Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:57 PM GMT

PDB ID	:	1HXM
Title	:	Crystal Structure of a Human Vgamma9/Vdelta2 T Cell Receptor
Authors	:	Allison, T.J.; Winter, C.C.; Fournie, J.J.; Bonneville, M.; Garboczi, D.N.
Deposited on	:	2001-01-16
Resolution	:	3.12 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:

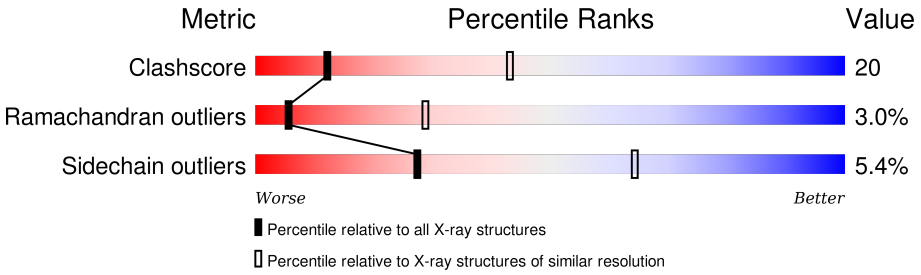
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.12 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	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)

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	229	61% 28% • 10%
1	C	229	58% 30% • 10%
1	E	229	55% 32% • 10%
1	G	229	60% 26% • 10%
2	B	242	57% 33% 5% 5%
2	D	242	59% 31% 5% 5%
2	F	242	60% 30% 5% 5%

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Mol	Chain	Length	Quality of chain
2	H	242	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13820 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

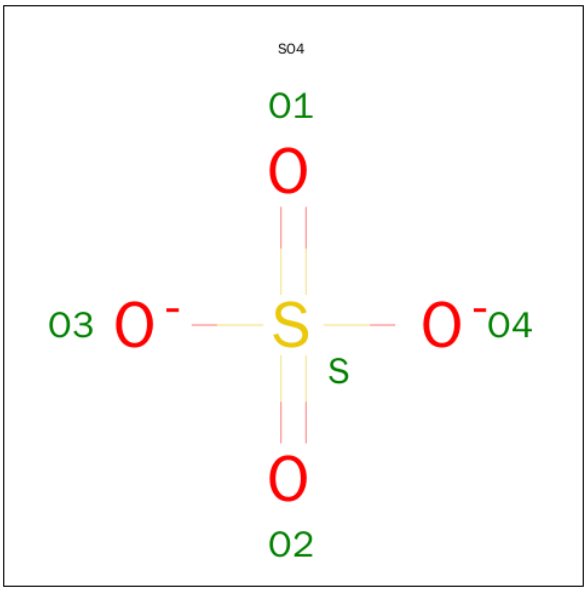
- Molecule 1 is a protein called GAMMA-DELTA T-CELL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1611	1022	270	310	9			
1	C	206	Total	C	N	O	S	0	0	0
			1611	1022	270	310	9			
1	E	206	Total	C	N	O	S	0	0	0
			1611	1022	270	310	9			
1	G	206	Total	C	N	O	S	0	0	0
			1611	1022	270	310	9			

- Molecule 2 is a protein called GAMMA-DELTA T-CELL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	230	Total	C	N	O	S	0	0	0
			1828	1167	304	351	6			
2	D	230	Total	C	N	O	S	0	0	0
			1828	1167	304	351	6			
2	F	230	Total	C	N	O	S	0	0	0
			1828	1167	304	351	6			
2	H	230	Total	C	N	O	S	0	0	0
			1828	1167	304	351	6			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	B	12	Total O 12 12	0	0
4	C	2	Total O 2 2	0	0
4	D	2	Total O 2 2	0	0
4	E	8	Total O 8 8	0	0
4	F	8	Total O 8 8	0	0
4	G	7	Total O 7 7	0	0
4	H	10	Total O 10 10	0	0

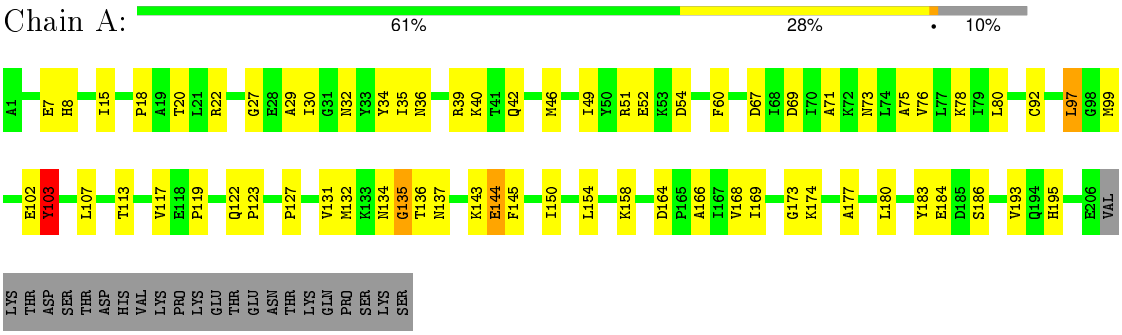
3 Residue-property plots (i)

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.

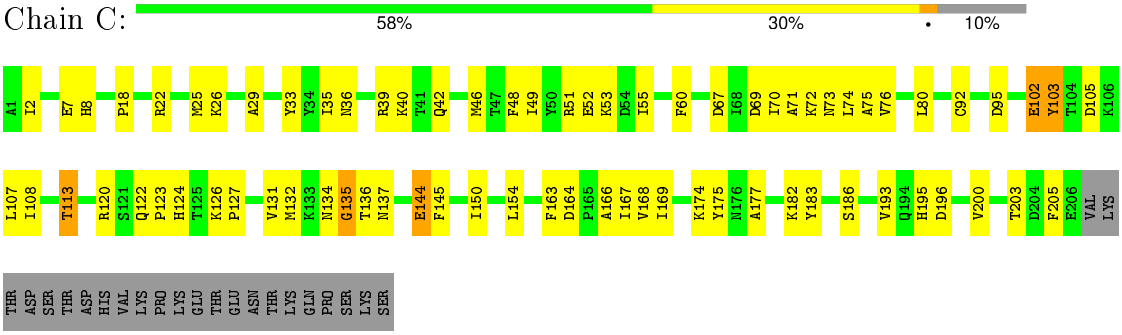
• Molecule 1: GAMMA-DELTA T-CELL RECEPTOR

Chain A:



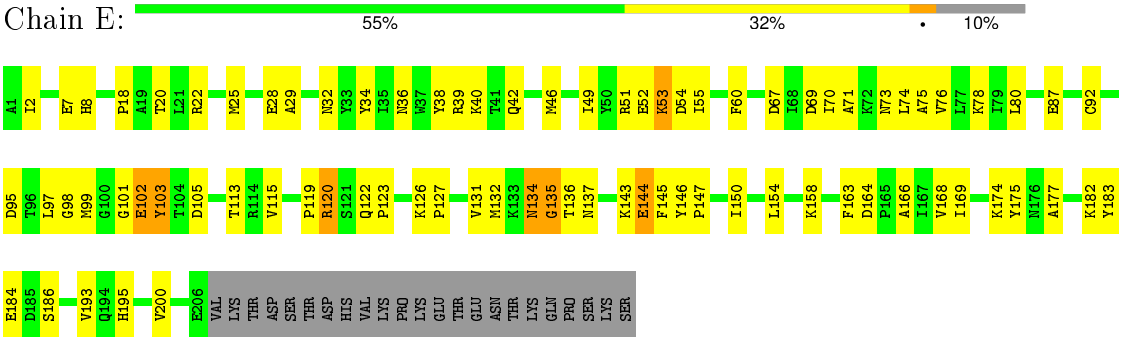
• Molecule 1: GAMMA-DELTA T-CELL RECEPTOR

Chain C:



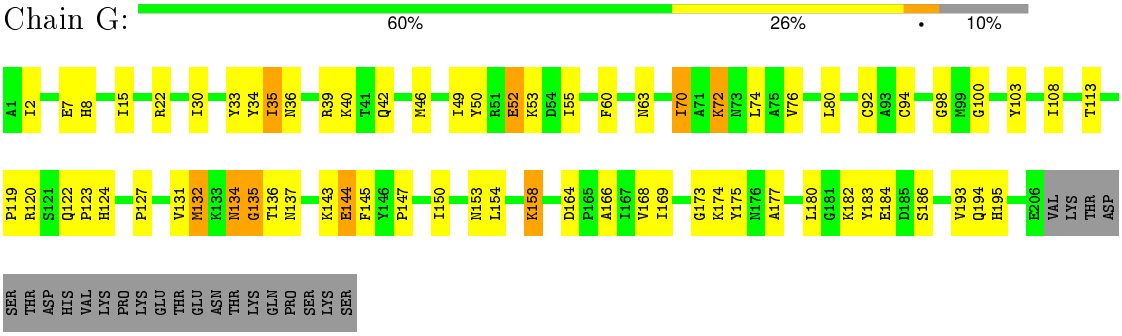
• Molecule 1: GAMMA-DELTA T-CELL RECEPTOR

Chain E:



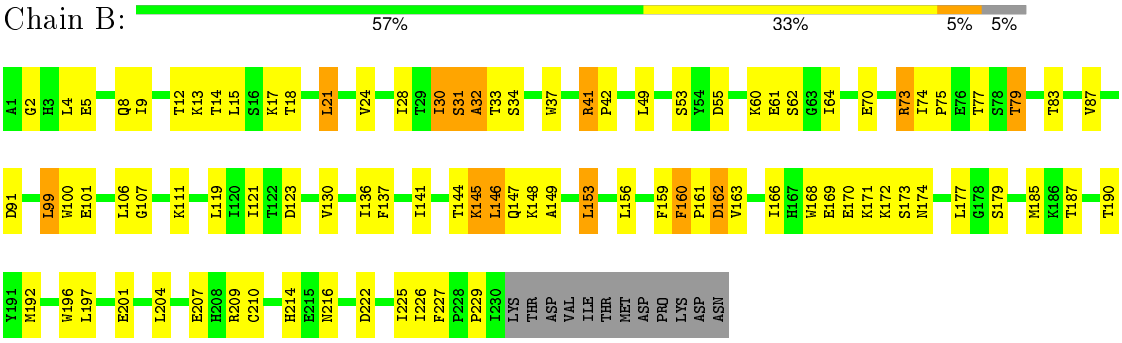
• Molecule 1: GAMMA-DELTA T-CELL RECEPTOR

Chain G:



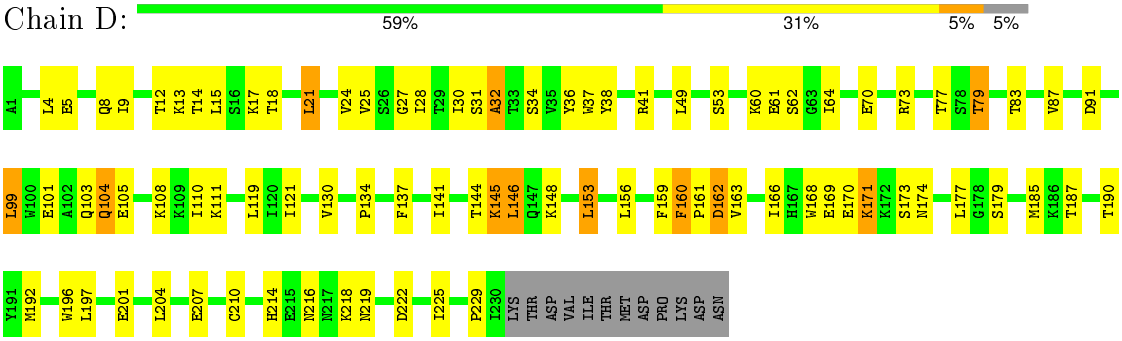
• Molecule 2: GAMMA-DELTA T-CELL RECEPTOR

Chain B:



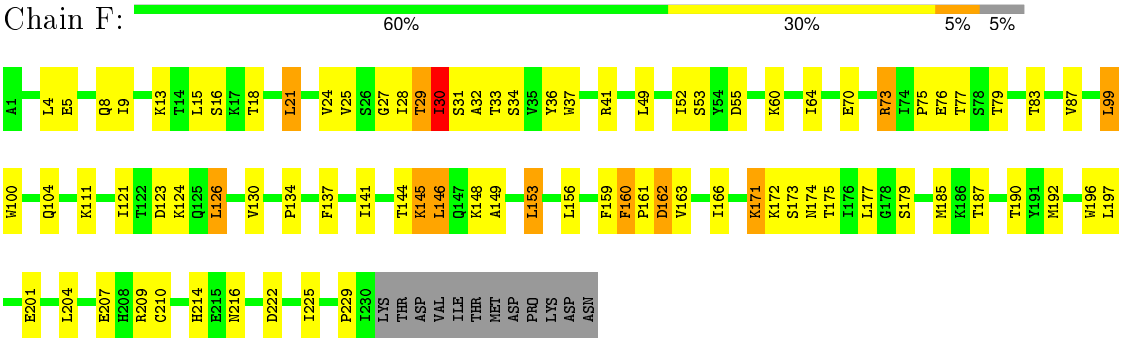
• Molecule 2: GAMMA-DELTA T-CELL RECEPTOR

Chain D:



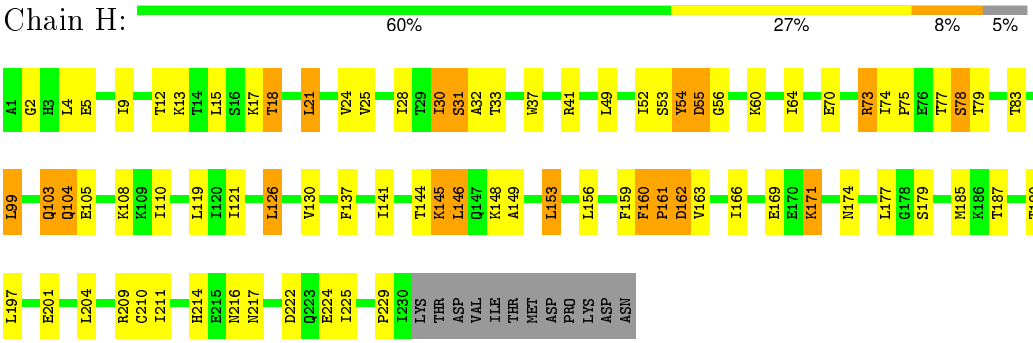
• Molecule 2: GAMMA-DELTA T-CELL RECEPTOR

Chain F:



• Molecule 2: GAMMA-DELTA T-CELL RECEPTOR

Chain H:


60%
27%
8%
5%
A1 G2 H3 L4 E5 I9 T12 K13 T14 L15 S16 K17 T18 L21 V24 V25 I28 T29 I30 S31 A32 T33 W37 R41 L49 I52 S53 Y54 D55 G56 K60 I64 E70 R73 I74 F75 E76 T77 S78 T79 T83 V87 D91
L99 Q103 Q104 E105 K108 K109 I110 L119 I120 I121 L126 V130 F137 I141 T144 K145 L146 Q147 K148 A149 L153 L156 F159 F160 P161 D162 V163 I166 E169 E170 K171 N174 L177 G178 S179 M185 K186 T187 T190 Y191 M192 W196
L197 E201 L204 R209 C210 I211 H214 E215 N216 N217 D222 Q223 E224 I225 P229 I230 LYS THR ASP VAL ILE THR MET ASP PRO LYS ASP ASN

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 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.05Å 151.74Å 97.87Å 90.00° 99.48° 90.00°	Depositor
Resolution (Å)	30.77 – 3.12	Depositor
% Data completeness (in resolution range)	99.0 (30.77-3.12)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.219 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13820	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.42	0/1646	0.65	0/2228
1	C	0.40	0/1646	0.65	0/2228
1	E	0.42	0/1646	0.65	0/2228
1	G	0.43	0/1646	0.69	0/2228
2	B	0.45	0/1867	0.70	1/2529 (0.0%)
2	D	0.43	0/1867	0.70	1/2529 (0.0%)
2	F	0.44	0/1867	0.70	1/2529 (0.0%)
2	H	0.43	0/1867	0.70	1/2529 (0.0%)
All	All	0.43	0/14052	0.68	4/19028 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	160	PHE	N-CA-C	5.80	126.66	111.00
2	F	160	PHE	N-CA-C	5.64	126.22	111.00
2	H	160	PHE	N-CA-C	5.60	126.11	111.00
2	B	160	PHE	N-CA-C	5.58	126.06	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1611	0	1597	54	0
1	C	1611	0	1597	57	0
1	E	1611	0	1597	72	0
1	G	1611	0	1597	56	0
2	B	1828	0	1848	100	0
2	D	1828	0	1848	81	0
2	F	1828	0	1848	86	0
2	H	1828	0	1848	81	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
4	A	5	0	0	0	0
4	B	12	0	0	2	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	8	0	0	2	0
4	F	8	0	0	1	0
4	G	7	0	0	0	0
4	H	10	0	0	0	0
All	All	13820	0	13780	545	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 20.

All (545) 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:F:153:LEU:HD12	2:F:196:TRP:HB3	1.42	1.02
1:C:127:PRO:HB3	1:C:145:PHE:HB3	1.38	1.02
1:A:127:PRO:HB3	1:A:145:PHE:HB3	1.39	1.00
1:E:127:PRO:HB3	1:E:145:PHE:HB3	1.38	0.99
2:D:153:LEU:HD12	2:D:196:TRP:HB3	1.40	0.99
2:H:153:LEU:HD12	2:H:196:TRP:HB3	1.45	0.99
1:A:36:ASN:HD21	1:A:51:ARG:HH11	1.04	0.98
1:G:127:PRO:HB3	1:G:145:PHE:HB3	1.41	0.98
2:B:153:LEU:HD12	2:B:196:TRP:HB3	1.47	0.97
2:B:30:ILE:HD12	2:B:30:ILE:H	1.28	0.96
2:H:171:LYS:HA	2:H:209:ARG:HH22	1.31	0.95
1:C:36:ASN:HD21	1:C:51:ARG:HH11	1.11	0.94
2:H:130:VAL:HG13	2:H:160:PHE:H	1.34	0.93
2:D:130:VAL:HG13	2:D:160:PHE:H	1.34	0.92
2:F:130:VAL:HG13	2:F:160:PHE:H	1.33	0.92
2:F:171:LYS:HG2	2:F:207:GLU:HB3	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ALA:HA	1:C:73:ASN:HD21	1.37	0.90
2:B:130:VAL:HG13	2:B:160:PHE:H	1.38	0.89
2:F:171:LYS:HA	2:F:209:ARG:HH12	1.36	0.89
1:C:39:ARG:HB3	1:C:49:ILE:HD11	1.56	0.88
2:D:171:LYS:HB2	2:D:207:GLU:HB3	1.53	0.87
1:G:164:ASP:H	2:H:185:MET:HE1	1.40	0.85
1:A:122:GLN:HB2	1:A:123:PRO:HD2	1.59	0.84
1:A:39:ARG:HB3	1:A:49:ILE:HD11	1.59	0.82
1:A:20:THR:HG22	1:A:78:LYS:HG3	1.60	0.81
1:A:22:ARG:HG2	1:A:76:VAL:HG12	1.63	0.80
1:E:39:ARG:HB3	1:E:49:ILE:HD11	1.64	0.79
1:G:30:ILE:HD11	1:G:35:ILE:HD11	1.65	0.78
1:E:22:ARG:HG2	1:E:76:VAL:HG12	1.65	0.78
1:G:39:ARG:HB3	1:G:49:ILE:HD11	1.65	0.78
2:H:30:ILE:H	2:H:30:ILE:HD12	1.48	0.77
2:F:130:VAL:HG11	2:F:160:PHE:HB3	1.66	0.77
1:C:22:ARG:HG2	1:C:76:VAL:HG12	1.66	0.77
2:H:130:VAL:HG11	2:H:160:PHE:HB3	1.67	0.76
1:G:164:ASP:N	2:H:185:MET:HE1	2.00	0.76
2:H:209:ARG:HD2	2:H:224:GLU:HG2	1.67	0.76
1:G:22:ARG:HG2	1:G:76:VAL:HG12	1.68	0.75
1:A:36:ASN:HD21	1:A:51:ARG:NH1	1.83	0.75
1:A:164:ASP:H	2:B:185:MET:HE1	1.51	0.75
1:E:158:LYS:HE2	1:E:184:GLU:HG3	1.70	0.74
2:F:171:LYS:HD2	2:F:172:LYS:HG3	1.70	0.74
2:D:30:ILE:H	2:D:30:ILE:HD12	1.53	0.74
2:B:156:LEU:HD12	2:B:166:ILE:HD11	1.70	0.73
2:B:187:THR:O	2:B:190:THR:HG22	1.89	0.73
2:F:130:VAL:HG13	2:F:160:PHE:N	2.03	0.72
2:H:187:THR:O	2:H:190:THR:HG22	1.88	0.72
1:C:122:GLN:HB2	1:C:123:PRO:HD2	1.72	0.72
1:C:36:ASN:HD21	1:C:51:ARG:NH1	1.88	0.72
2:D:130:VAL:HG11	2:D:160:PHE:HB3	1.70	0.72
1:C:36:ASN:ND2	1:C:51:ARG:HH11	1.88	0.71
2:H:130:VAL:HG13	2:H:160:PHE:N	2.06	0.71
2:B:185:MET:CE	4:B:2004:HOH:O	2.38	0.71
2:D:130:VAL:HG13	2:D:160:PHE:N	2.05	0.71
2:H:126:LEU:HD13	2:H:126:LEU:H	1.54	0.70
2:F:187:THR:O	2:F:190:THR:HG22	1.90	0.70
1:A:40:LYS:HG2	1:A:46:MET:H	1.56	0.70
2:B:130:VAL:HG11	2:B:160:PHE:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:9:ILE:CG2	2:H:163:VAL:HG12	2.22	0.69
2:B:34:SER:OG	2:B:53:SER:HA	1.91	0.69
2:D:103:GLN:HB3	2:D:104:GLN:OE1	1.93	0.69
2:B:185:MET:HE2	4:B:2004:HOH:O	1.93	0.68
2:F:9:ILE:CG2	2:F:163:VAL:HG12	2.23	0.68
1:G:40:LYS:HG2	1:G:46:MET:H	1.58	0.68
1:C:72:LYS:HA	1:C:72:LYS:HE2	1.74	0.68
1:A:122:GLN:HE22	1:A:174:LYS:HG2	1.59	0.67
1:C:144:GLU:OE1	1:C:174:LYS:HD2	1.95	0.67
2:H:156:LEU:HD12	2:H:166:ILE:HD11	1.76	0.67
2:D:187:THR:O	2:D:190:THR:HG22	1.95	0.67
2:B:130:VAL:HG13	2:B:160:PHE:N	2.10	0.67
1:C:95:ASP:HB3	1:C:107:LEU:HD23	1.76	0.67
1:E:36:ASN:HD21	1:E:51:ARG:HH11	1.43	0.67
2:B:30:ILE:CD1	2:B:30:ILE:H	2.01	0.67
2:D:137:PHE:HB2	2:D:153:LEU:O	1.94	0.67
1:E:99:MET:HG3	1:E:101:GLY:H	1.61	0.66
1:E:144:GLU:OE1	1:E:174:LYS:HD2	1.96	0.66
2:D:144:THR:O	2:D:148:LYS:HA	1.95	0.66
2:D:15:LEU:HD12	2:D:15:LEU:H	1.59	0.66
2:F:156:LEU:HD12	2:F:166:ILE:HD11	1.76	0.66
1:E:40:LYS:HG2	1:E:46:MET:H	1.61	0.66
1:C:2:ILE:HD12	1:C:33:TYR:CE2	2.31	0.66
2:B:209:ARG:NH1	2:B:226:ILE:HG12	2.11	0.65
1:C:40:LYS:HG2	1:C:46:MET:H	1.61	0.65
1:E:154:LEU:HD13	1:E:183:TYR:OH	1.97	0.65
1:C:22:ARG:HB3	1:C:74:LEU:HD21	1.79	0.65
2:H:74:ILE:HD12	2:H:74:ILE:H	1.60	0.65
2:D:77:THR:OG1	2:D:79:THR:HG23	1.96	0.65
2:F:124:LYS:HZ1	1:G:120:ARG:HG2	1.61	0.65
2:F:15:LEU:HD12	2:F:15:LEU:H	1.60	0.65
2:B:144:THR:O	2:B:148:LYS:HA	1.95	0.65
1:A:49:ILE:HG23	1:A:60:PHE:CD2	2.32	0.65
2:F:179:SER:HB3	2:F:197:LEU:HD13	1.78	0.65
2:H:30:ILE:HG22	2:H:73:ARG:HH21	1.61	0.64
2:H:73:ARG:HD3	2:H:73:ARG:O	1.97	0.64
2:H:144:THR:O	2:H:148:LYS:HA	1.97	0.64
2:F:126:LEU:HD12	2:F:126:LEU:H	1.61	0.64
2:D:5:GLU:HB2	2:D:24:VAL:HG22	1.78	0.64
2:F:144:THR:O	2:F:148:LYS:HA	1.98	0.64
2:F:130:VAL:O	2:F:159:PHE:HA	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:LEU:H	2:B:15:LEU:HD12	1.62	0.64
2:H:103:GLN:HB2	2:H:108:LYS:O	1.98	0.64
1:A:164:ASP:N	2:B:185:MET:HE1	2.13	0.63
2:B:77:THR:O	2:B:79:THR:HG22	1.98	0.63
2:D:4:LEU:HD22	2:D:25:VAL:HG12	1.80	0.63
2:H:99:LEU:HD23	2:H:99:LEU:O	1.98	0.63
1:A:34:TYR:HE1	1:A:97:LEU:HB3	1.64	0.63
2:H:15:LEU:HD12	2:H:15:LEU:H	1.64	0.63
2:H:5:GLU:HB2	2:H:24:VAL:HG22	1.80	0.63
2:D:87:VAL:HG21	2:D:121:ILE:HD11	1.80	0.63
1:E:120:ARG:HB3	1:E:120:ARG:NH1	2.14	0.63
1:G:49:ILE:HG23	1:G:60:PHE:CD2	2.34	0.63
1:A:144:GLU:OE1	1:A:174:LYS:HD2	1.99	0.62
1:C:154:LEU:HD13	1:C:183:TYR:OH	1.98	0.62
2:B:24:VAL:HG23	2:B:24:VAL:O	1.99	0.62
2:B:87:VAL:HG21	2:B:121:ILE:HD11	1.82	0.62
1:A:143:LYS:NZ	2:B:146:LEU:HD23	2.15	0.62
2:D:179:SER:HB3	2:D:197:LEU:HD13	1.81	0.62
2:F:137:PHE:HB2	2:F:153:LEU:O	1.99	0.62
2:H:130:VAL:O	2:H:159:PHE:HA	1.99	0.62
1:E:105:ASP:HB2	2:F:36:TYR:OH	1.99	0.62
2:D:9:ILE:CG2	2:D:163:VAL:HG12	2.29	0.62
1:C:69:ASP:OD1	1:C:71:ALA:HB3	2.00	0.62
2:D:214:HIS:CD2	2:D:216:ASN:H	2.18	0.62
1:E:74:LEU:HD12	1:E:75:ALA:N	2.14	0.62
1:G:144:GLU:OE1	1:G:174:LYS:HD2	1.99	0.61
1:E:38:TYR:OH	2:F:111:LYS:HB3	1.99	0.61
1:C:49:ILE:HG23	1:C:60:PHE:CD2	2.35	0.61
2:B:33:THR:HG22	2:B:34:SER:N	2.16	0.61
2:D:210:CYS:HB3	2:D:225:ILE:HB	1.82	0.61
1:G:2:ILE:HD12	1:G:33:TYR:CZ	2.35	0.61
2:F:161:PRO:HD2	2:F:214:HIS:NE2	2.15	0.61
2:D:130:VAL:O	2:D:159:PHE:HA	2.01	0.61
2:B:214:HIS:CD2	2:B:216:ASN:H	2.19	0.61
2:F:156:LEU:HD12	2:F:166:ILE:CD1	2.31	0.61
2:F:16:SER:OG	1:G:80:LEU:HB2	2.01	0.61
2:B:130:VAL:O	2:B:159:PHE:HA	2.01	0.60
2:D:30:ILE:N	2:D:30:ILE:HD12	2.15	0.60
2:H:137:PHE:HB2	2:H:153:LEU:O	2.00	0.60
2:B:179:SER:HB3	2:B:197:LEU:HD13	1.82	0.60
2:F:214:HIS:CD2	2:F:216:ASN:H	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:PHE:HB2	2:B:153:LEU:O	2.02	0.60
2:H:214:HIS:CD2	2:H:216:ASN:H	2.19	0.60
2:F:5:GLU:HB2	2:F:24:VAL:HG22	1.83	0.60
2:B:170:GLU:HB2	2:B:173:SER:O	2.01	0.60
2:B:5:GLU:HB2	2:B:24:VAL:HG22	1.83	0.60
1:G:55:ILE:HD11	2:H:108:LYS:HD2	1.82	0.59
2:D:77:THR:HG21	1:G:194:GLN:OE1	2.02	0.59
1:E:120:ARG:HH11	1:E:120:ARG:HB3	1.67	0.59
1:A:36:ASN:ND2	1:A:51:ARG:HH11	1.88	0.59
2:F:130:VAL:CG1	2:F:160:PHE:HB3	2.31	0.59
1:G:35:ILE:HD12	1:G:94:CYS:SG	2.43	0.59
1:E:102:GLU:H	1:E:102:GLU:CD	2.05	0.59
2:B:209:ARG:HH12	2:B:226:ILE:HG12	1.67	0.59
4:E:2030:HOH:O	2:F:185:MET:HE2	2.02	0.59
2:F:137:PHE:CD2	2:F:153:LEU:HD23	2.38	0.59
1:E:137:ASN:HD21	1:E:182:LYS:HZ3	1.49	0.59
1:C:103:TYR:H	1:C:103:TYR:HD2	1.49	0.59
2:B:161:PRO:HD2	2:B:214:HIS:NE2	2.18	0.59
1:C:55:ILE:HG12	2:D:108:LYS:HE3	1.84	0.59
1:C:124:HIS:HD1	1:C:196:ASP:CG	2.06	0.58
2:H:156:LEU:HD12	2:H:166:ILE:CD1	2.32	0.58
2:B:99:LEU:O	2:B:99:LEU:HD23	2.03	0.58
2:D:156:LEU:HD12	2:D:166:ILE:HD11	1.84	0.58
2:B:60:LYS:HD2	2:B:64:ILE:HB	1.86	0.58
1:A:42:GLN:O	1:A:42:GLN:HG3	2.04	0.58
1:G:7:GLU:HG2	1:G:8:HIS:CE1	2.39	0.58
2:D:161:PRO:HD2	2:D:214:HIS:NE2	2.18	0.58
1:G:34:TYR:HD2	1:G:52:GLU:HG2	1.68	0.58
1:E:36:ASN:HD21	1:E:51:ARG:NH1	2.02	0.58
2:B:31:SER:O	2:B:32:ALA:HB2	2.04	0.58
2:H:130:VAL:CG1	2:H:160:PHE:HB3	2.33	0.58
1:C:120:ARG:HG2	1:C:120:ARG:HH11	1.69	0.58
2:D:103:GLN:HB2	2:D:108:LYS:HB3	1.85	0.58
1:E:122:GLN:HB2	1:E:123:PRO:HD2	1.86	0.58
1:G:137:ASN:HD21	1:G:182:LYS:HZ1	1.52	0.58
2:F:173:SER:O	2:F:175:THR:HG23	2.04	0.57
1:E:42:GLN:HG3	1:E:42:GLN:O	2.05	0.57
1:A:150:ILE:HD11	1:A:193:VAL:HG11	1.86	0.57
2:B:2:GLY:HA3	2:B:28:ILE:HG12	1.85	0.57
1:E:49:ILE:HG23	1:E:60:PHE:CD2	2.39	0.57
1:C:74:LEU:HD23	1:C:75:ALA:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:ILE:N	2:B:74:ILE:HD12	2.20	0.57
4:E:2030:HOH:O	2:F:185:MET:CE	2.52	0.57
2:D:169:GLU:OE1	2:D:174:ASN:HB2	2.05	0.57
1:G:150:ILE:HD11	1:G:193:VAL:HG11	1.86	0.57
2:B:130:VAL:CG1	2:B:160:PHE:HB3	2.33	0.57
2:F:130:VAL:CG1	2:F:160:PHE:H	2.13	0.57
1:A:29:ALA:HA	1:A:73:ASN:HD21	1.70	0.57
2:H:87:VAL:HG21	2:H:121:ILE:HD11	1.87	0.57
2:B:9:ILE:CG2	2:B:163:VAL:HG12	2.35	0.57
1:E:20:THR:HG22	1:E:78:LYS:HG3	1.86	0.57
1:G:136:THR:HA	1:G:186:SER:HB3	1.87	0.56
2:D:130:VAL:CG1	2:D:130:VAL:O	2.53	0.56
2:B:156:LEU:HD12	2:B:166:ILE:CD1	2.35	0.56
2:H:179:SER:HB3	2:H:197:LEU:HD13	1.85	0.56
2:F:87:VAL:HG21	2:F:121:ILE:HD11	1.86	0.56
1:A:119:PRO:HB3	1:A:173:GLY:O	2.06	0.56
1:E:168:VAL:HG12	1:E:169:ILE:N	2.21	0.56
1:G:154:LEU:HD13	1:G:183:TYR:OH	2.05	0.56
1:A:122:GLN:HB2	1:A:123:PRO:CD	2.32	0.56
1:C:135:GLY:C	1:C:137:ASN:H	2.10	0.55
2:D:156:LEU:HD12	2:D:166:ILE:CD1	2.36	0.55
2:H:162:ASP:OD2	2:H:162:ASP:C	2.45	0.55
2:D:201:GLU:O	2:D:204:LEU:HD13	2.07	0.55
2:B:55:ASP:N	2:B:55:ASP:OD2	2.39	0.55
2:H:177:LEU:HD12	2:H:177:LEU:N	2.22	0.55
1:A:107:LEU:HD11	2:B:111:LYS:HD3	1.88	0.55
1:G:143:LYS:NZ	2:H:146:LEU:HD23	2.22	0.55
2:F:210:CYS:HB3	2:F:225:ILE:HB	1.88	0.55
2:F:201:GLU:O	2:F:204:LEU:HD13	2.07	0.55
2:F:9:ILE:HG22	2:F:163:VAL:HG12	1.89	0.54
1:G:168:VAL:HG12	1:G:169:ILE:N	2.22	0.54
1:A:34:TYR:CE1	1:A:97:LEU:HB3	2.42	0.54
2:B:24:VAL:CG2	2:B:24:VAL:O	2.56	0.54
2:D:77:THR:HA	1:G:153:ASN:ND2	2.23	0.54
2:F:99:LEU:O	2:F:99:LEU:HD23	2.07	0.54
2:B:141:ILE:HG22	2:B:145:LYS:HE3	1.88	0.54
2:D:70:GLU:HB2	2:D:83:THR:HB	1.89	0.54
1:G:35:ILE:H	1:G:52:GLU:HB2	1.73	0.54
2:B:137:PHE:CD2	2:B:153:LEU:HD23	2.41	0.54
2:D:130:VAL:CG1	2:D:160:PHE:HB3	2.36	0.54
2:H:9:ILE:HG22	2:H:163:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:177:LEU:HD12	2:F:177:LEU:N	2.23	0.54
2:H:210:CYS:HB3	2:H:225:ILE:HB	1.88	0.54
1:C:136:THR:HA	1:C:186:SER:HB3	1.90	0.54
1:E:135:GLY:C	1:E:137:ASN:H	2.12	0.54
1:E:136:THR:HA	1:E:186:SER:HB3	1.89	0.54
2:B:130:VAL:CG1	2:B:130:VAL:O	2.56	0.54
2:F:30:ILE:HD12	2:F:30:ILE:N	2.23	0.53
1:C:105:ASP:HB3	2:D:36:TYR:OH	2.09	0.53
1:E:32:ASN:O	1:E:97:LEU:HB2	2.09	0.53
1:A:135:GLY:C	1:A:137:ASN:H	2.11	0.53
1:A:122:GLN:NE2	1:A:174:LYS:HG2	2.22	0.53
2:H:99:LEU:C	2:H:99:LEU:HD23	2.29	0.53
1:A:30:ILE:H	1:A:73:ASN:CG	2.11	0.53
1:C:150:ILE:HD11	1:C:193:VAL:HG11	1.90	0.53
1:E:150:ILE:HD11	1:E:193:VAL:HG11	1.91	0.53
1:C:42:GLN:O	1:C:42:GLN:HG3	2.08	0.53
1:A:136:THR:HA	1:A:186:SER:HB3	1.90	0.53
2:D:170:GLU:HB2	2:D:173:SER:O	2.09	0.53
1:E:20:THR:HG22	1:E:78:LYS:CG	2.39	0.53
1:E:119:PRO:HD2	1:E:175:TYR:OH	2.08	0.53
2:H:171:LYS:HA	2:H:209:ARG:NH2	2.12	0.53
2:B:209:ARG:HH11	2:B:209:ARG:HG2	1.73	0.53
2:D:99:LEU:HD23	2:D:99:LEU:O	2.09	0.53
2:B:177:LEU:HD12	2:B:177:LEU:N	2.24	0.53
2:B:210:CYS:HB3	2:B:225:ILE:HB	1.90	0.53
2:H:70:GLU:HB2	2:H:83:THR:HB	1.90	0.53
1:G:135:GLY:C	1:G:137:ASN:H	2.12	0.53
1:E:28:GLU:HG2	1:E:29:ALA:H	1.73	0.52
2:B:30:ILE:HG22	2:B:73:ARG:HH21	1.75	0.52
1:G:2:ILE:HD13	1:G:108:ILE:HD12	1.89	0.52
2:D:137:PHE:CD2	2:D:153:LEU:HD23	2.44	0.52
2:B:100:TRP:CZ2	2:B:111:LYS:HD2	2.44	0.52
1:A:168:VAL:HG12	1:A:169:ILE:N	2.25	0.52
2:D:34:SER:OG	2:D:53:SER:HA	2.09	0.52
1:G:158:LYS:HB2	1:G:184:GLU:HB2	1.92	0.52
2:H:209:ARG:HG3	2:H:209:ARG:HH11	1.74	0.52
2:H:201:GLU:O	2:H:204:LEU:HD13	2.10	0.52
1:A:158:LYS:HB2	1:A:184:GLU:HB2	1.92	0.52
1:E:164:ASP:H	2:F:185:MET:HE1	1.75	0.52
2:D:104:GLN:HG2	2:D:105:GLU:H	1.75	0.52
1:A:35:ILE:HG21	1:A:75:ALA:HB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HD13	1:A:183:TYR:OH	2.09	0.52
1:G:42:GLN:O	1:G:42:GLN:HG3	2.10	0.52
1:E:22:ARG:HG2	1:E:74:LEU:HD11	1.91	0.51
2:D:28:ILE:HD12	2:D:101:GLU:HG3	1.92	0.51
2:F:60:LYS:HD2	2:F:64:ILE:HB	1.93	0.51
2:F:24:VAL:HG23	2:F:24:VAL:O	2.10	0.51
2:H:161:PRO:HD2	2:H:214:HIS:NE2	2.26	0.51
1:G:63:ASN:O	1:G:80:LEU:HG	2.11	0.51
1:C:168:VAL:HG12	1:C:169:ILE:N	2.25	0.51
2:D:103:GLN:HB2	2:D:108:LYS:CB	2.41	0.51
2:F:70:GLU:HB2	2:F:83:THR:HB	1.92	0.51
2:D:130:VAL:CG1	2:D:160:PHE:H	2.15	0.51
2:D:177:LEU:HD12	2:D:177:LEU:N	2.25	0.51
2:H:60:LYS:HD2	2:H:64:ILE:HB	1.93	0.51
2:H:171:LYS:HB2	2:H:209:ARG:HH12	1.76	0.50
1:E:51:ARG:HG3	1:E:51:ARG:HH11	1.77	0.50
1:A:143:LYS:HZ3	2:B:146:LEU:HD23	1.76	0.50
1:A:7:GLU:HG2	1:A:8:HIS:CE1	2.46	0.50
2:H:21:LEU:CD1	2:H:21:LEU:N	2.74	0.50
2:B:201:GLU:O	2:B:204:LEU:HD13	2.12	0.50
1:C:120:ARG:HG2	1:C:120:ARG:NH1	2.26	0.50
2:B:168:TRP:O	2:B:169:GLU:HG3	2.12	0.50
2:B:171:LYS:HG2	2:B:209:ARG:NH2	2.27	0.50
2:F:75:PRO:HG2	2:F:76:GLU:OE1	2.11	0.50
2:H:130:VAL:CG1	2:H:160:PHE:H	2.17	0.49
1:E:137:ASN:HB3	2:F:137:PHE:HZ	1.78	0.49
1:G:137:ASN:HD21	1:G:182:LYS:NZ	2.10	0.49
1:E:103:TYR:H	1:E:103:TYR:HD2	1.60	0.49
1:G:15:ILE:HD11	1:G:169:ILE:HG21	1.93	0.49
1:C:48:PHE:CE2	2:D:110:ILE:HD13	2.46	0.49
1:G:35:ILE:CD1	1:G:94:CYS:SG	3.00	0.49
2:F:126:LEU:HD12	2:F:126:LEU:N	2.26	0.49
2:D:77:THR:O	2:D:79:THR:HG22	2.12	0.49
2:F:9:ILE:HG22	2:F:163:VAL:CG1	2.43	0.49
2:B:171:LYS:HD3	2:B:171:LYS:C	2.33	0.49
2:B:99:LEU:C	2:B:99:LEU:HD23	2.33	0.49
2:D:60:LYS:HD2	2:D:64:ILE:HB	1.95	0.49
2:H:160:PHE:HB3	2:H:161:PRO:HD3	1.94	0.49
2:B:70:GLU:HB2	2:B:83:THR:HB	1.93	0.49
1:C:51:ARG:HG3	1:C:51:ARG:HH11	1.77	0.49
1:E:105:ASP:HB3	2:F:100:TRP:NE1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:TYR:OH	2:D:111:LYS:NZ	2.41	0.49
2:F:37:TRP:O	2:F:49:LEU:HB3	2.13	0.48
2:B:21:LEU:CD1	2:B:21:LEU:N	2.76	0.48
1:C:102:GLU:H	1:C:102:GLU:CD	2.15	0.48
1:C:22:ARG:CB	1:C:74:LEU:HD21	2.43	0.48
1:G:122:GLN:HB2	1:G:123:PRO:CD	2.42	0.48
1:A:137:ASN:HB3	2:B:137:PHE:CZ	2.48	0.48
1:E:36:ASN:ND2	1:E:51:ARG:HH11	2.10	0.48
2:D:91:ASP:O	2:D:119:LEU:HD23	2.13	0.48
1:E:18:PRO:HG3	1:E:80:LEU:O	2.14	0.48
2:H:54:TYR:C	2:H:56:GLY:H	2.17	0.48
2:H:171:LYS:HD3	2:H:209:ARG:NH1	2.28	0.48
2:B:169:GLU:OE1	2:B:174:ASN:HB2	2.14	0.48
2:F:73:ARG:HG3	2:F:73:ARG:O	2.14	0.48
2:D:21:LEU:CD1	2:D:21:LEU:N	2.77	0.48
1:E:164:ASP:N	2:F:185:MET:HE1	2.29	0.48
2:H:130:VAL:O	2:H:130:VAL:CG1	2.62	0.48
1:E:51:ARG:HB3	1:E:55:ILE:HB	1.96	0.48
2:F:16:SER:OG	1:G:80:LEU:CB	2.62	0.48
2:D:162:ASP:C	2:D:162:ASP:OD2	2.52	0.48
2:H:137:PHE:CD2	2:H:153:LEU:HD23	2.49	0.47
2:F:160:PHE:O	2:F:161:PRO:C	2.52	0.47
2:D:30:ILE:CD1	2:D:30:ILE:H	2.25	0.47
1:G:124:HIS:CD2	1:G:147:PRO:HD3	2.49	0.47
1:E:137:ASN:HD21	1:E:182:LYS:NZ	2.12	0.47
2:B:160:PHE:O	2:B:161:PRO:C	2.52	0.47
2:D:146:LEU:C	2:D:148:LYS:H	2.18	0.47
1:G:166:ALA:O	1:G:177:ALA:HA	2.14	0.47
1:C:166:ALA:O	1:C:177:ALA:HA	2.14	0.47
2:H:209:ARG:HD2	2:H:224:GLU:CG	2.40	0.47
1:E:105:ASP:HB3	2:F:100:TRP:HE1	1.79	0.47
1:A:15:ILE:HD11	1:A:169:ILE:HG21	1.96	0.47
2:F:28:ILE:HG22	2:F:29:THR:N	2.30	0.47
2:B:33:THR:HG22	2:B:34:SER:H	1.79	0.47
1:E:53:LYS:O	1:E:55:ILE:HG13	2.14	0.47
2:D:73:ARG:HG3	2:D:73:ARG:O	2.13	0.47
2:D:31:SER:O	2:D:32:ALA:HB2	2.15	0.47
1:C:7:GLU:HG2	1:C:8:HIS:CE1	2.49	0.47
2:F:130:VAL:O	2:F:130:VAL:CG1	2.63	0.47
2:H:141:ILE:HG22	2:H:145:LYS:HE3	1.96	0.47
1:A:166:ALA:O	1:A:177:ALA:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:37:TRP:O	2:H:49:LEU:HB3	2.15	0.47
2:F:145:LYS:HB2	4:F:2002:HOH:O	2.15	0.47
2:B:14:THR:O	2:B:17:LYS:HB2	2.15	0.47
1:G:180:LEU:HD11	2:H:153:LEU:HD21	1.97	0.47
2:H:160:PHE:O	2:H:162:ASP:N	2.48	0.47
2:F:15:LEU:N	2:F:15:LEU:HD12	2.28	0.47
2:F:24:VAL:O	2:F:24:VAL:CG2	2.63	0.47
2:F:4:LEU:HD22	2:F:25:VAL:HG12	1.97	0.47
1:G:53:LYS:HD3	1:G:53:LYS:HA	1.58	0.47
2:B:91:ASP:O	2:B:119:LEU:HD23	2.15	0.47
2:H:9:ILE:HG22	2:H:163:VAL:CG1	2.45	0.47
2:H:160:PHE:O	2:H:161:PRO:C	2.53	0.46
1:C:137:ASN:HD21	1:C:182:LYS:NZ	2.13	0.46
2:B:9:ILE:HG22	2:B:163:VAL:HG12	1.96	0.46
1:A:117:VAL:O	1:A:169:ILE:HD11	2.15	0.46
1:G:137:ASN:HB3	2:H:137:PHE:CZ	2.50	0.46
2:B:15:LEU:CD1	2:B:15:LEU:H	2.28	0.46
2:D:13:LYS:O	2:D:121:ILE:HA	2.15	0.46
2:H:169:GLU:HG3	2:H:211:ILE:HD12	1.97	0.46
2:F:126:LEU:H	2:F:126:LEU:CD1	2.27	0.46
2:H:4:LEU:HD22	2:H:25:VAL:HG12	1.97	0.46
1:G:119:PRO:HD2	1:G:175:TYR:OH	2.16	0.46
2:F:52:ILE:O	2:F:52:ILE:HG23	2.16	0.46
2:H:73:ARG:O	2:H:75:PRO:HD3	2.15	0.46
2:F:141:ILE:HG22	2:F:145:LYS:HE3	1.96	0.46
1:G:143:LYS:HZ3	2:H:146:LEU:HD23	1.80	0.46
1:G:122:GLN:HE22	1:G:174:LYS:HG2	1.81	0.46
2:F:53:SER:HB3	2:F:55:ASP:OD2	2.15	0.46
1:G:72:LYS:HE2	1:G:72:LYS:HA	1.95	0.46
2:H:91:ASP:O	2:H:119:LEU:HD23	2.16	0.46
1:E:7:GLU:HG2	1:E:8:HIS:CE1	2.51	0.46
2:B:28:ILE:HD11	2:B:101:GLU:OE1	2.16	0.46
1:G:134:ASN:O	1:G:137:ASN:HB2	2.16	0.46
1:G:136:THR:O	1:G:182:LYS:HA	2.14	0.46
2:B:162:ASP:OD2	2:B:162:ASP:C	2.54	0.46
2:B:4:LEU:HD11	2:B:99:LEU:HD22	1.97	0.46
2:H:2:GLY:HA3	2:H:28:ILE:HG12	1.97	0.46
2:D:160:PHE:O	2:D:161:PRO:C	2.53	0.46
1:E:99:MET:HB3	1:E:103:TYR:CG	2.50	0.46
2:B:37:TRP:O	2:B:49:LEU:HB3	2.16	0.46
1:E:166:ALA:O	1:E:177:ALA:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:MET:HG3	1:E:101:GLY:N	2.29	0.46
1:A:127:PRO:HD3	1:A:195:HIS:CD2	2.51	0.45
2:B:169:GLU:HA	2:B:177:LEU:CD1	2.46	0.45
2:B:74:ILE:CD1	2:B:74:ILE:N	2.79	0.45
1:G:127:PRO:HD3	1:G:195:HIS:CD2	2.51	0.45
1:E:67:ASP:O	1:E:76:VAL:HG22	2.17	0.45
2:D:15:LEU:N	2:D:15:LEU:HD12	2.29	0.45
2:D:24:VAL:HG23	2:D:24:VAL:O	2.14	0.45
2:B:100:TRP:CE2	2:B:111:LYS:HD2	2.50	0.45
2:H:52:ILE:HG23	2:H:52:ILE:O	2.16	0.45
2:H:24:VAL:O	2:H:24:VAL:HG23	2.17	0.45
2:B:73:ARG:HD3	2:B:73:ARG:O	2.17	0.45
2:F:21:LEU:N	2:F:21:LEU:CD1	2.80	0.45
1:E:137:ASN:HB3	2:F:137:PHE:CZ	2.52	0.45
1:E:98:GLY:HA2	1:E:103:TYR:CE1	2.52	0.45
1:A:122:GLN:HE22	1:A:174:LYS:HE2	1.82	0.45
1:A:20:THR:CG2	1:A:78:LYS:HG3	2.39	0.45
1:E:134:ASN:O	1:E:137:ASN:HB2	2.16	0.45
1:E:99:MET:HB3	1:E:103:TYR:CD2	2.52	0.45
2:D:141:ILE:HG22	2:D:145:LYS:HE3	1.99	0.44
2:B:146:LEU:C	2:B:148:LYS:H	2.20	0.44
2:F:146:LEU:C	2:F:148:LYS:H	2.21	0.44
1:E:34:TYR:HB2	1:E:95:ASP:OD1	2.18	0.44
2:B:73:ARG:O	2:B:75:PRO:HD3	2.18	0.44
2:F:162:ASP:C	2:F:162:ASP:OD2	2.56	0.44
1:E:137:ASN:ND2	1:E:182:LYS:HZ3	2.15	0.44
2:B:171:LYS:HB2	2:B:207:GLU:HB3	2.00	0.44
2:H:146:LEU:C	2:H:148:LYS:H	2.20	0.44
2:H:4:LEU:HD11	2:H:99:LEU:HD22	1.99	0.44
1:C:137:ASN:HD21	1:C:182:LYS:HZ3	1.64	0.44
2:H:13:LYS:O	2:H:121:ILE:HA	2.17	0.44
1:C:164:ASP:N	2:D:185:MET:HE1	2.32	0.44
2:D:37:TRP:O	2:D:49:LEU:HB3	2.17	0.44
2:B:13:LYS:O	2:B:121:ILE:HA	2.17	0.44
2:F:13:LYS:O	2:F:121:ILE:HA	2.17	0.44
2:B:8:GLN:OE1	2:B:21:LEU:HA	2.17	0.44
1:A:136:THR:HA	1:A:183:TYR:O	2.18	0.44
1:A:102:GLU:CD	1:A:102:GLU:H	2.20	0.44
2:H:77:THR:O	2:H:79:THR:HG22	2.17	0.44
2:B:171:LYS:HG3	2:B:207:GLU:OE2	2.17	0.44
1:C:18:PRO:HG3	1:C:80:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:53:SER:HB2	2:H:55:ASP:OD2	2.18	0.44
1:G:137:ASN:HB3	2:H:137:PHE:HZ	1.83	0.44
2:B:146:LEU:HG	2:B:147:GLN:HG3	1.98	0.44
2:B:15:LEU:N	2:B:15:LEU:HD12	2.30	0.44
1:C:67:ASP:O	1:C:76:VAL:HG22	2.18	0.43
1:A:69:ASP:OD1	1:A:71:ALA:HB3	2.18	0.43
2:H:209:ARG:HG3	2:H:209:ARG:NH1	2.33	0.43
2:F:160:PHE:O	2:F:162:ASP:N	2.51	0.43
1:C:136:THR:HA	1:C:183:TYR:O	2.18	0.43
2:D:210:CYS:SG	2:D:225:ILE:HD12	2.58	0.43
2:D:61:GLU:HG3	2:D:62:SER:N	2.32	0.43
1:G:30:ILE:HD11	1:G:35:ILE:CD1	2.44	0.43
2:F:4:LEU:HD11	2:F:99:LEU:HD22	2.01	0.43
1:A:137:ASN:HB3	2:B:137:PHE:HZ	1.83	0.43
2:H:30:ILE:HB	2:H:31:SER:H	1.61	0.43
2:D:13:LYS:HD2	2:D:17:LYS:HE2	2.00	0.43
1:A:107:LEU:HD21	2:B:100:TRP:CZ2	2.53	0.43
2:B:136:ILE:HG23	2:B:227:PHE:CE1	2.54	0.43
1:G:34:TYR:CD2	1:G:52:GLU:HG2	2.52	0.43
2:H:17:LYS:HG3	2:H:18:THR:H	1.82	0.43
1:A:20:THR:HG22	1:A:78:LYS:CG	2.42	0.43
1:C:136:THR:O	1:C:182:LYS:HA	2.18	0.43
1:E:32:ASN:HA	1:E:97:LEU:HD12	1.99	0.43
2:D:8:GLN:OE1	2:D:21:LEU:HA	2.19	0.43
2:F:171:LYS:HD2	2:F:172:LYS:HZ2	1.84	0.43
1:E:74:LEU:HD12	1:E:75:ALA:H	1.79	0.43
2:H:144:THR:HA	2:H:149:ALA:O	2.19	0.43
2:B:12:THR:O	2:B:13:LYS:HD3	2.18	0.43
2:D:218:LYS:O	2:D:219:ASN:HB2	2.18	0.43
1:E:2:ILE:HD11	1:E:25:MET:HE1	2.01	0.43
1:E:136:THR:O	1:E:182:LYS:HA	2.18	0.43
1:E:127:PRO:HD3	1:E:195:HIS:CD2	2.54	0.43
1:G:55:ILE:CG2	2:H:110:ILE:HD11	2.49	0.43
1:E:70:ILE:H	1:E:70:ILE:HG13	1.52	0.43
2:B:33:THR:CG2	2:B:34:SER:N	2.82	0.43
2:D:14:THR:OG1	2:D:17:LYS:HD3	2.19	0.43
1:E:163:PHE:HB3	2:F:185:MET:HE1	2.01	0.43
1:A:99:MET:HB3	1:A:103:TYR:HB3	2.00	0.43
1:E:163:PHE:HB3	2:F:185:MET:CE	2.49	0.42
2:H:104:GLN:HB2	2:H:105:GLU:OE1	2.19	0.42
2:D:12:THR:O	2:D:13:LYS:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:ARG:HH11	2:B:73:ARG:HG2	1.83	0.42
2:B:160:PHE:HB3	2:B:161:PRO:HD3	2.01	0.42
1:E:52:GLU:O	1:E:53:LYS:HB2	2.19	0.42
2:B:106:LEU:HD12	2:B:107:GLY:N	2.34	0.42
1:A:180:LEU:HD11	2:B:153:LEU:HD21	2.01	0.42
1:E:143:LYS:NZ	2:F:146:LEU:HD23	2.35	0.42
1:E:38:TYR:HH	2:F:111:LYS:HB3	1.83	0.42
1:E:28:GLU:HG2	1:E:29:ALA:N	2.34	0.42
2:F:27:GLY:O	2:F:28:ILE:HD13	2.18	0.42
2:F:145:LYS:HD2	2:F:145:LYS:N	2.33	0.42
2:B:160:PHE:O	2:B:162:ASP:N	2.52	0.42
2:B:171:LYS:HD3	2:B:172:LYS:N	2.35	0.42
1:C:70:ILE:HG12	1:C:70:ILE:O	2.18	0.42
1:A:18:PRO:HG3	1:A:80:LEU:O	2.20	0.42
2:D:104:GLN:CD	2:D:104:GLN:H	2.21	0.42
1:C:127:PRO:HD3	1:C:195:HIS:CD2	2.55	0.42
2:F:15:LEU:CD1	2:F:15:LEU:H	2.28	0.42
1:A:30:ILE:HG22	1:A:73:ASN:OD1	2.20	0.42
2:B:145:LYS:N	2:B:145:LYS:HD2	2.34	0.42
1:C:8:HIS:O	1:C:113:THR:HB	2.19	0.42
1:G:136:THR:HA	1:G:183:TYR:O	2.19	0.42
2:F:8:GLN:OE1	2:F:21:LEU:HA	2.20	0.42
2:B:144:THR:HA	2:B:149:ALA:O	2.20	0.42
2:F:30:ILE:O	2:F:32:ALA:N	2.52	0.42
1:A:35:ILE:HD12	1:A:35:ILE:N	2.34	0.42
1:G:119:PRO:HB3	1:G:173:GLY:O	2.20	0.42
2:D:4:LEU:HD21	2:D:99:LEU:HD22	2.00	0.42
2:F:33:THR:O	2:F:73:ARG:NH2	2.53	0.42
2:B:53:SER:HB2	2:B:55:ASP:OD2	2.20	0.41
1:C:53:LYS:O	1:C:55:ILE:HG13	2.20	0.41
2:B:209:ARG:HG2	2:B:209:ARG:NH1	2.35	0.41
2:H:12:THR:O	2:H:13:LYS:HD3	2.20	0.41
1:E:119:PRO:HD2	1:E:175:TYR:CZ	2.54	0.41
2:F:144:THR:HA	2:F:149:ALA:O	2.20	0.41
1:G:150:ILE:HD11	1:G:193:VAL:CG1	2.48	0.41
2:F:15:LEU:O	2:F:16:SER:HB2	2.19	0.41
1:C:164:ASP:H	2:D:185:MET:HE1	1.84	0.41
1:A:29:ALA:HB3	1:A:32:ASN:ND2	2.35	0.41
2:H:145:LYS:HD2	2:H:145:LYS:N	2.35	0.41
2:F:34:SER:OG	2:F:53:SER:HA	2.21	0.41
1:C:2:ILE:HD13	1:C:108:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:77:THR:OG1	2:F:79:THR:HG22	2.20	0.41
2:B:41:ARG:HG3	2:B:42:PRO:HD2	2.03	0.41
2:B:61:GLU:HG3	2:B:62:SER:N	2.34	0.41
1:E:99:MET:C	1:E:101:GLY:H	2.24	0.41
2:F:171:LYS:HD3	2:F:209:ARG:HH22	1.86	0.41
2:D:5:GLU:HB2	2:D:24:VAL:CG2	2.46	0.41
2:D:87:VAL:CG2	2:D:121:ILE:HD11	2.49	0.41
2:D:177:LEU:HD22	2:D:197:LEU:HD21	2.02	0.41
2:B:31:SER:O	2:B:32:ALA:CB	2.68	0.41
2:H:177:LEU:HD22	2:H:197:LEU:HD21	2.02	0.41
1:E:69:ASP:OD1	1:E:71:ALA:HB3	2.21	0.41
1:E:87:GLU:HG3	1:E:115:VAL:O	2.21	0.41
1:C:167:ILE:N	1:C:167:ILE:HD12	2.36	0.41
1:C:126:LYS:HE3	1:C:200:VAL:HG22	2.01	0.41
1:E:126:LYS:HE3	1:E:200:VAL:HG22	2.03	0.41
1:C:203:THR:C	1:C:205:PHE:H	2.25	0.41
2:B:4:LEU:HD21	2:B:99:LEU:HD22	2.03	0.41
2:B:17:LYS:HA	2:B:17:LYS:HD2	1.85	0.41
2:D:145:LYS:HD2	2:D:145:LYS:N	2.36	0.41
1:G:132:MET:HG2	1:G:132:MET:H	1.64	0.41
1:C:145:PHE:O	1:C:175:TYR:HB2	2.21	0.40
1:A:67:ASP:O	1:A:76:VAL:HG22	2.21	0.40
2:D:15:LEU:H	2:D:15:LEU:CD1	2.29	0.40
1:C:25:MET:HG2	1:C:26:LYS:N	2.36	0.40
2:D:168:TRP:O	2:D:169:GLU:HG3	2.21	0.40
1:C:163:PHE:HB3	2:D:185:MET:CE	2.52	0.40
1:C:36:ASN:ND2	1:C:51:ARG:HG3	2.37	0.40
2:H:214:HIS:H	2:H:217:ASN:ND2	2.18	0.40
1:C:55:ILE:CG1	2:D:108:LYS:HE3	2.51	0.40
1:G:36:ASN:HA	1:G:50:TYR:O	2.21	0.40
1:E:146:TYR:CG	1:E:147:PRO:HA	2.55	0.40
1:E:136:THR:HA	1:E:183:TYR:O	2.21	0.40
2:F:137:PHE:HB2	2:F:153:LEU:HB3	2.04	0.40
1:A:122:GLN:NE2	1:A:174:LYS:HE2	2.36	0.40
1:C:135:GLY:C	1:C:137:ASN:N	2.75	0.40
2:D:24:VAL:CG2	2:D:24:VAL:O	2.69	0.40
2:D:27:GLY:O	2:D:28:ILE:HD13	2.21	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	204/229 (89%)	178 (87%)	19 (9%)	7 (3%)	5 25
1	C	204/229 (89%)	184 (90%)	16 (8%)	4 (2%)	9 39
1	E	204/229 (89%)	180 (88%)	18 (9%)	6 (3%)	6 30
1	G	204/229 (89%)	179 (88%)	17 (8%)	8 (4%)	4 22
2	B	228/242 (94%)	191 (84%)	33 (14%)	4 (2%)	11 43
2	D	228/242 (94%)	199 (87%)	25 (11%)	4 (2%)	11 43
2	F	228/242 (94%)	199 (87%)	22 (10%)	7 (3%)	5 28
2	H	228/242 (94%)	188 (82%)	29 (13%)	11 (5%)	3 17
All	All	1728/1884 (92%)	1498 (87%)	179 (10%)	51 (3%)	5 29

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	32	ALA
2	D	171	LYS
2	F	30	ILE
2	F	31	SER
2	F	171	LYS
2	H	30	ILE
2	H	32	ALA
2	H	171	LYS
2	H	174	ASN
1	A	27	GLY
1	A	52	GLU
1	A	54	ASP
1	A	135	GLY
2	B	229	PRO
1	C	135	GLY
2	D	32	ALA
2	D	229	PRO

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Mol	Chain	Res	Type
1	E	73	ASN
1	E	135	GLY
2	F	229	PRO
1	G	100	GLY
1	G	135	GLY
2	H	31	SER
2	H	229	PRO
1	A	134	ASN
1	C	52	GLU
1	E	54	ASP
1	E	134	ASN
2	F	126	LEU
2	F	174	ASN
2	H	55	ASP
1	A	144	GLU
2	B	31	SER
1	C	134	ASN
2	D	146	LEU
1	E	53	LYS
1	E	144	GLU
2	F	146	LEU
1	G	52	GLU
1	G	103	TYR
1	G	134	ASN
1	G	144	GLU
2	B	146	LEU
1	C	144	GLU
1	G	98	GLY
2	H	78	SER
2	H	103	GLN
2	H	146	LEU
1	A	103	TYR
1	G	70	ILE
2	H	161	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	180/203 (89%)	174 (97%)	6 (3%)	45 79
1	C	180/203 (89%)	173 (96%)	7 (4%)	39 75
1	E	180/203 (89%)	173 (96%)	7 (4%)	39 75
1	G	180/203 (89%)	171 (95%)	9 (5%)	30 68
2	B	208/220 (94%)	195 (94%)	13 (6%)	22 58
2	D	208/220 (94%)	196 (94%)	12 (6%)	25 61
2	F	208/220 (94%)	193 (93%)	15 (7%)	18 53
2	H	208/220 (94%)	193 (93%)	15 (7%)	18 53
All	All	1552/1692 (92%)	1468 (95%)	84 (5%)	27 64

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	CYS
1	A	97	LEU
1	A	103	TYR
1	A	113	THR
1	A	131	VAL
1	A	132	MET
2	B	18	THR
2	B	21	LEU
2	B	30	ILE
2	B	41	ARG
2	B	73	ARG
2	B	79	THR
2	B	99	LEU
2	B	123	ASP
2	B	145	LYS
2	B	153	LEU
2	B	162	ASP
2	B	192	MET
2	B	222	ASP
1	C	35	ILE
1	C	92	CYS
1	C	102	GLU
1	C	103	TYR
1	C	113	THR
1	C	131	VAL
1	C	132	MET
2	D	18	THR

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Mol	Chain	Res	Type
2	D	21	LEU
2	D	41	ARG
2	D	79	THR
2	D	99	LEU
2	D	104	GLN
2	D	134	PRO
2	D	145	LYS
2	D	153	LEU
2	D	162	ASP
2	D	192	MET
2	D	222	ASP
1	E	92	CYS
1	E	102	GLU
1	E	103	TYR
1	E	113	THR
1	E	120	ARG
1	E	131	VAL
1	E	132	MET
2	F	18	THR
2	F	21	LEU
2	F	29	THR
2	F	30	ILE
2	F	41	ARG
2	F	73	ARG
2	F	99	LEU
2	F	104	GLN
2	F	123	ASP
2	F	134	PRO
2	F	145	LYS
2	F	153	LEU
2	F	162	ASP
2	F	192	MET
2	F	222	ASP
1	G	35	ILE
1	G	70	ILE
1	G	72	LYS
1	G	74	LEU
1	G	92	CYS
1	G	113	THR
1	G	131	VAL
1	G	132	MET
1	G	158	LYS

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Mol	Chain	Res	Type
2	H	18	THR
2	H	21	LEU
2	H	33	THR
2	H	41	ARG
2	H	54	TYR
2	H	73	ARG
2	H	78	SER
2	H	99	LEU
2	H	104	GLN
2	H	126	LEU
2	H	145	LYS
2	H	153	LEU
2	H	162	ASP
2	H	192	MET
2	H	222	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	32	ASN
1	A	36	ASN
1	A	122	GLN
1	A	137	ASN
2	B	3	HIS
2	B	90	GLN
2	B	147	GLN
2	B	214	HIS
2	B	216	ASN
2	B	223	GLN
1	C	8	HIS
1	C	32	ASN
1	C	36	ASN
1	C	73	ASN
1	C	122	GLN
1	C	137	ASN
2	D	3	HIS
2	D	90	GLN
2	D	216	ASN
2	D	223	GLN
1	E	8	HIS
1	E	36	ASN

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Mol	Chain	Res	Type
1	E	122	GLN
1	E	137	ASN
1	E	153	ASN
2	F	3	HIS
2	F	90	GLN
2	F	103	GLN
2	F	147	GLN
2	F	208	HIS
2	F	214	HIS
2	F	216	ASN
1	G	8	HIS
1	G	9	GLN
1	G	122	GLN
1	G	137	ASN
1	G	195	HIS
2	H	90	GLN
2	H	214	HIS
2	H	216	ASN
2	H	217	ASN

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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	D	1002	-	4,4,4	0.07	0	6,6,6	0.14	0
3	SO4	F	1001	-	4,4,4	0.28	0	6,6,6	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	D	1002	-	-	0/0/0/0	0/0/0/0
3	SO4	F	1001	-	-	0/0/0/0	0/0/0/0

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.