Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:58 AM GMT

PDB ID	:	2JIX
Title	:	Crystal structure of ABT-007 FAB fragment with the soluble domain of EPO receptor
Authors	:	Liu, Z.; Stoll, V.S.; DeVries, P.; Jakob, C.G.; Xie, N.; Simmer, R.L.; Lacy, S.E.; Egan, D.A.; Harlan, J.E.; Lesniewski, R.R.; Reilly, E.B.
Deposited on	:	2007-07-02
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

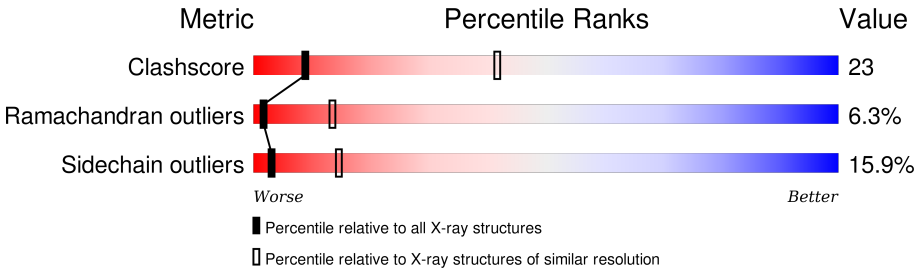
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.20 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))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	58% 35% 7%
1	G	214	54% 40% 7%
1	L	214	62% 30% 7%
2	B	225	46% 38% 11%
2	C	225	50% 30% 13%
2	E	225	53% 33% 8%
3	D	217	46% 41% 12%

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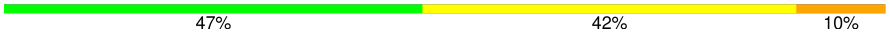
Mol	Chain	Length	Quality of chain
3	F	217	
3	H	217	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14781 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 ABT-007 FAB FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1642	1023	281	333	5			
1	G	214	Total	C	N	O	S	0	0	0
			1642	1023	281	333	5			
1	L	214	Total	C	N	O	S	0	0	0
			1642	1023	281	333	5			

- Molecule 2 is a protein called ERYTHROPOIETIN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	1
			1680	1065	297	311	7			
2	C	215	Total	C	N	O	S	0	0	1
			1665	1056	295	307	7			
2	E	217	Total	C	N	O	S	0	0	1
			1680	1065	297	311	7			

- Molecule 3 is a protein called ABT-007 FAB FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	217	Total	C	N	O	S	0	0	1
			1607	1015	268	320	4			
3	F	217	Total	C	N	O	S	0	0	1
			1607	1015	268	320	4			
3	H	217	Total	C	N	O	S	0	0	0
			1616	1021	269	322	4			

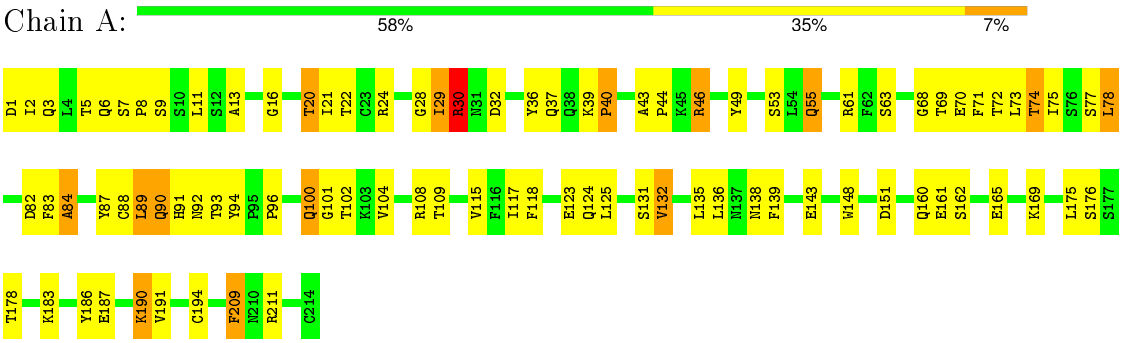
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

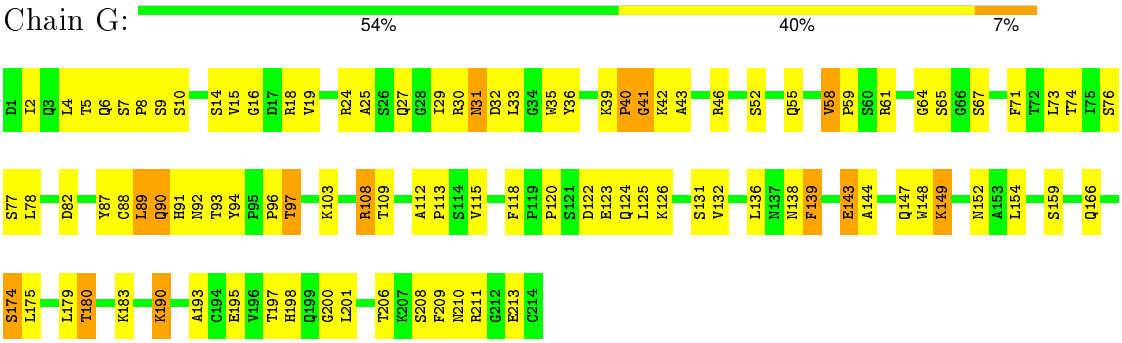
- Molecule 1: ABT-007 FAB FRAGMENT

Chain A:



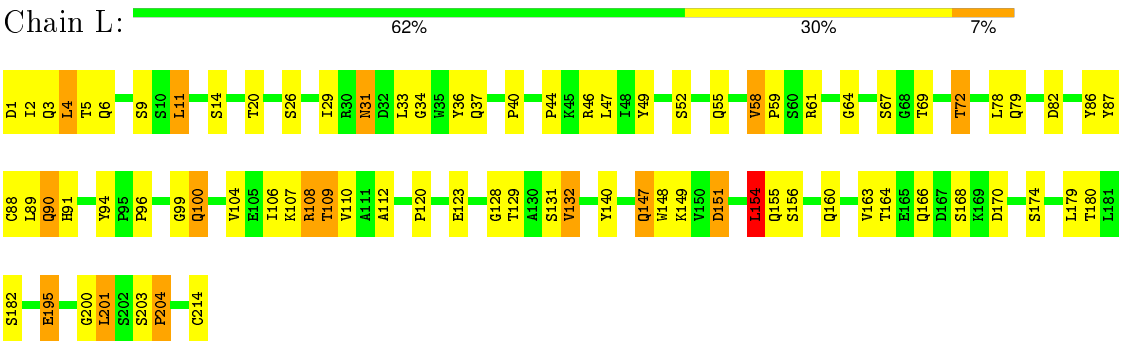
- Molecule 1: ABT-007 FAB FRAGMENT

Chain G:



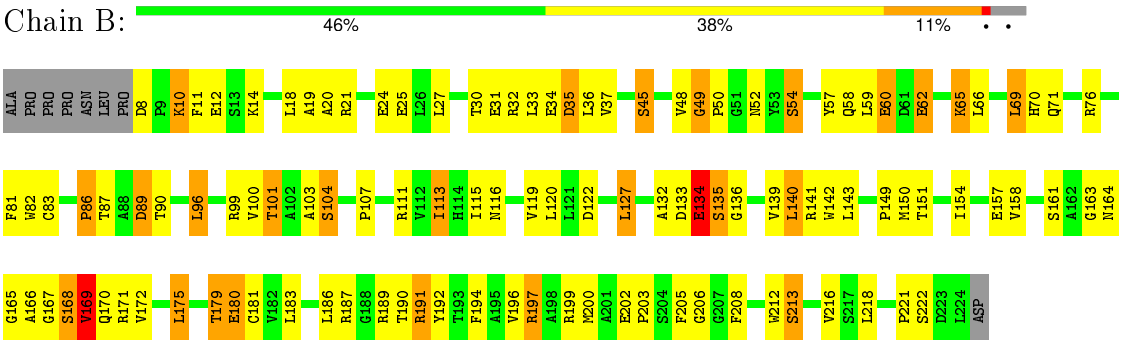
- Molecule 1: ABT-007 FAB FRAGMENT

Chain L:



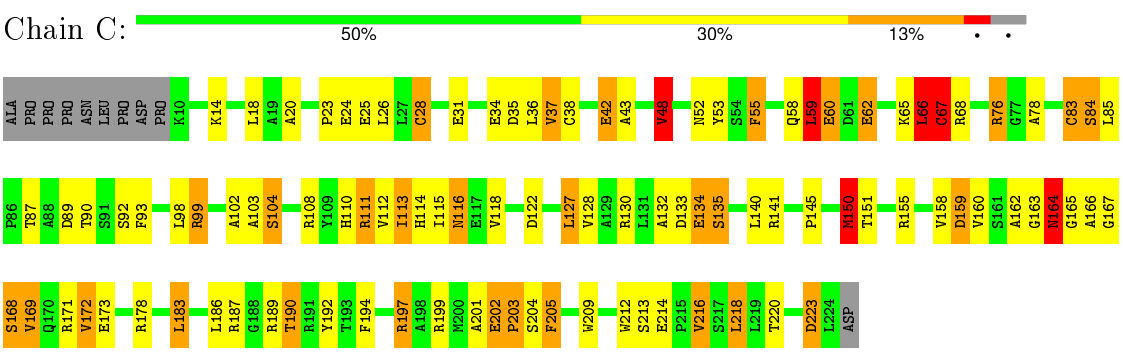
• Molecule 2: ERYTHROPOIETIN RECEPTOR

Chain B:



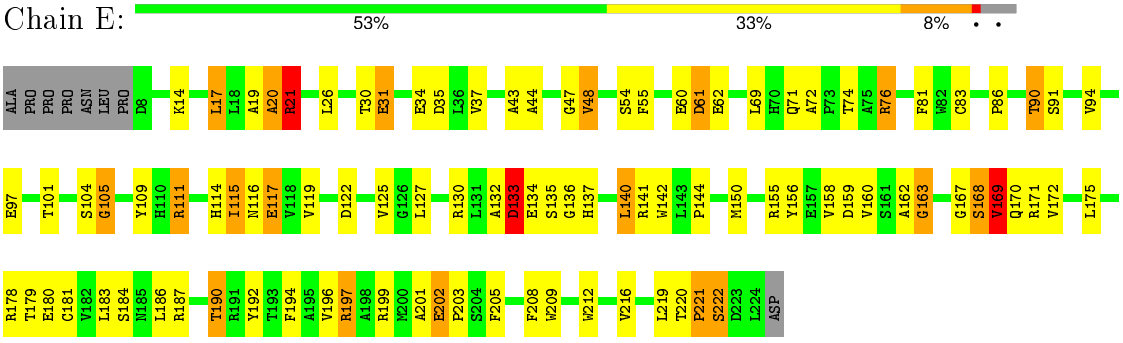
• Molecule 2: ERYTHROPOIETIN RECEPTOR

Chain C:



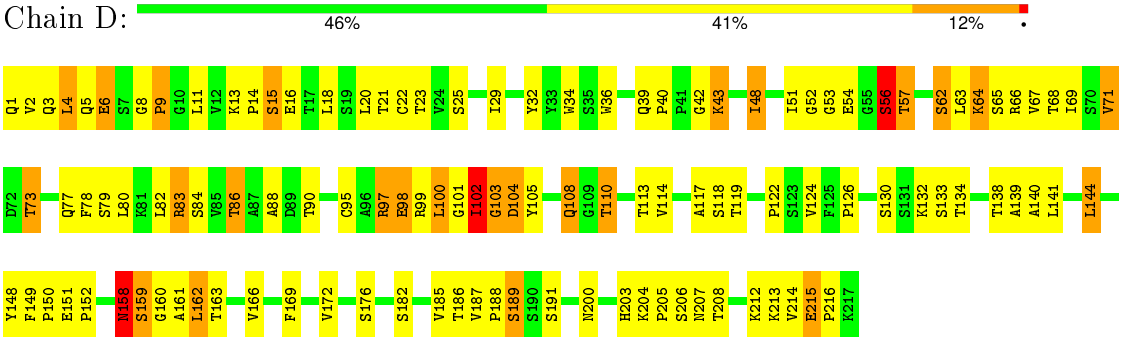
• Molecule 2: ERYTHROPOIETIN RECEPTOR

Chain E:



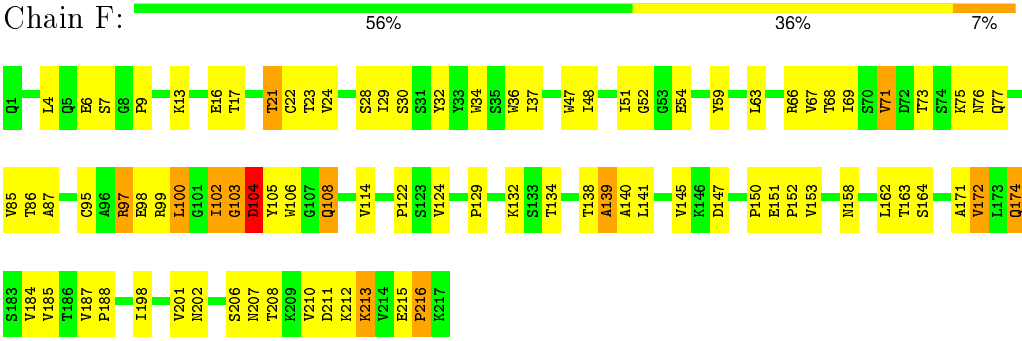
• Molecule 3: ABT-007 FAB FRAGMENT

Chain D:



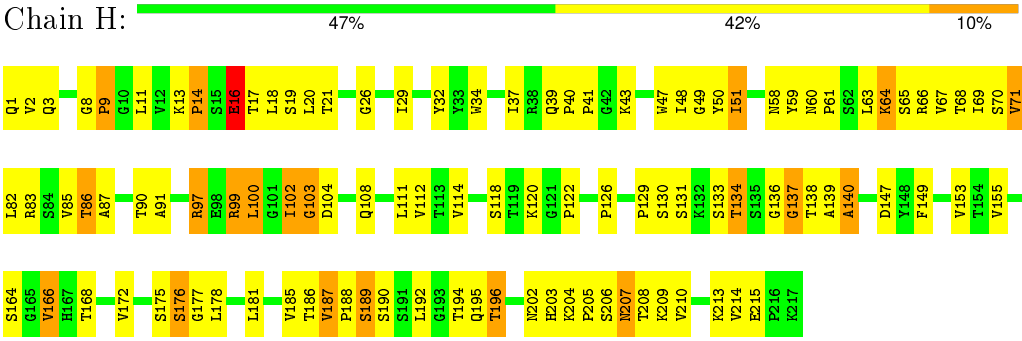
• Molecule 3: ABT-007 FAB FRAGMENT

Chain F:



• Molecule 3: ABT-007 FAB FRAGMENT

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.95Å 156.17Å 164.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.23 – 3.20	Depositor
% Data completeness (in resolution range)	97.3 (113.23-3.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.257 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14781	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.60	3/1677 (0.2%)	3.73	17/2275 (0.7%)
1	G	0.66	3/1677 (0.2%)	3.74	16/2275 (0.7%)
1	L	0.53	0/1677	0.67	0/2275
2	B	0.70	0/1726	0.82	1/2356 (0.0%)
2	C	0.83	2/1710 (0.1%)	0.80	3/2333 (0.1%)
2	E	0.70	0/1726	0.76	0/2356
3	D	0.56	0/1646	0.73	2/2249 (0.1%)
3	F	0.50	0/1646	0.66	0/2249
3	H	0.54	0/1655	0.70	0/2258
All	All	0.63	8/15140 (0.1%)	1.87	39/20626 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	67	CYS	CB-SG	16.80	2.10	1.82
1	A	209	PHE	CD1-CE1	5.63	1.50	1.39
1	G	139	PHE	CD1-CE1	5.43	1.50	1.39
1	A	139	PHE	CD1-CE1	5.25	1.49	1.39
1	G	209	PHE	CD2-CE2	5.18	1.49	1.39
2	C	28	CYS	CB-SG	5.06	1.90	1.82
1	G	209	PHE	CD1-CE1	5.05	1.49	1.39
1	A	139	PHE	CD2-CE2	5.02	1.49	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	209	PHE	CZ-CE2-CD2	-58.96	49.35	120.10
1	A	139	PHE	CZ-CE2-CD2	-58.49	49.91	120.10
1	G	209	PHE	CD1-CE1-CZ	-58.43	49.99	120.10
1	G	139	PHE	CZ-CE2-CD2	-58.35	50.08	120.10
1	G	139	PHE	CD1-CE1-CZ	-58.12	50.36	120.10
1	G	209	PHE	CZ-CE2-CD2	-58.05	50.44	120.10
1	A	139	PHE	CD1-CE1-CZ	-57.88	50.64	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	209	PHE	CD1-CE1-CZ	-57.63	50.95	120.10
1	G	209	PHE	CG-CD1-CE1	-50.14	65.64	120.80
1	A	209	PHE	CG-CD2-CE2	-50.13	65.66	120.80
1	A	139	PHE	CG-CD2-CE2	-50.12	65.67	120.80
1	G	139	PHE	CG-CD2-CE2	-49.98	65.82	120.80
1	G	209	PHE	CG-CD2-CE2	-49.91	65.90	120.80
1	A	139	PHE	CG-CD1-CE1	-49.79	66.03	120.80
1	G	139	PHE	CG-CD1-CE1	-49.63	66.21	120.80
1	A	209	PHE	CG-CD1-CE1	-49.44	66.42	120.80
1	A	139	PHE	CE1-CZ-CE2	-42.53	43.45	120.00
1	A	209	PHE	CE1-CZ-CE2	-42.52	43.46	120.00
1	G	139	PHE	CE1-CZ-CE2	-42.52	43.46	120.00
1	G	209	PHE	CE1-CZ-CE2	-42.48	43.54	120.00
1	G	139	PHE	CD1-CG-CD2	-26.19	84.25	118.30
1	A	209	PHE	CD1-CG-CD2	-26.15	84.31	118.30
1	A	139	PHE	CD1-CG-CD2	-26.04	84.45	118.30
1	G	209	PHE	CD1-CG-CD2	-25.98	84.53	118.30
1	A	209	PHE	CB-CG-CD1	24.29	137.81	120.80
1	G	209	PHE	CB-CG-CD1	24.25	137.78	120.80
1	G	209	PHE	CB-CG-CD2	24.03	137.62	120.80
1	A	139	PHE	CB-CG-CD2	23.93	137.56	120.80
1	G	139	PHE	CB-CG-CD1	23.93	137.55	120.80
1	A	139	PHE	CB-CG-CD1	23.89	137.53	120.80
1	G	139	PHE	CB-CG-CD2	23.72	137.41	120.80
1	A	209	PHE	CB-CG-CD2	23.30	137.11	120.80
2	C	67	CYS	CA-CB-SG	7.08	126.75	114.00
2	C	67	CYS	N-CA-C	-5.91	95.04	111.00
2	B	49	GLY	N-CA-C	-5.74	98.76	113.10
3	D	4	LEU	CA-CB-CG	5.67	128.33	115.30
2	C	66	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	89	LEU	CA-CB-CG	5.07	126.96	115.30
3	D	102	ILE	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1642	0	1599	78	0
1	G	1642	0	1599	72	0
1	L	1642	0	1599	56	0
2	B	1680	0	1633	89	0
2	C	1665	0	1624	100	0
2	E	1680	0	1633	65	0
3	D	1607	0	1592	84	0
3	F	1607	0	1592	102	0
3	H	1616	0	1605	79	0
All	All	14781	0	14476	685	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (685) 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)
2:C:67:CYS:SG	2:C:67:CYS:CB	2.10	1.38
2:E:201:ALA:O	2:E:205:PHE:HD1	1.32	1.11
3:H:102:ILE:HG22	3:H:103:GLY:H	1.06	1.11
3:F:102:ILE:HG13	3:F:106:TRP:HE1	0.99	1.10
2:B:87:THR:HA	2:B:90:THR:OG1	1.55	1.07
3:F:102:ILE:HG12	3:F:103:GLY:N	1.72	1.02
3:D:29:ILE:HA	3:D:34:TRP:CH2	1.94	1.01
2:B:132:ALA:HB1	2:B:134:GLU:HG2	1.41	0.99
1:L:4:LEU:HD21	1:L:90:GLN:HB3	1.45	0.99
1:A:46:ARG:HG3	3:F:102:ILE:HG21	1.44	0.98
2:E:190:THR:H	2:E:220:THR:HG22	1.29	0.96
1:G:2:ILE:HD12	1:G:93:THR:HB	1.46	0.96
2:C:130:ARG:HH21	2:C:141:ARG:HH21	1.12	0.96
3:H:202:ASN:HB3	3:H:209:LYS:HD3	1.49	0.95
3:F:102:ILE:HG13	3:F:106:TRP:NE1	1.81	0.95
2:E:201:ALA:O	2:E:205:PHE:CD1	2.23	0.92
3:D:99:ARG:O	3:D:101:GLY:N	2.03	0.92
2:C:55:PHE:CE1	2:C:67:CYS:HB2	2.06	0.91
3:F:103:GLY:O	3:F:105:TYR:N	2.04	0.90
3:H:102:ILE:HG22	3:H:103:GLY:N	1.81	0.90
2:E:130:ARG:HH12	2:E:141:ARG:HH21	1.20	0.90
3:H:102:ILE:CG2	3:H:103:GLY:H	1.85	0.90
1:A:30:ARG:HD2	2:C:25:GLU:OE2	1.73	0.89
1:A:132:VAL:HB	1:A:148:TRP:CH2	2.09	0.88
2:E:168:SER:O	2:E:169:VAL:HG13	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:29:ILE:HD11	3:D:73:THR:HA	1.56	0.87
2:E:202:GLU:HB2	2:E:203:PRO:HA	1.54	0.87
2:E:43:ALA:HB2	1:L:59:PRO:HA	1.56	0.87
3:F:102:ILE:CG1	3:F:106:TRP:HE1	1.87	0.86
3:H:206:SER:O	3:H:207:ASN:HB2	1.75	0.86
3:D:51:ILE:HG12	3:D:71:VAL:HG22	1.59	0.85
3:D:56:SER:O	3:D:57:THR:HB	1.76	0.84
3:F:29:ILE:HA	3:F:34:TRP:HH2	1.43	0.83
3:H:90:THR:HB	3:H:114:VAL:HG12	1.58	0.83
3:F:29:ILE:HA	3:F:34:TRP:CH2	2.14	0.82
3:F:162:LEU:HD21	3:F:185:VAL:HG21	1.59	0.82
3:F:97:ARG:O	3:F:103:GLY:HA2	1.78	0.82
1:A:30:ARG:HA	1:A:68:GLY:H	1.45	0.81
3:D:13:LYS:HG2	3:D:16:GLU:HB2	1.62	0.80
2:B:70:HIS:HD2	2:B:82:TRP:CH2	2.00	0.80
2:C:183:LEU:HD12	2:C:194:PHE:HE2	1.47	0.79
1:A:11:LEU:HB3	1:A:104:VAL:HG12	1.62	0.79
1:A:46:ARG:HB3	1:A:55:GLN:NE2	1.97	0.79
1:L:89:LEU:HG	1:L:90:GLN:N	1.98	0.79
3:D:122:PRO:HB3	3:D:148:TYR:HB3	1.63	0.79
1:L:108:ARG:HG2	1:L:109:THR:H	1.48	0.78
2:B:186:LEU:HB3	2:B:192:TYR:CE2	2.20	0.77
2:C:190:THR:H	2:C:220:THR:HG22	1.50	0.77
2:C:202:GLU:HG3	2:C:203:PRO:HA	1.65	0.77
2:B:186:LEU:HB3	2:B:192:TYR:HE2	1.49	0.77
3:D:3:GLN:HB2	3:D:25:SER:HB2	1.67	0.76
3:D:52:GLY:C	3:D:54:GLU:H	1.88	0.76
3:D:8:GLY:N	3:D:9:PRO:HD3	2.00	0.76
3:F:75:LYS:HE3	3:F:77:GLN:HB2	1.67	0.76
2:C:130:ARG:HH21	2:C:141:ARG:NH2	1.83	0.76
3:F:32:TYR:HD1	3:F:97:ARG:HD2	1.51	0.75
1:G:36:TYR:CE2	1:G:46:ARG:HG3	2.21	0.75
3:H:50:TYR:CE1	3:H:58:ASN:HB3	2.21	0.75
1:A:118:PHE:HZ	3:F:140:ALA:HB3	1.52	0.75
1:L:164:THR:HG22	1:L:174:SER:H	1.52	0.75
2:B:18:LEU:HD22	2:B:21:ARG:HH12	1.52	0.74
1:L:4:LEU:HD21	1:L:90:GLN:CB	2.18	0.74
2:C:132:ALA:HB1	2:C:134:GLU:HG2	1.68	0.74
3:F:102:ILE:CG1	3:F:103:GLY:N	2.40	0.73
2:E:134:GLU:O	2:E:135:SER:OG	2.06	0.73
1:L:89:LEU:HG	1:L:90:GLN:H	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:103:GLY:C	3:F:105:TYR:H	1.92	0.73
1:G:2:ILE:CD1	1:G:93:THR:HB	2.17	0.73
2:E:60:GLU:HB3	2:E:94:VAL:HG11	1.69	0.73
2:C:202:GLU:CB	2:C:203:PRO:HA	2.19	0.73
2:C:163:GLY:O	2:C:166:ALA:N	2.21	0.73
3:D:163:THR:O	3:D:166:VAL:HG12	1.89	0.73
2:B:103:ALA:O	2:B:104:SER:HB3	1.88	0.73
2:C:55:PHE:CE1	2:C:67:CYS:CB	2.72	0.73
1:L:4:LEU:CD2	1:L:90:GLN:HB3	2.18	0.72
2:C:197:ARG:HD2	2:C:212:TRP:CH2	2.24	0.72
3:F:32:TYR:CD1	3:F:97:ARG:HD2	2.24	0.72
3:H:29:ILE:O	3:H:34:TRP:HZ3	1.70	0.72
3:F:97:ARG:HB3	3:F:97:ARG:HH11	1.55	0.71
2:B:140:LEU:O	2:B:180:GLU:HA	1.89	0.71
2:B:167:GLY:O	2:B:168:SER:O	2.07	0.71
3:D:29:ILE:HD12	3:D:71:VAL:HG12	1.70	0.71
3:H:187:VAL:HG22	3:H:188:PRO:HD2	1.71	0.71
2:C:25:GLU:OE2	2:C:111:ARG:NH2	2.23	0.71
2:C:202:GLU:CG	2:C:203:PRO:HA	2.20	0.70
2:E:60:GLU:O	2:E:62:GLU:N	2.24	0.70
2:C:34:GLU:HB2	2:C:87:THR:OG1	1.91	0.70
3:F:23:THR:HA	3:F:77:GLN:HG2	1.73	0.70
2:C:48:VAL:HA	2:C:52:ASN:HD22	1.57	0.70
2:C:55:PHE:CD1	2:C:67:CYS:HB2	2.25	0.70
3:D:83:ARG:HH11	3:D:83:ARG:HB3	1.56	0.70
2:B:175:LEU:H	2:B:175:LEU:CD2	2.04	0.70
2:C:164:ASN:HD22	2:C:165:GLY:N	1.90	0.69
1:G:108:ARG:HG2	1:G:109:THR:N	2.08	0.69
2:B:127:LEU:HD23	2:B:216:VAL:HG12	1.74	0.69
3:F:97:ARG:O	3:F:103:GLY:CA	2.40	0.69
2:B:25:GLU:HG2	2:B:111:ARG:HH12	1.56	0.69
3:H:51:ILE:HG12	3:H:71:VAL:HG13	1.74	0.69
1:G:33:LEU:HD13	1:G:71:PHE:CD1	2.28	0.69
2:C:66:LEU:O	2:C:68:ARG:N	2.25	0.69
1:G:89:LEU:HD22	1:G:97:THR:O	1.92	0.69
3:F:181:LEU:O	3:F:182:SER:HB2	1.91	0.69
3:D:48:ILE:HD11	3:D:80:LEU:HD13	1.74	0.68
2:B:49:GLY:O	2:B:52:ASN:HB2	1.92	0.68
2:E:190:THR:H	2:E:220:THR:CG2	2.04	0.68
2:C:197:ARG:HD2	2:C:212:TRP:CZ3	2.28	0.68
2:E:130:ARG:HH12	2:E:141:ARG:NH2	1.89	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:130:SER:HB3	3:D:133:SER:HB3	1.74	0.67
3:F:63:LEU:HB3	3:F:67:VAL:HG23	1.76	0.67
1:A:20:THR:HG23	1:A:74:THR:HB	1.75	0.67
2:C:132:ALA:C	2:C:134:GLU:H	1.98	0.67
1:L:6:GLN:NE2	1:L:88:CYS:H	1.91	0.67
1:A:89:LEU:HD22	1:A:90:GLN:H	1.60	0.67
2:C:183:LEU:HD12	2:C:194:PHE:CE2	2.28	0.66
2:B:52:ASN:O	2:B:103:ALA:HB2	1.94	0.66
2:C:116:ASN:H	2:C:116:ASN:HD22	1.41	0.66
1:A:44:PRO:HD2	3:F:106:TRP:CE3	2.31	0.66
3:H:149:PHE:HB2	3:H:178:LEU:HD22	1.76	0.66
3:F:99:ARG:O	3:F:100:LEU:HB2	1.93	0.66
3:F:97:ARG:HH11	3:F:97:ARG:CB	2.09	0.66
1:L:112:ALA:HB1	1:L:201:LEU:HD22	1.78	0.66
1:G:210:ASN:HB2	1:G:213:GLU:OE1	1.96	0.66
1:A:124:GLN:HE22	1:A:131:SER:HB2	1.60	0.66
2:E:127:LEU:HD12	2:E:142:TRP:HB3	1.77	0.65
1:A:49:TYR:HB2	3:F:100:LEU:HD22	1.77	0.65
3:H:86:THR:O	3:H:114:VAL:HG11	1.96	0.65
3:F:36:TRP:HB2	3:F:48:ILE:HD11	1.78	0.65
2:B:115:ILE:HD12	2:B:115:ILE:H	1.61	0.65
2:C:190:THR:H	2:C:220:THR:CG2	2.09	0.65
2:B:58:GLN:HG2	2:B:60:GLU:H	1.62	0.65
3:F:97:ARG:CG	3:F:97:ARG:HH11	2.09	0.65
3:H:48:ILE:HG23	3:H:63:LEU:HD12	1.77	0.65
2:E:127:LEU:HD11	2:E:196:VAL:HG23	1.78	0.65
2:B:132:ALA:HB2	2:B:139:VAL:HG23	1.79	0.64
2:B:36:LEU:HD11	2:B:113:ILE:HD11	1.78	0.64
2:C:36:LEU:HD11	2:C:113:ILE:HD11	1.79	0.64
3:F:86:THR:O	3:F:114:VAL:HG11	1.97	0.64
3:H:59:TYR:CE1	3:H:69:ILE:HG12	2.33	0.63
3:F:36:TRP:CD1	3:F:69:ILE:HD12	2.34	0.63
3:F:102:ILE:HG23	3:F:103:GLY:H	1.63	0.63
1:G:120:PRO:HB3	1:G:124:GLN:OE1	1.99	0.63
1:L:132:VAL:HG23	1:L:179:LEU:HB3	1.80	0.63
1:G:113:PRO:HB3	1:G:139:PHE:HB3	1.80	0.63
3:D:138:THR:HA	3:D:189:SER:HB2	1.81	0.63
1:A:46:ARG:HB3	1:A:55:GLN:HE22	1.64	0.62
1:G:6:GLN:NE2	1:G:88:CYS:H	1.96	0.62
2:E:127:LEU:HD23	2:E:216:VAL:HG12	1.79	0.62
1:G:89:LEU:HD13	1:G:90:GLN:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:SER:HB3	2:B:76:ARG:HH11	1.64	0.62
2:C:190:THR:N	2:C:220:THR:HG22	2.14	0.62
2:C:197:ARG:HG3	2:C:209:TRP:CE3	2.35	0.62
2:C:48:VAL:HA	2:C:52:ASN:ND2	2.15	0.62
1:A:46:ARG:HB2	3:F:102:ILE:HD12	1.80	0.61
1:A:96:PRO:HD2	3:F:47:TRP:CE3	2.35	0.61
2:B:132:ALA:HB1	2:B:134:GLU:CG	2.23	0.61
2:C:127:LEU:HG	2:C:216:VAL:CG1	2.30	0.61
3:D:62:SER:HB2	3:D:63:LEU:HD12	1.80	0.61
1:A:151:ASP:HA	1:A:191:VAL:HB	1.81	0.61
2:B:158:VAL:HB	2:B:172:VAL:CG1	2.31	0.61
2:B:202:GLU:HB3	2:B:203:PRO:HA	1.82	0.61
3:F:16:GLU:O	3:F:85:VAL:HG23	2.00	0.61
2:E:162:ALA:O	2:E:163:GLY:O	2.19	0.61
1:G:108:ARG:HG2	1:G:109:THR:H	1.65	0.60
3:H:87:ALA:O	3:H:90:THR:HG22	2.00	0.60
3:D:13:LYS:O	3:D:15:SER:N	2.34	0.60
3:H:59:TYR:HE1	3:H:69:ILE:HG12	1.66	0.60
2:C:218:LEU:HD11	2:E:169:VAL:HB	1.83	0.60
1:G:125:LEU:HB3	1:G:183:LYS:HE3	1.84	0.60
2:C:134:GLU:O	2:C:135:SER:HB3	2.02	0.60
1:A:36:TYR:CE2	3:F:102:ILE:HB	2.37	0.60
3:D:9:PRO:HG3	3:D:110:THR:HG21	1.83	0.60
1:G:122:ASP:HA	1:G:125:LEU:HD12	1.84	0.60
1:A:61:ARG:NH1	1:A:82:ASP:OD1	2.35	0.60
1:A:6:GLN:HE22	1:A:87:TYR:HA	1.67	0.60
2:C:55:PHE:O	2:C:66:LEU:HA	2.02	0.59
1:A:20:THR:CG2	1:A:74:THR:HB	2.32	0.59
3:H:63:LEU:HB2	3:H:67:VAL:CG2	2.32	0.59
2:C:76:ARG:HH21	2:C:76:ARG:HB3	1.66	0.59
1:A:94:TYR:CD1	1:A:96:PRO:HD3	2.38	0.59
2:C:43:ALA:HB2	2:C:78:ALA:HA	1.83	0.59
1:A:87:TYR:CE1	1:A:101:GLY:HA3	2.37	0.59
3:F:102:ILE:CG1	3:F:103:GLY:H	2.15	0.59
2:C:127:LEU:HG	2:C:216:VAL:HG12	1.83	0.59
3:F:187:VAL:HG22	3:F:188:PRO:HD2	1.84	0.59
3:F:63:LEU:HB3	3:F:67:VAL:CG2	2.32	0.59
1:A:160:GLN:NE2	3:F:174:GLN:HG2	2.18	0.59
3:H:8:GLY:H	3:H:9:PRO:HD3	1.68	0.59
3:H:102:ILE:HD12	3:H:102:ILE:N	2.17	0.59
2:C:127:LEU:HD23	2:C:214:GLU:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:LYS:HB3	1:G:40:PRO:HD2	1.85	0.59
2:B:197:ARG:HD2	2:B:212:TRP:CH2	2.38	0.59
1:A:32:ASP:O	1:A:91:HIS:CD2	2.56	0.59
1:A:125:LEU:HD21	1:A:186:TYR:CD2	2.39	0.58
2:B:168:SER:O	2:B:169:VAL:HG13	2.03	0.58
3:H:63:LEU:O	3:H:65:SER:N	2.36	0.58
1:A:6:GLN:NE2	1:A:88:CYS:H	2.02	0.58
3:D:103:GLY:HA3	1:G:36:TYR:HE2	1.67	0.58
1:L:148:TRP:HB2	1:L:155:GLN:HG3	1.86	0.58
2:B:86:PRO:O	2:B:90:THR:HG23	2.03	0.58
3:H:29:ILE:O	3:H:34:TRP:CZ3	2.56	0.58
3:H:85:VAL:HG12	3:H:114:VAL:HG21	1.85	0.58
3:H:32:TYR:HB2	3:H:34:TRP:CH2	2.39	0.58
1:A:135:LEU:HD22	3:F:184:VAL:HG11	1.86	0.58
1:G:190:LYS:HG3	1:G:211:ARG:H	1.68	0.58
3:D:187:VAL:HB	3:D:188:PRO:HD2	1.85	0.58
3:H:130:SER:HB3	3:H:134:THR:HG23	1.86	0.58
2:E:74:THR:HB	2:E:76:ARG:HE	1.69	0.58
1:L:61:ARG:NH1	1:L:82:ASP:OD1	2.37	0.58
2:E:168:SER:O	2:E:169:VAL:CG1	2.51	0.58
1:A:83:PHE:O	1:A:84:ALA:HB2	2.02	0.58
2:B:86:PRO:O	2:B:90:THR:CG2	2.50	0.57
2:E:197:ARG:HD2	2:E:212:TRP:CH2	2.40	0.57
2:C:84:SER:O	2:C:85:LEU:HD23	2.04	0.57
3:D:97:ARG:HH12	3:D:105:TYR:HD1	1.52	0.57
3:D:4:LEU:HD12	3:D:22:CYS:SG	2.44	0.57
2:C:132:ALA:C	2:C:134:GLU:N	2.57	0.57
3:H:166:VAL:HB	3:H:185:VAL:HG23	1.85	0.57
3:H:29:ILE:HA	3:H:34:TRP:CH2	2.39	0.57
2:B:158:VAL:HG22	2:B:196:VAL:HG22	1.87	0.57
3:D:97:ARG:NH1	3:D:105:TYR:HD1	2.02	0.57
2:C:59:LEU:HD11	2:C:89:ASP:HB3	1.86	0.57
2:B:70:HIS:CD2	2:B:82:TRP:CH2	2.88	0.57
1:L:6:GLN:HE22	1:L:87:TYR:HA	1.69	0.57
3:D:43:LYS:HD2	3:D:43:LYS:O	2.05	0.57
1:A:36:TYR:CE2	1:A:46:ARG:HG3	2.40	0.57
3:H:102:ILE:CG2	3:H:103:GLY:N	2.52	0.57
2:C:34:GLU:O	2:C:87:THR:HA	2.05	0.57
2:C:187:ARG:O	2:C:220:THR:HG21	2.05	0.56
2:E:127:LEU:HD11	2:E:196:VAL:CG2	2.35	0.56
1:G:58:VAL:HG23	1:G:59:PRO:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:101:THR:HG21	2:E:105:GLY:HA2	1.85	0.56
2:E:187:ARG:O	2:E:220:THR:HG21	2.06	0.56
1:L:108:ARG:CG	1:L:109:THR:H	2.16	0.56
3:D:4:LEU:HD12	3:D:95:CYS:SG	2.46	0.56
1:G:4:LEU:HD21	1:G:90:GLN:HB3	1.86	0.56
3:H:63:LEU:O	3:H:66:ARG:N	2.39	0.56
3:D:124:VAL:HA	3:D:144:LEU:O	2.05	0.56
3:D:122:PRO:HD2	3:D:208:THR:HG21	1.88	0.56
3:H:47:TRP:CH2	3:H:49:GLY:HA2	2.41	0.56
3:F:181:LEU:O	3:F:182:SER:CB	2.54	0.56
3:H:8:GLY:N	3:H:9:PRO:HD3	2.21	0.56
3:D:97:ARG:O	3:D:104:ASP:HB3	2.05	0.56
3:D:169:PHE:HE1	1:G:174:SER:O	1.87	0.56
1:G:19:VAL:HG21	1:G:78:LEU:HG	1.88	0.56
3:D:32:TYR:HB2	3:D:34:TRP:CZ3	2.40	0.56
2:B:34:GLU:HG3	2:B:35:ASP:H	1.72	0.55
2:B:103:ALA:O	2:B:104:SER:CB	2.54	0.55
3:H:72:ASP:OD2	3:H:75:LYS:HE3	2.05	0.55
3:F:63:LEU:O	3:F:67:VAL:HG23	2.05	0.55
2:C:189:ARG:N	2:C:220:THR:HG23	2.21	0.55
2:C:134:GLU:O	2:C:135:SER:CB	2.53	0.55
1:L:55:GLN:HB3	1:L:58:VAL:CG1	2.36	0.55
3:D:100:LEU:HA	2:E:97:GLU:OE1	2.06	0.55
1:A:132:VAL:HB	1:A:148:TRP:HH2	1.67	0.55
3:H:139:ALA:HB3	3:H:187:VAL:O	2.06	0.55
2:C:159:ASP:C	2:C:159:ASP:OD2	2.44	0.55
2:B:36:LEU:HD11	2:B:113:ILE:CD1	2.37	0.55
3:F:7:SER:HB2	3:F:21:THR:HG23	1.88	0.55
2:E:60:GLU:C	2:E:62:GLU:H	2.08	0.55
2:C:164:ASN:ND2	2:C:165:GLY:N	2.54	0.55
1:A:63:SER:HB3	2:B:76:ARG:NH1	2.22	0.55
1:L:55:GLN:HB3	1:L:58:VAL:HG11	1.88	0.55
1:L:108:ARG:NH1	1:L:170:ASP:O	2.41	0.54
1:L:148:TRP:O	1:L:155:GLN:HG2	2.06	0.54
3:H:122:PRO:HD2	3:H:208:THR:CB	2.37	0.54
1:L:149:LYS:NZ	1:L:195:GLU:HG3	2.22	0.54
2:B:48:VAL:HA	2:B:52:ASN:ND2	2.23	0.54
3:D:203:HIS:CD2	3:D:205:PRO:HD2	2.42	0.54
2:C:162:ALA:O	2:C:166:ALA:HB3	2.07	0.54
2:B:183:LEU:HD13	2:B:194:PHE:CE2	2.43	0.54
2:C:127:LEU:HD22	2:C:213:SER:OG	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:THR:HA	2:B:154:ILE:HD12	1.90	0.54
3:D:141:LEU:HD23	3:D:214:VAL:HB	1.90	0.54
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.89	0.54
1:A:40:PRO:HB3	1:A:165:GLU:HG2	1.90	0.54
1:G:7:SER:HA	1:G:8:PRO:C	2.28	0.54
2:B:101:THR:HA	2:B:107:PRO:HA	1.88	0.53
2:E:197:ARG:HG3	2:E:209:TRP:CE3	2.43	0.53
2:C:28:CYS:HB2	2:C:113:ILE:HD13	1.91	0.53
3:D:52:GLY:C	3:D:54:GLU:N	2.59	0.53
3:D:48:ILE:HD11	3:D:80:LEU:CD1	2.38	0.53
3:F:13:LYS:O	3:F:16:GLU:HB2	2.08	0.53
1:A:49:TYR:HD2	3:F:100:LEU:HD21	1.73	0.53
2:C:59:LEU:CD1	2:C:89:ASP:HB3	2.38	0.53
3:F:52:GLY:C	3:F:54:GLU:H	2.11	0.53
1:A:90:GLN:O	1:A:96:PRO:HA	2.09	0.53
3:F:104:ASP:OD2	3:F:104:ASP:N	2.40	0.53
3:D:6:GLU:HG2	3:D:108:GLN:NE2	2.22	0.53
1:A:29:ILE:HB	1:A:92:ASN:HB2	1.91	0.53
3:H:137:GLY:O	3:H:189:SER:HB2	2.09	0.53
3:D:29:ILE:HD12	3:D:71:VAL:CG1	2.36	0.53
3:F:151:GLU:OE2	3:F:152:PRO:HA	2.08	0.53
3:H:102:ILE:O	3:H:104:ASP:N	2.42	0.53
3:H:100:LEU:HD23	1:L:49:TYR:CE2	2.43	0.53
3:F:51:ILE:HD11	3:F:71:VAL:HG22	1.90	0.53
2:E:104:SER:O	2:E:104:SER:OG	2.25	0.53
2:B:32:ARG:O	2:B:34:GLU:HG2	2.09	0.52
1:L:52:SER:HA	1:L:64:GLY:O	2.09	0.52
1:G:29:ILE:HD11	1:G:71:PHE:CE1	2.45	0.52
3:D:2:VAL:HG21	3:D:97:ARG:HH22	1.73	0.52
3:F:151:GLU:HB3	3:F:152:PRO:HA	1.91	0.52
3:H:163:THR:HG23	3:H:164:SER:H	1.74	0.52
2:C:55:PHE:CD1	2:C:67:CYS:CB	2.92	0.52
3:H:149:PHE:HB2	3:H:178:LEU:CD2	2.40	0.52
3:H:63:LEU:CB	3:H:67:VAL:HG23	2.39	0.52
2:B:36:LEU:CD1	2:B:113:ILE:HD11	2.39	0.52
3:F:163:THR:HG23	3:F:164:SER:H	1.74	0.52
3:D:63:LEU:O	3:D:66:ARG:N	2.42	0.52
2:B:24:GLU:HA	2:B:24:GLU:OE1	2.10	0.52
3:D:29:ILE:HA	3:D:34:TRP:CZ3	2.43	0.52
3:H:139:ALA:O	3:H:140:ALA:CB	2.57	0.52
1:L:107:LYS:HA	1:L:140:TYR:OH	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TYR:OH	3:F:102:ILE:HG22	2.09	0.52
1:G:132:VAL:HG23	1:G:179:LEU:HB3	1.91	0.52
2:C:66:LEU:HB3	2:C:68:ARG:HB2	1.92	0.52
3:H:32:TYR:HB2	3:H:34:TRP:CZ3	2.45	0.52
1:G:6:GLN:HE22	1:G:87:TYR:HA	1.75	0.52
1:A:24:ARG:HH12	1:A:69:THR:HG23	1.75	0.52
3:H:34:TRP:O	3:H:50:TYR:HA	2.11	0.51
2:C:164:ASN:ND2	2:C:165:GLY:H	2.07	0.51
3:F:97:ARG:HH11	3:F:97:ARG:HG2	1.74	0.51
3:F:124:VAL:HG11	3:F:210:VAL:HB	1.92	0.51
2:E:17:LEU:HD22	2:E:21:ARG:NH1	2.26	0.51
2:E:167:GLY:O	2:E:168:SER:HB3	2.11	0.51
3:H:206:SER:O	3:H:207:ASN:CB	2.53	0.51
3:F:36:TRP:HD1	3:F:69:ILE:HD12	1.74	0.51
3:H:63:LEU:HB2	3:H:67:VAL:HG23	1.90	0.51
1:L:2:ILE:HD13	1:L:29:ILE:HG22	1.91	0.51
2:C:14:LYS:NZ	2:C:31:GLU:HG2	2.24	0.51
1:L:129:THR:HG23	1:L:182:SER:HA	1.92	0.51
2:C:150:MET:CE	2:C:150:MET:HA	2.40	0.51
2:C:58:GLN:NE2	2:C:62:GLU:O	2.44	0.51
1:G:148:TRP:HB3	1:G:179:LEU:HD12	1.93	0.51
1:A:2:ILE:HD11	1:A:93:THR:HB	1.92	0.51
2:C:65:LYS:O	2:C:66:LEU:HD12	2.10	0.51
1:A:6:GLN:HB2	1:A:100:GLN:HG3	1.93	0.51
3:D:86:THR:O	3:D:114:VAL:HG11	2.11	0.51
1:G:16:GLY:HA2	1:G:77:SER:HB2	1.92	0.51
2:C:202:GLU:HB3	2:C:203:PRO:HA	1.92	0.51
3:D:130:SER:HB2	3:D:134:THR:HG23	1.93	0.51
1:L:6:GLN:N	1:L:100:GLN:OE1	2.40	0.51
1:G:6:GLN:NE2	1:G:88:CYS:N	2.59	0.51
1:A:2:ILE:CD1	1:A:93:THR:HB	2.41	0.51
1:L:11:LEU:HG	1:L:104:VAL:HG12	1.93	0.51
1:L:108:ARG:HG2	1:L:109:THR:N	2.23	0.51
3:D:63:LEU:O	3:D:65:SER:N	2.43	0.51
3:D:63:LEU:HB3	3:D:67:VAL:CG2	2.41	0.51
2:B:175:LEU:HD23	2:B:175:LEU:H	1.73	0.51
2:C:168:SER:O	2:C:169:VAL:HG13	2.11	0.51
3:H:114:VAL:O	3:H:114:VAL:HG13	2.11	0.50
2:C:158:VAL:HB	2:C:172:VAL:HG13	1.93	0.50
2:B:158:VAL:HB	2:B:172:VAL:HG12	1.93	0.50
2:C:160:VAL:O	2:C:169:VAL:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:LEU:HA	1:G:97:THR:O	2.11	0.50
2:E:190:THR:N	2:E:220:THR:HG22	2.13	0.50
3:F:124:VAL:HG13	3:F:212:LYS:HG3	1.92	0.50
2:C:103:ALA:O	2:C:104:SER:CB	2.60	0.50
3:F:215:GLU:HB2	3:F:216:PRO:HD2	1.93	0.50
1:G:131:SER:HB3	1:G:180:THR:HG23	1.92	0.50
2:C:187:ARG:NH2	2:C:223:ASP:OD2	2.44	0.50
3:D:6:GLU:HG2	3:D:108:GLN:HE21	1.76	0.50
1:L:4:LEU:O	1:L:99:GLY:HA2	2.11	0.50
3:F:171:ALA:HB1	3:F:179:TYR:HB3	1.93	0.50
2:B:50:PRO:C	2:B:52:ASN:H	2.15	0.50
3:D:40:PRO:HG2	3:D:43:LYS:HB3	1.94	0.50
1:G:149:LYS:HD3	1:G:152:ASN:HA	1.94	0.50
3:D:32:TYR:HB2	3:D:34:TRP:CH2	2.47	0.50
2:E:114:HIS:O	2:E:115:ILE:C	2.51	0.50
2:B:57:TYR:CE1	2:B:65:LYS:HB3	2.47	0.50
3:H:126:PRO:HB3	3:H:214:VAL:HG12	1.93	0.50
1:A:36:TYR:HE2	3:F:102:ILE:HB	1.77	0.49
2:B:35:ASP:OD1	2:B:35:ASP:N	2.45	0.49
3:D:102:ILE:HG13	3:D:103:GLY:N	2.27	0.49
1:L:164:THR:HG22	1:L:174:SER:N	2.26	0.49
2:B:49:GLY:O	2:B:52:ASN:CB	2.60	0.49
2:B:140:LEU:HD11	2:B:194:PHE:HB3	1.94	0.49
1:L:64:GLY:HA2	1:L:72:THR:O	2.12	0.49
2:E:114:HIS:HB2	2:E:117:GLU:HG3	1.94	0.49
3:D:98:GLU:HB3	3:D:102:ILE:HA	1.94	0.49
1:L:120:PRO:HD3	1:L:132:VAL:HG13	1.93	0.49
1:L:147:GLN:HG2	1:L:195:GLU:HB3	1.92	0.49
2:B:34:GLU:HB2	2:B:87:THR:CG2	2.42	0.49
3:D:8:GLY:N	3:D:9:PRO:CD	2.74	0.49
1:A:36:TYR:HE2	3:F:102:ILE:CB	2.25	0.49
3:H:47:TRP:CE3	1:L:96:PRO:HD2	2.47	0.49
1:A:30:ARG:HB3	1:A:68:GLY:HA2	1.94	0.49
3:H:59:TYR:HE1	3:H:69:ILE:CG1	2.24	0.49
3:D:130:SER:CB	3:D:133:SER:HB3	2.40	0.49
3:F:138:THR:HG22	3:F:139:ALA:H	1.78	0.49
1:A:16:GLY:O	1:A:77:SER:HA	2.12	0.49
3:D:126:PRO:HG3	3:D:212:LYS:HB3	1.95	0.49
2:B:120:LEU:HD12	2:B:208:PHE:HB2	1.95	0.49
3:H:102:ILE:O	3:H:103:GLY:C	2.50	0.49
2:B:168:SER:C	2:B:169:VAL:HG22	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:HA	1:A:100:GLN:HE22	1.78	0.49
2:E:14:LYS:HE2	2:E:122:ASP:OD2	2.13	0.49
2:C:36:LEU:CD1	2:C:113:ILE:HD11	2.42	0.49
2:B:166:ALA:C	2:B:168:SER:H	2.15	0.49
3:H:51:ILE:HD11	3:H:71:VAL:HG22	1.93	0.49
1:G:195:GLU:HG2	1:G:206:THR:OG1	2.13	0.49
2:E:30:THR:O	2:E:119:VAL:HA	2.13	0.49
3:H:67:VAL:HG12	3:H:68:THR:N	2.27	0.48
2:E:71:GLN:HB2	2:E:81:PHE:CE1	2.47	0.48
3:H:99:ARG:HB2	3:H:104:ASP:CB	2.42	0.48
3:F:171:ALA:HA	3:F:180:SER:O	2.13	0.48
2:C:28:CYS:HA	2:C:37:VAL:O	2.13	0.48
3:F:36:TRP:CZ3	3:F:95:CYS:HB3	2.48	0.48
2:E:141:ARG:HD3	2:E:180:GLU:OE1	2.13	0.48
1:G:6:GLN:HE22	1:G:88:CYS:N	2.11	0.48
1:G:94:TYR:CD2	1:G:96:PRO:HD3	2.48	0.48
1:G:112:ALA:HB2	1:G:200:GLY:C	2.34	0.48
3:F:201:VAL:HB	3:F:210:VAL:HG22	1.95	0.48
1:A:30:ARG:HB2	1:A:30:ARG:HE	1.55	0.48
1:G:90:GLN:O	1:G:96:PRO:HA	2.14	0.48
2:B:34:GLU:HB2	2:B:87:THR:OG1	2.13	0.48
1:G:144:ALA:HB2	1:G:198:HIS:HD2	1.78	0.48
2:C:130:ARG:NH2	2:C:141:ARG:HH21	1.95	0.48
3:F:22:CYS:HB2	3:F:36:TRP:CH2	2.49	0.48
3:D:203:HIS:HD2	3:D:206:SER:H	1.62	0.48
2:E:144:PRO:HB3	2:E:156:TYR:OH	2.14	0.48
1:A:46:ARG:HB2	3:F:102:ILE:CD1	2.44	0.47
3:D:32:TYR:HD1	3:D:34:TRP:CH2	2.32	0.47
2:C:163:GLY:O	2:C:167:GLY:N	2.38	0.47
1:L:108:ARG:CG	1:L:109:THR:N	2.77	0.47
2:C:202:GLU:CB	2:C:203:PRO:CA	2.91	0.47
2:C:122:ASP:O	2:C:145:PRO:HB3	2.14	0.47
2:B:8:ASP:HB2	2:B:10:LYS:HE3	1.96	0.47
1:G:136:LEU:HD13	1:G:175:LEU:HB3	1.96	0.47
3:D:36:TRP:HD1	3:D:69:ILE:HD13	1.79	0.47
2:C:186:LEU:HD22	2:C:192:TYR:CE2	2.50	0.47
3:D:83:ARG:HB3	3:D:83:ARG:NH1	2.27	0.47
3:D:215:GLU:HB2	3:D:216:PRO:HD2	1.97	0.47
3:H:102:ILE:HD13	1:L:91:HIS:HB3	1.97	0.47
2:E:202:GLU:HB2	2:E:203:PRO:CA	2.37	0.47
3:D:102:ILE:HD11	1:G:89:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:VAL:O	2:B:213:SER:HB3	2.15	0.47
2:B:59:LEU:HD23	2:B:96:LEU:HD12	1.96	0.47
2:C:128:VAL:HG13	2:C:141:ARG:HB2	1.97	0.47
2:B:18:LEU:HB3	2:B:27:LEU:HD13	1.96	0.47
1:A:136:LEU:HD13	1:A:175:LEU:HB3	1.96	0.47
2:E:160:VAL:O	2:E:169:VAL:HA	2.15	0.47
3:D:103:GLY:HA3	1:G:36:TYR:CE2	2.49	0.47
3:F:129:PRO:HD3	3:F:141:LEU:HD23	1.96	0.47
3:F:206:SER:O	3:F:208:THR:N	2.48	0.47
2:C:67:CYS:HB3	2:C:83:CYS:SG	2.54	0.47
3:D:8:GLY:H	3:D:9:PRO:HD3	1.79	0.47
3:D:66:ARG:NH1	3:D:82:LEU:HD11	2.30	0.47
1:G:147:GLN:HB3	1:G:154:LEU:HD22	1.96	0.47
3:H:40:PRO:O	3:H:43:LYS:HB2	2.15	0.46
3:F:198:ILE:HG12	3:F:213:LYS:HB3	1.96	0.46
3:F:162:LEU:HD21	3:F:185:VAL:CG2	2.40	0.46
3:D:39:GLN:HA	3:D:40:PRO:HD2	1.71	0.46
1:G:193:ALA:HB2	1:G:208:SER:HB3	1.98	0.46
2:B:175:LEU:HD22	2:B:175:LEU:H	1.79	0.46
1:L:148:TRP:CB	1:L:155:GLN:HG3	2.45	0.46
3:D:117:ALA:HB3	3:D:149:PHE:CE2	2.51	0.46
1:A:22:THR:HA	1:A:71:PHE:O	2.15	0.46
2:B:127:LEU:HD12	2:B:142:TRP:HB3	1.97	0.46
1:A:9:SER:O	1:A:102:THR:HA	2.16	0.46
3:D:52:GLY:O	3:D:54:GLU:N	2.49	0.46
3:F:138:THR:HA	3:F:188:PRO:HA	1.97	0.46
2:E:186:LEU:HB3	2:E:192:TYR:CE2	2.51	0.46
3:F:132:LYS:HB2	3:F:134:THR:HG22	1.96	0.46
3:H:99:ARG:HB2	3:H:104:ASP:HB2	1.97	0.46
1:L:112:ALA:HB2	1:L:200:GLY:HA3	1.98	0.46
1:G:10:SER:HB2	1:G:103:LYS:HB3	1.97	0.46
2:C:28:CYS:HA	2:C:38:CYS:HA	1.98	0.46
3:D:63:LEU:O	3:D:64:LYS:C	2.54	0.46
3:D:126:PRO:HB3	3:D:214:VAL:HG22	1.97	0.46
2:E:111:ARG:NH2	1:G:31:ASN:ND2	2.64	0.46
1:G:29:ILE:O	1:G:30:ARG:HG3	2.16	0.45
1:G:89:LEU:HD13	1:G:89:LEU:C	2.36	0.45
1:G:6:GLN:HE22	1:G:88:CYS:H	1.63	0.45
1:G:190:LYS:HE2	1:G:211:ARG:HB3	1.98	0.45
2:E:114:HIS:O	2:E:116:ASN:N	2.49	0.45
1:L:131:SER:OG	1:L:180:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:68:THR:HB	3:F:81:LYS:HB2	1.97	0.45
3:D:158:ASN:ND2	3:D:161:ALA:HB3	2.31	0.45
1:L:55:GLN:O	1:L:58:VAL:HG13	2.17	0.45
3:H:163:THR:HG23	3:H:164:SER:N	2.31	0.45
1:G:132:VAL:CG2	1:G:179:LEU:HB3	2.46	0.45
3:D:34:TRP:HB3	3:D:78:PHE:CZ	2.50	0.45
2:E:133:ASP:C	2:E:134:GLU:OE1	2.54	0.45
1:G:61:ARG:NH1	1:G:82:ASP:OD1	2.50	0.45
3:F:102:ILE:HD13	3:F:104:ASP:N	2.31	0.45
3:F:122:PRO:HD2	3:F:208:THR:OG1	2.17	0.45
2:E:47:GLY:O	2:E:48:VAL:HG13	2.17	0.45
3:H:63:LEU:HB2	3:H:67:VAL:HG21	1.98	0.45
2:E:155:ARG:NE	2:E:199:ARG:HD3	2.32	0.45
1:G:25:ALA:C	1:G:27:GLN:H	2.18	0.45
2:C:155:ARG:HH21	2:C:199:ARG:HD2	1.82	0.45
1:A:96:PRO:HD2	3:F:47:TRP:CZ3	2.51	0.45
1:A:37:GLN:OE1	1:A:39:LYS:HE2	2.17	0.45
2:B:14:LYS:HE3	2:B:122:ASP:OD2	2.17	0.45
1:G:29:ILE:HG21	1:G:90:GLN:HG3	1.98	0.45
1:A:118:PHE:CZ	3:F:140:ALA:HB3	2.41	0.45
3:D:188:PRO:HG2	3:D:191:SER:OG	2.17	0.45
1:A:187:GLU:HA	1:A:211:ARG:NH2	2.32	0.45
2:B:205:PHE:HB3	2:B:206:GLY:H	1.63	0.45
1:G:32:ASP:HB2	1:G:92:ASN:HB2	1.99	0.45
1:G:36:TYR:HE1	1:G:89:LEU:HB3	1.82	0.45
1:L:2:ILE:HD13	1:L:29:ILE:CG2	2.47	0.45
1:A:28:GLY:HA2	1:A:68:GLY:O	2.17	0.45
3:F:4:LEU:CD2	3:F:24:VAL:HG22	2.47	0.45
2:E:158:VAL:HG22	2:E:196:VAL:HG22	1.98	0.45
2:C:168:SER:C	2:C:169:VAL:HG22	2.37	0.45
2:E:19:ALA:O	2:E:21:ARG:N	2.47	0.45
3:D:158:ASN:C	3:D:160:GLY:H	2.21	0.45
3:H:2:VAL:HG21	3:H:97:ARG:HH22	1.81	0.45
2:B:183:LEU:HD13	2:B:194:PHE:HE2	1.82	0.44
2:B:45:SER:O	2:B:48:VAL:HG22	2.18	0.44
1:A:78:LEU:CD2	1:A:82:ASP:HB2	2.47	0.44
3:D:22:CYS:O	3:D:77:GLN:HB2	2.17	0.44
2:C:58:GLN:O	2:C:60:GLU:N	2.50	0.44
3:H:136:GLY:O	3:H:138:THR:N	2.49	0.44
3:F:97:ARG:NH1	3:F:97:ARG:HG2	2.30	0.44
3:H:202:ASN:HB3	3:H:209:LYS:CD	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:158:VAL:HB	2:E:172:VAL:HG13	1.99	0.44
2:E:55:PHE:HB2	2:E:69:LEU:HD21	1.99	0.44
1:G:35:TRP:CD2	1:G:73:LEU:HB2	2.53	0.44
3:H:39:GLN:C	3:H:91:ALA:HB1	2.36	0.44
3:D:6:GLU:HG3	3:D:110:THR:OG1	2.17	0.44
2:E:133:ASP:N	2:E:133:ASP:OD1	2.34	0.44
1:L:33:LEU:HG	1:L:34:GLY:N	2.32	0.44
2:B:163:GLY:HA3	2:B:191:ARG:NH1	2.32	0.44
2:B:216:VAL:HG13	2:B:216:VAL:O	2.18	0.44
1:A:125:LEU:HD21	1:A:186:TYR:HD2	1.80	0.44
1:A:36:TYR:HE1	1:A:89:LEU:HB3	1.83	0.44
2:B:133:ASP:OD2	2:C:187:ARG:HD3	2.18	0.44
1:A:13:ALA:HB3	1:A:78:LEU:HD12	2.00	0.44
1:G:39:LYS:O	1:G:41:GLY:N	2.50	0.44
3:H:17:THR:HG22	3:H:83:ARG:HA	1.99	0.44
3:H:139:ALA:O	3:H:140:ALA:HB2	2.17	0.44
2:C:116:ASN:ND2	2:C:116:ASN:H	2.11	0.44
1:A:162:SER:HB3	1:A:176:SER:HB3	2.00	0.44
2:B:119:VAL:HG11	2:B:200:MET:HG3	2.00	0.44
2:C:92:SER:HB3	2:C:116:ASN:HB3	1.99	0.43
1:G:39:LYS:CB	1:G:40:PRO:HD2	2.45	0.43
1:A:190:LYS:CE	1:A:211:ARG:H	2.31	0.43
3:H:153:VAL:HG23	3:H:203:HIS:HB2	2.00	0.43
2:C:66:LEU:C	2:C:68:ARG:N	2.70	0.43
2:B:31:GLU:C	2:B:32:ARG:HD2	2.39	0.43
2:B:54:SER:O	2:B:100:VAL:HA	2.18	0.43
2:C:194:PHE:CD1	2:C:194:PHE:N	2.85	0.43
3:D:67:VAL:HG12	3:D:68:THR:N	2.32	0.43
2:B:120:LEU:CD1	2:B:208:PHE:HB2	2.47	0.43
1:A:1:ASP:O	1:A:3:GLN:NE2	2.51	0.43
3:F:103:GLY:C	3:F:105:TYR:N	2.61	0.43
3:F:145:VAL:HB	3:F:181:LEU:HB3	2.00	0.43
2:B:113:ILE:O	2:B:113:ILE:HG13	2.10	0.43
1:A:83:PHE:O	1:A:84:ALA:CB	2.66	0.43
3:F:97:ARG:NH1	3:F:97:ARG:HB3	2.29	0.43
3:D:204:LYS:N	3:D:205:PRO:CD	2.82	0.43
1:L:37:GLN:HG3	1:L:86:TYR:CZ	2.54	0.43
2:B:135:SER:HB2	2:B:136:GLY:H	1.61	0.43
2:E:221:PRO:HB2	2:E:222:SER:H	1.67	0.43
2:E:132:ALA:HB3	2:E:137:HIS:HB2	2.01	0.43
1:A:161:GLU:O	3:F:172:VAL:HG11	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:GLN:HE21	2:B:62:GLU:H	1.65	0.43
2:C:67:CYS:HB3	2:C:83:CYS:HG	1.84	0.43
1:A:43:ALA:HA	1:A:44:PRO:HD3	1.80	0.43
1:G:190:LYS:HE2	1:G:211:ARG:CB	2.49	0.43
2:E:20:ALA:O	2:E:21:ARG:HG3	2.19	0.43
2:B:218:LEU:HD12	2:B:218:LEU:HA	1.86	0.43
2:B:134:GLU:O	2:B:135:SER:HB3	2.18	0.43
2:E:167:GLY:O	2:E:168:SER:CB	2.67	0.43
3:F:4:LEU:HA	3:F:23:THR:O	2.19	0.43
3:F:59:TYR:HE1	3:F:69:ILE:HG12	1.84	0.43
3:H:168:THR:HG23	3:H:181:LEU:HD21	2.01	0.43
1:G:46:ARG:HD2	1:G:55:GLN:OE1	2.19	0.43
2:E:91:SER:O	2:E:94:VAL:HG23	2.18	0.43
2:C:92:SER:O	2:C:93:PHE:HB3	2.18	0.43
2:B:157:GLU:OE1	2:B:197:ARG:HD3	2.19	0.43
1:A:32:ASP:O	1:A:91:HIS:HD2	1.99	0.43
2:E:71:GLN:HG3	2:E:72:ALA:N	2.33	0.43
2:B:149:PRO:O	2:B:150:MET:HB2	2.19	0.43
1:A:36:TYR:CE2	3:F:102:ILE:HG21	2.54	0.42
1:A:49:TYR:CD2	3:F:100:LEU:HD21	2.54	0.42
3:F:97:ARG:O	3:F:99:ARG:N	2.52	0.42
2:E:168:SER:O	2:E:169:VAL:HG22	2.19	0.42
2:C:127:LEU:CD2	2:C:213:SER:OG	2.66	0.42
1:L:106:ILE:H	1:L:166:GLN:HE22	1.66	0.42
1:G:52:SER:HA	1:G:64:GLY:O	2.19	0.42
3:D:18:LEU:HD21	3:D:20:LEU:HG	2.01	0.42
3:F:17:THR:HA	3:F:82:LEU:O	2.19	0.42
1:L:90:GLN:O	1:L:96:PRO:HA	2.18	0.42
2:B:50:PRO:HB3	2:B:69:LEU:O	2.18	0.42
1:G:143:GLU:CD	1:G:143:GLU:N	2.72	0.42
3:D:9:PRO:HG3	3:D:110:THR:CG2	2.48	0.42
1:L:3:GLN:HB2	1:L:26:SER:HB3	2.01	0.42
2:C:159:ASP:OD2	2:C:160:VAL:N	2.52	0.42
3:H:16:GLU:HB3	3:H:17:THR:H	1.67	0.42
2:C:53:TYR:CD1	2:C:102:ALA:HA	2.54	0.42
2:C:52:ASN:OD1	2:C:103:ALA:HB2	2.19	0.42
3:H:122:PRO:HD2	3:H:208:THR:HB	2.01	0.42
2:C:87:THR:HA	2:C:90:THR:OG1	2.19	0.42
2:C:14:LYS:HZ2	2:C:31:GLU:HG2	1.83	0.42
2:C:99:ARG:HG3	2:C:110:HIS:CD2	2.55	0.42
3:H:60:ASN:HA	3:H:61:PRO:HD2	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:LEU:O	2:C:173:GLU:HG2	2.19	0.42
2:E:14:LYS:HZ2	2:E:31:GLU:HB3	1.84	0.42
2:E:26:LEU:HB2	2:E:109:TYR:CD2	2.55	0.42
2:C:114:HIS:O	2:C:115:ILE:C	2.58	0.42
3:D:15:SER:O	3:D:84:SER:HA	2.20	0.42
3:H:67:VAL:CG1	3:H:68:THR:N	2.82	0.42
2:B:197:ARG:HD2	2:B:212:TRP:CZ3	2.54	0.42
2:B:8:ASP:HB2	2:B:10:LYS:HD2	2.02	0.42
1:A:117:ILE:O	1:A:117:ILE:HG23	2.19	0.42
1:G:89:LEU:HD13	1:G:90:GLN:C	2.40	0.42
3:F:66:ARG:HG2	3:F:83:ARG:O	2.20	0.42
2:B:199:ARG:HG2	2:B:200:MET:N	2.35	0.42
2:E:175:LEU:HD12	2:E:178:ARG:HD3	2.02	0.42
2:C:38:CYS:HB2	2:C:83:CYS:SG	2.60	0.41
3:F:187:VAL:CG2	3:F:188:PRO:HD2	2.49	0.41
2:C:24:GLU:OE2	2:C:42:GLU:HB2	2.20	0.41
1:L:151:ASP:N	1:L:151:ASP:OD1	2.53	0.41
3:H:204:LYS:N	3:H:205:PRO:CD	2.83	0.41
3:D:13:LYS:HG2	3:D:16:GLU:CB	2.41	0.41
3:F:215:GLU:CB	3:F:216:PRO:HD2	2.50	0.41
2:E:137:HIS:HA	2:E:183:LEU:O	2.20	0.41
1:L:203:SER:HA	1:L:204:PRO:HD2	1.82	0.41
3:F:36:TRP:O	3:F:37:ILE:HG13	2.20	0.41
2:E:140:LEU:HD11	2:E:194:PHE:HB3	2.02	0.41
2:C:26:LEU:CD2	2:C:98:LEU:HD11	2.49	0.41
3:H:13:LYS:HA	3:H:14:PRO:HD3	1.77	0.41
1:G:36:TYR:N	1:G:36:TYR:CD1	2.87	0.41
3:D:130:SER:HB3	3:D:133:SER:CB	2.49	0.41
1:A:100:GLN:HG3	1:A:101:GLY:H	1.85	0.41
3:F:52:GLY:C	3:F:54:GLU:N	2.73	0.41
2:C:112:VAL:CG2	3:F:100:LEU:HG	2.50	0.41
1:G:55:GLN:O	1:G:58:VAL:CG1	2.68	0.41
2:B:141:ARG:HG2	2:B:180:GLU:HB2	2.02	0.41
1:G:149:LYS:HG3	1:G:193:ALA:HB3	2.01	0.41
2:C:36:LEU:HG	2:C:37:VAL:N	2.36	0.41
2:B:175:LEU:N	2:B:175:LEU:CD2	2.79	0.41
3:F:86:THR:HB	3:F:87:ALA:H	1.67	0.41
2:C:18:LEU:C	2:C:20:ALA:N	2.74	0.41
1:G:91:HIS:CD2	1:G:91:HIS:O	2.74	0.41
1:A:36:TYR:HE2	3:F:102:ILE:HG21	1.85	0.41
3:F:97:ARG:O	3:F:97:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:122:PRO:CB	3:D:148:TYR:HB3	2.43	0.41
1:G:123:GLU:HA	1:G:126:LYS:HG2	2.02	0.41
3:H:20:LEU:HD11	3:H:112:VAL:HG21	2.01	0.41
3:H:176:SER:O	3:H:178:LEU:N	2.53	0.41
2:C:55:PHE:CZ	2:C:67:CYS:CB	3.04	0.41
2:B:142:TRP:CE3	2:B:196:VAL:HG21	2.56	0.41
2:B:127:LEU:HD23	2:B:216:VAL:CG1	2.49	0.41
3:F:138:THR:O	3:F:139:ALA:HB2	2.21	0.41
1:A:125:LEU:HD11	1:A:186:TYR:HE2	1.86	0.41
1:L:79:GLN:O	1:L:82:ASP:HB2	2.21	0.41
1:G:78:LEU:HD23	1:G:78:LEU:HA	1.91	0.41
3:H:122:PRO:HD2	3:H:208:THR:OG1	2.21	0.41
2:C:18:LEU:C	2:C:20:ALA:H	2.23	0.41
3:D:162:LEU:CD2	3:D:185:VAL:HG21	2.51	0.41
1:L:154:LEU:HG	1:L:154:LEU:H	1.69	0.41
1:L:31:ASN:O	1:L:31:ASN:CG	2.58	0.41
2:B:71:GLN:HB2	2:B:81:PHE:CD1	2.55	0.41
3:H:194:THR:O	3:H:195:GLN:HB2	2.21	0.41
1:L:78:LEU:HA	1:L:78:LEU:HD23	1.82	0.41
3:H:103:GLY:O	1:L:36:TYR:HE2	2.04	0.41
1:L:100:GLN:H	1:L:100:GLN:HG3	1.63	0.41
3:H:195:GLN:HG2	3:H:196:THR:N	2.36	0.41
3:D:151:GLU:HB3	3:D:152:PRO:HA	2.03	0.41
3:H:1:GLN:HE21	3:H:3:GLN:HB2	1.86	0.41
3:H:1:GLN:O	3:H:26:GLY:HA3	2.20	0.41
1:A:21:ILE:O	1:A:72:THR:HA	2.21	0.41
2:B:70:HIS:HD2	2:B:82:TRP:CZ3	2.39	0.40
1:G:46:ARG:NH1	1:G:55:GLN:OE1	2.54	0.40
2:B:142:TRP:NE1	2:B:179:THR:HG22	2.37	0.40
3:F:6:GLU:HA	3:F:21:THR:O	2.21	0.40
2:B:33:LEU:CD2	2:B:119:VAL:HG21	2.51	0.40
2:E:219:LEU:HD23	2:E:220:THR:O	2.21	0.40
3:D:108:GLN:HA	1:G:43:ALA:HB2	2.04	0.40
3:F:145:VAL:HG11	3:F:153:VAL:HG21	2.02	0.40
1:A:29:ILE:HB	1:A:92:ASN:CB	2.51	0.40
1:L:94:TYR:CD2	1:L:96:PRO:HD3	2.56	0.40
2:E:74:THR:HB	2:E:76:ARG:HH21	1.86	0.40
1:G:35:TRP:CE2	1:G:73:LEU:HB2	2.56	0.40
1:A:7:SER:HA	1:A:8:PRO:C	2.41	0.40
1:G:4:LEU:HD21	1:G:90:GLN:CB	2.50	0.40
1:A:49:TYR:HB2	3:F:100:LEU:CD2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:134:GLU:C	2:E:135:SER:HG	2.16	0.40
3:F:201:VAL:HG12	3:F:202:ASN:N	2.37	0.40
2:B:59:LEU:HD13	2:B:89:ASP:HB3	2.03	0.40
1:A:190:LYS:HE2	1:A:211:ARG:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	212/214 (99%)	176 (83%)	30 (14%)	6 (3%)	6 37
1	G	212/214 (99%)	178 (84%)	27 (13%)	7 (3%)	5 32
1	L	212/214 (99%)	188 (89%)	17 (8%)	7 (3%)	5 32
2	B	215/225 (96%)	172 (80%)	28 (13%)	15 (7%)	1 10
2	C	213/225 (95%)	163 (76%)	33 (16%)	17 (8%)	1 7
2	E	215/225 (96%)	169 (79%)	30 (14%)	16 (7%)	1 9
3	D	215/217 (99%)	163 (76%)	31 (14%)	21 (10%)	1 4
3	F	215/217 (99%)	164 (76%)	37 (17%)	14 (6%)	1 13
3	H	215/217 (99%)	161 (75%)	36 (17%)	18 (8%)	1 6
All	All	1924/1968 (98%)	1534 (80%)	269 (14%)	121 (6%)	2 13

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	123	GLU
2	B	116	ASN
2	B	168	SER

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Mol	Chain	Res	Type
2	C	23	PRO
2	C	42	GLU
2	C	60	GLU
2	C	135	SER
2	C	164	ASN
2	C	201	ALA
2	C	204	SER
3	D	9	PRO
3	D	57	THR
3	D	100	LEU
3	D	102	ILE
3	D	150	PRO
2	E	86	PRO
2	E	163	GLY
2	E	168	SER
2	E	221	PRO
3	F	98	GLU
3	F	150	PRO
3	F	182	SER
3	F	207	ASN
3	H	9	PRO
3	H	64	LYS
3	H	102	ILE
3	H	129	PRO
3	H	140	ALA
3	H	158	ASN
3	H	207	ASN
1	L	156	SER
1	A	84	ALA
1	A	143	GLU
2	B	104	SER
2	B	134	GLU
2	B	135	SER
2	C	59	LEU
2	C	67	CYS
2	C	104	SER
2	C	133	ASP
2	C	150	MET
2	C	205	PHE
3	D	15	SER
3	D	42	GLY
3	D	104	ASP

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Mol	Chain	Res	Type
3	D	140	ALA
3	D	159	SER
3	D	207	ASN
2	E	115	ILE
2	E	133	ASP
3	F	100	LEU
3	F	104	ASP
1	G	166	GLN
3	H	103	GLY
3	H	131	SER
3	H	137	GLY
3	H	177	GLY
3	H	190	SER
1	L	40	PRO
1	L	154	LEU
2	B	11	PHE
2	B	20	ALA
2	B	86	PRO
2	B	165	GLY
2	B	170	GLN
2	C	151	THR
3	D	14	PRO
3	D	56	SER
3	D	103	GLY
3	D	139	ALA
3	D	158	ASN
2	E	35	ASP
2	E	105	GLY
2	E	136	GLY
2	E	181	CYS
3	F	9	PRO
3	F	108	GLN
3	F	147	ASP
3	F	158	ASN
1	G	40	PRO
1	G	143	GLU
3	H	16	GLU
3	H	108	GLN
3	H	147	ASP
3	H	176	SER
1	L	204	PRO
2	B	12	GLU

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Mol	Chain	Res	Type
2	B	221	PRO
3	D	62	SER
3	D	88	ALA
2	E	20	ALA
2	E	21	ARG
2	E	44	ALA
2	E	61	ASP
2	E	90	THR
3	F	103	GLY
3	F	174	GLN
1	G	67	SER
1	L	44	PRO
1	A	138	ASN
2	B	19	ALA
2	B	60	GLU
2	C	48	VAL
2	C	83	CYS
3	D	64	LYS
3	F	139	ALA
1	G	138	ASN
1	L	110	VAL
3	D	53	GLY
3	D	176	SER
3	H	14	PRO
1	G	15	VAL
1	G	41	GLY
1	A	40	PRO
2	B	169	VAL
3	F	216	PRO
3	H	41	PRO
1	L	128	GLY
2	E	169	VAL
2	C	203	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	187/187 (100%)	163 (87%)	24 (13%)	5 25
1	G	187/187 (100%)	163 (87%)	24 (13%)	5 25
1	L	187/187 (100%)	159 (85%)	28 (15%)	3 17
2	B	178/186 (96%)	143 (80%)	35 (20%)	1 8
2	C	176/186 (95%)	141 (80%)	35 (20%)	1 8
2	E	178/186 (96%)	150 (84%)	28 (16%)	3 15
3	D	184/185 (100%)	149 (81%)	35 (19%)	2 10
3	F	184/185 (100%)	168 (91%)	16 (9%)	13 45
3	H	185/185 (100%)	148 (80%)	37 (20%)	1 8
All	All	1646/1674 (98%)	1384 (84%)	262 (16%)	3 14

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	20	THR
1	A	29	ILE
1	A	30	ARG
1	A	46	ARG
1	A	53	SER
1	A	55	GLN
1	A	70	GLU
1	A	73	LEU
1	A	74	THR
1	A	75	ILE
1	A	78	LEU
1	A	90	GLN
1	A	100	GLN
1	A	108	ARG
1	A	109	THR
1	A	115	VAL
1	A	132	VAL
1	A	169	LYS
1	A	178	THR
1	A	183	LYS
1	A	190	LYS
1	A	194	CYS
1	A	209	PHE
2	B	10	LYS
2	B	30	THR

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Mol	Chain	Res	Type
2	B	35	ASP
2	B	37	VAL
2	B	45	SER
2	B	54	SER
2	B	62	GLU
2	B	65	LYS
2	B	66	LEU
2	B	69	LEU
2	B	83	CYS
2	B	89	ASP
2	B	96	LEU
2	B	99	ARG
2	B	101	THR
2	B	113	ILE
2	B	127	LEU
2	B	134	GLU
2	B	140	LEU
2	B	143	LEU
2	B	161	SER
2	B	164	ASN
2	B	169	VAL
2	B	171	ARG
2	B	175	LEU
2	B	179	THR
2	B	180	GLU
2	B	181	CYS
2	B	187	ARG
2	B	189	ARG
2	B	190	THR
2	B	191	ARG
2	B	197	ARG
2	B	213	SER
2	B	222	SER
2	C	35	ASP
2	C	37	VAL
2	C	48	VAL
2	C	55	PHE
2	C	59	LEU
2	C	62	GLU
2	C	66	LEU
2	C	67	CYS
2	C	76	ARG

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Mol	Chain	Res	Type
2	C	84	SER
2	C	99	ARG
2	C	108	ARG
2	C	111	ARG
2	C	113	ILE
2	C	116	ASN
2	C	118	VAL
2	C	127	LEU
2	C	134	GLU
2	C	140	LEU
2	C	150	MET
2	C	159	ASP
2	C	164	ASN
2	C	168	SER
2	C	169	VAL
2	C	171	ARG
2	C	172	VAL
2	C	178	ARG
2	C	183	LEU
2	C	190	THR
2	C	197	ARG
2	C	202	GLU
2	C	205	PHE
2	C	216	VAL
2	C	218	LEU
2	C	223	ASP
3	D	1	GLN
3	D	5	GLN
3	D	6	GLU
3	D	11	LEU
3	D	21	THR
3	D	23	THR
3	D	43	LYS
3	D	48	ILE
3	D	56	SER
3	D	71	VAL
3	D	73	THR
3	D	79	SER
3	D	83	ARG
3	D	86	THR
3	D	90	THR
3	D	97	ARG

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Mol	Chain	Res	Type
3	D	98	GLU
3	D	102	ILE
3	D	108	GLN
3	D	110	THR
3	D	113	THR
3	D	118	SER
3	D	119	THR
3	D	132	LYS
3	D	144	LEU
3	D	158	ASN
3	D	159	SER
3	D	162	LEU
3	D	172	VAL
3	D	182	SER
3	D	186	THR
3	D	189	SER
3	D	200	ASN
3	D	213	LYS
3	D	215	GLU
2	E	17	LEU
2	E	21	ARG
2	E	31	GLU
2	E	34	GLU
2	E	37	VAL
2	E	48	VAL
2	E	54	SER
2	E	61	ASP
2	E	76	ARG
2	E	83	CYS
2	E	90	THR
2	E	111	ARG
2	E	117	GLU
2	E	125	VAL
2	E	133	ASP
2	E	140	LEU
2	E	150	MET
2	E	159	ASP
2	E	169	VAL
2	E	170	GLN
2	E	171	ARG
2	E	179	THR
2	E	184	SER

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Mol	Chain	Res	Type
2	E	190	THR
2	E	197	ARG
2	E	202	GLU
2	E	208	PHE
2	E	222	SER
3	F	21	THR
3	F	28	SER
3	F	30	SER
3	F	71	VAL
3	F	73	THR
3	F	76	ASN
3	F	80	LEU
3	F	82	LEU
3	F	83	ARG
3	F	97	ARG
3	F	102	ILE
3	F	104	ASP
3	F	108	GLN
3	F	172	VAL
3	F	211	ASP
3	F	213	LYS
1	G	5	THR
1	G	9	SER
1	G	14	SER
1	G	18	ARG
1	G	24	ARG
1	G	31	ASN
1	G	42	LYS
1	G	58	VAL
1	G	65	SER
1	G	74	THR
1	G	76	SER
1	G	89	LEU
1	G	90	GLN
1	G	97	THR
1	G	108	ARG
1	G	115	VAL
1	G	118	PHE
1	G	149	LYS
1	G	159	SER
1	G	174	SER
1	G	180	THR

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Mol	Chain	Res	Type
1	G	190	LYS
1	G	197	THR
1	G	201	LEU
3	H	11	LEU
3	H	16	GLU
3	H	18	LEU
3	H	19	SER
3	H	21	THR
3	H	37	ILE
3	H	51	ILE
3	H	64	LYS
3	H	70	SER
3	H	71	VAL
3	H	73	THR
3	H	75	LYS
3	H	82	LEU
3	H	86	THR
3	H	97	ARG
3	H	99	ARG
3	H	100	LEU
3	H	111	LEU
3	H	118	SER
3	H	120	LYS
3	H	133	SER
3	H	134	THR
3	H	155	VAL
3	H	158	ASN
3	H	159	SER
3	H	162	LEU
3	H	166	VAL
3	H	172	VAL
3	H	175	SER
3	H	186	THR
3	H	187	VAL
3	H	189	SER
3	H	192	LEU
3	H	196	THR
3	H	210	VAL
3	H	213	LYS
3	H	215	GLU
1	L	1	ASP
1	L	4	LEU

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Mol	Chain	Res	Type
1	L	5	THR
1	L	9	SER
1	L	11	LEU
1	L	14	SER
1	L	20	THR
1	L	31	ASN
1	L	46	ARG
1	L	58	VAL
1	L	67	SER
1	L	69	THR
1	L	72	THR
1	L	90	GLN
1	L	100	GLN
1	L	108	ARG
1	L	109	THR
1	L	123	GLU
1	L	132	VAL
1	L	147	GLN
1	L	151	ASP
1	L	154	LEU
1	L	160	GLN
1	L	163	VAL
1	L	168	SER
1	L	195	GLU
1	L	201	LEU
1	L	214	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	55	GLN
1	A	91	HIS
1	A	100	GLN
1	A	124	GLN
1	A	158	ASN
1	A	160	GLN
1	A	166	GLN
2	B	58	GLN
2	B	70	HIS
2	C	52	ASN
2	C	116	ASN

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Mol	Chain	Res	Type
2	C	164	ASN
3	D	1	GLN
3	D	108	GLN
3	D	158	ASN
3	D	203	HIS
2	E	170	GLN
3	F	5	GLN
1	G	6	GLN
1	G	31	ASN
1	G	91	HIS
1	G	138	ASN
1	G	199	GLN
3	H	1	GLN
3	H	3	GLN
1	L	6	GLN
1	L	31	ASN
1	L	160	GLN
1	L	166	GLN
1	L	189	HIS

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

There are no ligands in this entry.

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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.