76:SER:O	1:A:77:SER:HB2	2.08	0.52
2:B:154:PHE:HB2	2:B:183:LEU:HD23	1.90	0.52
3:I:189:ARG:N	3:I:189:ARG:HD2	2.23	0.52
2:H:196:SER:HB2	2:H:200:GLN:HG3	1.90	0.52
2:H:55:ASP:O	2:H:56:SER:HB2	2.09	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
1:L:188:LYS:HB2	1:L:188:LYS:HZ3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:247:ASN:C	3:I:247:ASN:HD22	2.12	0.52
3:J:233:VAL:CG1	3:J:234:LEU:N	2.72	0.52
2:H:68:PHE:CE2	2:H:83:MET:HG2	2.44	0.52
1:L:187:GLU:HA	1:L:211:ARG:CD	2.40	0.52
1:A:150:VAL:O	1:A:151:ASP:HB2	2.10	0.52
1:L:184:ALA:O	1:L:188:LYS:NZ	2.42	0.52
1:A:142:ARG:HB2	1:A:173:TYR:CE1	2.45	0.52
2:H:72:VAL:HG22	2:H:73:ASP:N	2.25	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:262:GLY:O	3:J:264:HIS:N	2.40	0.52
3:J:139:SER:OG	3:J:142:LEU:HD23	2.09	0.52
2:B:55:ASP:OD1	3:J:197:LYS:HE3	2.09	0.52
3:I:132:LEU:HD23	3:I:133:VAL:N	2.25	0.52
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:106:ILE:H	1:L:166:GLN:HE22	1.56	0.51
1:L:193:ALA:CA	1:L:208:SER:HB3	2.35	0.51
1:L:21:ILE:O	1:L:72:THR:HG23	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
3:I:291:THR:HB	3:I:293:GLU:OE1	2.10	0.51
2:H:208:HIS:CD2	2:H:210:PRO:HD2	2.46	0.51
1:L:149:LYS:HE2	1:L:154:LEU:CD1	2.40	0.51
2:H:72:VAL:HG22	2:H:73:ASP:H	1.74	0.51
1:A:113:PRO:HA	1:A:139:PHE:HB3	1.93	0.51
1:A:48:ILE:HA	1:A:53:THR:O	2.10	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:J:247:ASN:C	3:J:247:ASN:HD22	2.13	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
3:I:280:LYS:HA	3:I:281:PRO:C	2.31	0.50
3:J:188:LYS:HD3	3:J:189:ARG:HD2	1.92	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:CD	2.41	0.50
1:L:201:LEU:HD13	1:L:205:VAL:HG23	1.93	0.50
1:A:148:TRP:CZ3	1:A:194:CYS:HB2	2.46	0.50
3:I:174:SER:HA	3:I:205:LEU:O	2.12	0.50
3:J:149:LYS:HE2	3:J:293:GLU:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:150:VAL:HG22	1:L:192:TYR:CE2	2.46	0.50
2:H:83:MET:HE3	2:H:94:TYR:CZ	2.46	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
2:B:163:ASN:O	2:B:166:ALA:HB3	2.12	0.50
3:I:162:SER:O	3:I:163:ASN:HB3	2.11	0.50
1:L:21:ILE:HD12	1:L:73:LEU:HD23	1.94	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
2:H:40:ALA:O	2:H:41:PRO:C	2.49	0.49
1:L:170:ASP:O	1:L:171:SER:HB2	2.12	0.49
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:302:LEU:HD23	3:J:305:LYS:CD	2.34	0.49
2:B:178:LEU:HD13	2:B:184:TYR:CE2	2.47	0.49
2:H:158:VAL:CG2	2:H:186:LEU:HD21	2.43	0.49
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.48	0.49
3:I:188:LYS:HE2	3:I:189:ARG:NH1	2.28	0.49
1:A:209:PHE:CD1	1:A:209:PHE:C	2.86	0.49
2:B:8:GLY:O	2:B:18:LEU:HD11	2.13	0.49
3:I:263:LYS:NZ	3:I:291:THR:HG22	2.28	0.49
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
3:J:184:SER:O	3:J:187:VAL:HG22	2.12	0.48
1:A:13:ALA:HB3	1:A:78:LEU:HD22	1.96	0.48
3:I:171:VAL:CG2	3:I:219:VAL:HG21	2.41	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
2:H:57:GLU:CD	3:I:198:HIS:HE2	2.16	0.48
3:I:129:ASN:HB2	3:I:227:ARG:CZ	2.44	0.48
2:B:203:ILE:HA	2:B:218:LYS:HA	1.96	0.48
2:B:55:ASP:OD1	3:J:194:ALA:HB1	2.14	0.48
2:H:36:TRP:CE2	2:H:81:LEU:HB2	2.49	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: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
2:B:39:GLN:C	2:B:92:ALA:HB1	2.35	0.47
2:H:39:GLN:C	2:H:92:ALA:HB1	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:160:LYS:HB2	3:I:160:LYS:NZ	2.29	0.47
3:J:256:ARG:NH2	3:J:278:ALA:O	2.47	0.47
1:L:146:VAL:HA	1:L:195:GLU:O	2.15	0.47
2:B:57:GLU:OE1	3:J:198:HIS:NE2	2.36	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
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
1:A:106:ILE:HG22	1:A:107:LYS:N	2.27	0.47
2:H:179:GLN:HG2	2:H:183:LEU:O	2.15	0.47
3:I:151:LEU:HA	3:I:154:MET:HE2	1.97	0.47
1:L:186:TYR:C	1:L:188:LYS:H	2.16	0.47
2:H:132:LEU:HB2	2:H:147:GLY:C	2.35	0.47
3:I:151:LEU:O	3:I:155:LYS:HG3	2.15	0.47
3:J:172:GLN:CD	3:J:202:MET:HG3	2.34	0.47
1:L:61:ARG:NH2	1:L:61:ARG:HG2	2.30	0.47
1:A:164:THR:HG23	1:A:165:GLU:O	2.15	0.47
2:H:91:THR:HG23	2:H:117:VAL:O	2.14	0.47
3:J:247:ASN:C	3:J:247:ASN:ND2	2.68	0.47
1:L:135:LEU:C	1:L:136:LEU:HD23	2.35	0.47
1:L:161:GLU:HB3	1:L:175:LEU:HD21	1.95	0.47
2:B:156:GLU:HB3	2:B:157:PRO:HA	1.97	0.47
2:B:196:SER:HB2	2:B:200:GLN:CG	2.45	0.47
2:B:51:ILE:HG13	2:B:52:HIS:N	2.30	0.47
2:H:162:TRP:CZ3	2:H:204:CYS:HB3	2.50	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:131:SER:HA	1:L:179:LEU:O	2.15	0.47
3:I:258:ILE:HG22	3:I:278:ALA:HB2	1.95	0.47
3:J:236:ILE:O	3:J:259:ILE:N	2.47	0.47
1:L:83:PHE:O	1:L:84:ALA:HB2	2.15	0.47
2:H:192:VAL:HB	2:H:193:PRO:CD	2.45	0.46
2:H:51:ILE:HG13	2:H:52:HIS:H	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
2:B:113:GLN:NE2	2:B:113:GLN:N	2.60	0.46
3:J:189:ARG:HG3	3:J:189:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:33:LEU:HD12	1:L:90:GLN:HA	1.98	0.46
1:A:158:ASN:HD21	1:A:179:LEU:HD11	1.81	0.46
2:H:51:ILE:HD11	2:H:56:SER:CA	2.46	0.46
2:B:87:ARG:HD2	2:B:89:GLU:HG2	1.96	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
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
1:L:11:LEU:HD12	1:L:11:LEU:C	2.36	0.46
2:H:203:ILE:HG23	2:H:218:LYS:CA	2.46	0.45
2:H:69:THR:HB	2:H:82:GLN:HB3	1.98	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:CE	3:I:252:LYS:HA	2.46	0.45
3:J:271:GLN:NE2	3:J:288:ILE:HD13	2.32	0.45
3:J:236:ILE:HB	3:J:258:ILE:HA	1.98	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
2:B:144:ALA:CB	2:B:197:LEU:HD11	2.46	0.45
2:B:27:TYR:CE1	2:B:98:ARG:HD2	2.51	0.45
2:H:196:SER:HB2	2:H:200:GLN:CG	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
2:H:127:PRO:HB2	2:H:150:VAL:HG13	1.99	0.45
1:L:151:ASP:OD1	1:L:191:VAL:HB	2.17	0.45
3:J:296:LYS:O	3:J:299:PHE:HB3	2.17	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
2:B:57:GLU:HB2	3:J:197:LYS:HE2	1.97	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:CA	3:J:252:LYS:HE3	2.46	0.45
3:J:262:GLY:C	3:J:264:HIS:H	2.20	0.45
2:B:40:ALA:O	2:B:41:PRO:C	2.55	0.44
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.99	0.44
2:H:57:GLU:OE2	3:I:198:HIS:CE1	2.70	0.44
1:L:175:LEU:HD23	1:L:176:SER:C	2.37	0.44
2:B:67:ARG:NE	2:B:87:ARG:HH22	2.15	0.44
2:H:127:PRO:HB3	2:H:153:TYR:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:135:LEU:HD13	3:J:215:VAL:HG21	2.00	0.44
1:L:164:THR:HG22	1:L:174:SER:N	2.31	0.44
1:L:30:SER:HB3	1:L:31:LYS:H	1.52	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
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
1:L:76:SER:O	1:L:77:SER:CB	2.63	0.44
3:J:133:VAL:HG12	3:J:134:PHE:N	2.32	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:19:VAL:HG12	1:L:20:THR:N	2.33	0.44
1:A:98:PHE:CZ	2:B:108:PHE:HE1	2.30	0.44
3:I:129:ASN:ND2	3:I:129:ASN:N	2.66	0.44
2:H:57:GLU:CD	3:I:198:HIS:NE2	2.72	0.44
3:I:255:ILE:HG23	3:I:285:PHE:CE2	2.53	0.44
3:J:129:ASN:N	3:J:129:ASN:HD22	2.15	0.44
1:L:61:ARG:HH21	1:L:61:ARG:HG2	1.83	0.44
1:A:39:LYS:NZ	1:A:81:GLU:O	2.47	0.44
3:I:129:ASN:HD22	3:I:129:ASN:N	2.16	0.44
3:J:188:LYS:O	3:J:188:LYS:HG2	2.18	0.44
1:L:27:LYS:O	1:L:28:THR:O	2.36	0.44
1:A:115:VAL:HG22	1:A:136:LEU:CD2	2.48	0.43
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
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:HD1	3:I:136:PHE:H	1.64	0.43
3:J:136:PHE:CZ	3:J:172:GLN:HB2	2.53	0.43
1:A:38:GLN:HE21	1:A:44:PRO:HD3	1.83	0.43
2:H:132:LEU:HB2	2:H:147:GLY:O	2.18	0.43
2:H:3:GLN:HB3	2:H:3:GLN:HE21	1.55	0.43
2:H:98:ARG:NH1	2:H:110:TYR:HD2	2.17	0.43
3:I:263:LYS:HZ3	3:I:291:THR:HG22	1.83	0.43
3:J:291:THR:HB	3:J:293:GLU:OE1	2.17	0.43
1:L:133:VAL:HG22	1:L:178:THR:HG23	2.00	0.43
1:L:2:ILE:HG21	1:L:90:GLN:HG2	2.00	0.43
2:B:61:ASN:O	2:B:62:GLN:C	2.57	0.43
1:L:100:GLN:HE21	1:L:100:GLN:HB3	1.60	0.43
2:B:190:VAL:O	2:B:190:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:203:ILE:HG23	2:H:218:LYS:N	2.33	0.43
1:L:108:ARG:HH21	1:L:172:THR:HG23	1.84	0.43
1:L:175:LEU:HD23	1:L:176:SER:CA	2.46	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
3:I:164:THR:HG23	3:I:166:TYR:HB2	1.99	0.43
1:A:148:TRP:CE2	1:A:179:LEU:HB2	2.53	0.43
2:H:181:SER:OG	2:H:183:LEU:HD12	2.18	0.43
2:H:203:ILE:HG23	2:H:217:LYS:C	2.39	0.43
3:J:239:ASP:OD1	3:J:239:ASP:N	2.50	0.43
1:L:140:TYR:HA	1:L:141:PRO:C	2.38	0.43
1:A:154:LEU:HD12	1:A:154:LEU:N	2.32	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
3:J:233:VAL:CG1	3:J:234:LEU:H	2.31	0.43
1:L:103:LYS:CD	1:L:103:LYS:H	2.29	0.43
3:J:224:LEU:HD12	3:J:224:LEU:N	2.34	0.43
1:L:3:GLN:N	1:L:26:SER:HB2	2.33	0.43
2:B:116:LEU:HD23	2:B:117:VAL:N	2.34	0.42
1:L:46:LEU:CD2	1:L:47:LEU:N	2.73	0.42
1:A:8:PRO:O	1:A:102:THR:HB	2.18	0.42
2:B:131:PRO:HD3	2:B:217:LYS:CE	2.47	0.42
1:L:111:ALA:HB3	1:L:140:TYR:N	2.34	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
1:L:184:ALA:O	1:L:188:LYS:HB2	2.19	0.42
1:A:94:TYR:HB3	1:A:95:PRO:HA	2.02	0.42
2:B:186:LEU:HD12	2:B:186:LEU:C	2.40	0.42
2:B:205:ASN:OD1	2:B:216:ASP:OD1	2.37	0.42
2:B:30:THR:HA	2:B:53:PRO:HB2	2.01	0.42
2:B:5:VAL:HG12	2:B:6:GLU:N	2.34	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:186:TYR:C	1:A:188:LYS:H	2.22	0.42
2:B:170:GLY:O	2:B:190:VAL:HA	2.19	0.42
3:I:194:ALA:O	3:I:197:LYS:HG2	2.18	0.42
3:J:188:LYS:HE2	3:J:189:ARG:CZ	2.49	0.42
3:J:171:VAL:HG21	3:J:219:VAL:HG21	2.02	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
2:H:186:LEU:C	2:H:186:LEU:CD1	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:285:PHE:N	3:J:285:PHE:CD1	2.86	0.42
1:L:102:THR:OG1	1:L:102:THR:O	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
1:L:32:TYR:HD2	1:L:91:HIS:CE1	2.37	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:I:158:MET:HG2	3:I:168:PHE:CD1	2.55	0.42
2:B:97:ALA:HB1	2:B:108:PHE:HB3	2.02	0.42
2:H:153:TYR:CD1	2:H:153:TYR:C	2.93	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
1:L:27:LYS:O	1:L:28:THR:C	2.58	0.42
3:J:178:LYS:HB2	3:J:202:MET:CE	2.50	0.41
1:A:28:THR:HG23	1:A:28:THR:O	2.20	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
3:J:299:PHE:O	3:J:302:LEU:N	2.51	0.41
1:L:192:TYR:O	1:L:208:SER:HB2	2.19	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:A:36:TYR:HA	1:A:45:LYS:O	2.21	0.41
3:I:184:SER:HA	3:I:187:VAL:HG12	2.02	0.41
3:J:177:TYR:OH	3:J:210:GLY:HA3	2.19	0.41
1:A:11:LEU:HD12	1:A:11:LEU:C	2.40	0.41
2:H:6:GLU:HG3	2:H:113:GLN:OE1	2.21	0.41
1:L:162:SER:HB3	2:H:174:PHE:HB3	2.03	0.41
2:H:51:ILE:CD1	2:H:58:THR:HG22	2.35	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
3:I:158:MET:HG2	3:I:168:PHE:CE1	2.56	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
2:B:159:THR:HG1	2:B:207:ASN:HB3	1.85	0.41
2:H:4:LEU:HA	2:H:4:LEU:HD23	1.92	0.41
3:I:129:ASN:HD22	3:I:129:ASN:H	1.68	0.41
2:B:108:PHE:HB2	2:B:111:TRP:NE1	2.36	0.41
1:A:46:LEU:HG	2:B:108:PHE:O	2.21	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)
1:A:90:GLN:O	1:A:90:GLN:OE1	2.39	0.41
2:B:177:VAL:O	2:B:177:VAL:HG13	2.20	0.41
2:H:199:THR:HG23	2:H:200:GLN:HG2	2.03	0.41
3:I:243:THR:O	3:I:243:THR:HG22	2.21	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:J:206:THR:HG22	3:J:206:THR:O	2.21	0.41
2:B:154:PHE:HA	2:B:155:PRO:HA	1.76	0.41
2:H:101:TYR:O	3:I:200:LYS:NZ	2.43	0.41
2:H:87:ARG:HG3	2:H:89:GLU:HG3	2.03	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
1:L:2:ILE:HD11	1:L:93:GLU:OE2	2.21	0.41
1:A:30:SER:HB3	1:A:31:LYS:H	1.36	0.40
2:H:129:VAL:CG2	2:H:206:VAL:HG21	2.52	0.40
1:L:175:LEU:CD2	1:L:176:SER:N	2.66	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
3:J:132:LEU:C	3:J:132:LEU:CD2	2.89	0.40
2:H:68:PHE:CD2	2:H:83:MET:HG2	2.57	0.40
1:A:24:ARG:HE	1:A:24:ARG:HB2	1.29	0.40
2:H:129:VAL:HG21	2:H:206:VAL:HG21	2.04	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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	212/214 (99%)	193 (91%)	17 (8%)	2 (1%)	17 57
1	L	212/214 (99%)	182 (86%)	22 (10%)	8 (4%)	3 27
2	B	211/220 (96%)	183 (87%)	22 (10%)	6 (3%)	5 34
2	H	211/220 (96%)	191 (90%)	16 (8%)	4 (2%)	8 42
3	I	177/181 (98%)	157 (89%)	16 (9%)	4 (2%)	6 38
3	J	177/181 (98%)	158 (89%)	16 (9%)	3 (2%)	9 45
All	All	1200/1230 (98%)	1064 (89%)	109 (9%)	27 (2%)	6 38

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
2	H	155	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	189/189 (100%)	172 (91%)	17 (9%)	9 39
1	L	189/189 (100%)	178 (94%)	11 (6%)	20 55
2	B	182/186 (98%)	176 (97%)	6 (3%)	38 69
2	H	182/186 (98%)	168 (92%)	14 (8%)	13 45
3	I	159/161 (99%)	148 (93%)	11 (7%)	15 49
3	J	159/161 (99%)	144 (91%)	15 (9%)	8 38
All	All	1060/1072 (99%)	986 (93%)	74 (7%)	15 48

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
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	136	LEU
1	L	159	SER
1	L	170	ASP
1	L	188	LYS
2	H	3	GLN
2	H	6	GLU
2	H	19	ARG
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

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Mol	Chain	Res	Type
2	H	155	PRO
2	H	157	PRO
2	H	177	VAL
3	I	129	ASN
3	I	142	LEU
3	I	143	GLN
3	I	160	LYS
3	I	189	ARG
3	I	247	ASN
3	I	252	LYS
3	I	256	ARG
3	I	263	LYS
3	I	288	ILE
3	I	297	ASP
1	A	2	ILE
1	A	3	GLN
1	A	8	PRO
1	A	23	CYS
1	A	26	SER
1	A	30	SER
1	A	46	LEU
1	A	50	SER
1	A	60	SER
1	A	88	CYS
1	A	100	GLN
1	A	125	LEU
1	A	137	ASN
1	A	164	THR
1	A	170	ASP
1	A	175	LEU
1	A	188	LYS
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	160	LYS
3	J	177	TYR

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Mol	Chain	Res	Type
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	256	ARG
3	J	263	LYS
3	J	272	GLU
3	J	279	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	100	GLN
1	L	137	ASN
1	L	152	ASN
1	L	166	GLN
1	L	199	GLN
2	H	3	GLN
2	H	39	GLN
2	H	77	ASN
2	H	172	HIS
3	I	129	ASN
3	I	143	GLN
3	I	167	GLN
3	I	247	ASN
3	I	266	GLN
1	A	3	GLN
1	A	38	GLN
1	A	89	GLN
1	A	100	GLN
1	A	137	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

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Mol	Chain	Res	Type
2	B	205	ASN
3	J	129	ASN
3	J	143	GLN
3	J	247	ASN
3	J	266	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 carbohydrates 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

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, 95^{th} 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%)	0.56	23 (10%) 6 3	54, 102, 134, 155	0
1	L	214/214 (100%)	0.15	5 (2%) 60 44	72, 101, 129, 144	0
2	B	215/220 (97%)	0.67	32 (14%) 2 1	52, 104, 132, 159	0
2	H	215/220 (97%)	0.15	4 (1%) 66 51	53, 95, 121, 136	0
3	I	179/181 (98%)	0.12	4 (2%) 62 45	26, 91, 122, 137	0
3	J	179/181 (98%)	0.08	3 (1%) 70 55	26, 86, 118, 137	0
All	All	1216/1230 (98%)	0.30	71 (5%) 23 13	26, 96, 130, 159	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	306	ILE	8.9
3	I	304	LYS	7.9
1	A	129	THR	5.6
1	A	214	CYS	4.9
2	B	142	GLY	4.8
1	A	181	LEU	4.6
2	B	134	PRO	4.4
2	B	182	GLY	4.4
2	B	132	LEU	4.3
1	A	128	GLY	4.2
2	B	155	PRO	4.1
3	I	303	GLN	4.0
1	A	194	CYS	3.6
1	A	1	ASP	3.6
1	A	134	CYS	3.5
3	I	305	LYS	3.5
2	H	197	LEU	3.5
2	B	220	GLU	3.5
1	A	182	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	L	214	CYS	3.3
2	B	147	GLY	3.3
2	B	194	SER	3.3
1	A	156	SER	3.2
1	A	213	GLU	3.2
2	B	210	PRO	3.2
2	B	215	VAL	3.1
1	A	155	GLN	3.1
1	L	209	PHE	3.1
2	B	191	THR	3.1
1	A	125	LEU	3.1
2	B	219	VAL	3.0
2	B	170	GLY	3.0
2	B	148	CYS	3.0
2	B	133	ALA	3.0
1	A	127	SER	3.0
2	B	166	ALA	2.9
2	B	131	PRO	2.8
1	L	148	TRP	2.8
3	J	303	GLN	2.8
2	B	149	LEU	2.8
2	B	206	VAL	2.7
2	B	136	SER	2.7
1	A	124	GLN	2.7
1	A	154	LEU	2.7
2	B	187	SER	2.7
2	B	169	SER	2.7
1	A	212	GLY	2.6
2	B	181	SER	2.6
1	A	135	LEU	2.6
2	B	146	LEU	2.6
2	B	172	HIS	2.6
2	B	160	VAL	2.5
2	B	130	PHE	2.5
2	B	216	ASP	2.5
1	A	131	SER	2.5
2	B	198	GLY	2.5
1	A	152	ASN	2.4
2	H	202	TYR	2.3
1	A	130	ALA	2.3
1	L	180	THR	2.2
1	A	126	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	143	THR	2.2
2	H	151	LYS	2.2
3	J	306	ILE	2.2
2	H	143	THR	2.2
2	B	197	LEU	2.1
1	A	177	SER	2.1
1	L	194	CYS	2.1
1	A	118	PHE	2.0
2	B	156	GLU	2.0
3	J	297	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
4	ZN	I	1	1/1	0.84	0.28	99,99,99,99	0
4	ZN	J	2	1/1	0.97	0.25	99,99,99,99	0

6.5 Other polymers (i)

There are no such residues in this entry.