Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 06:30 PM EDT

PDB ID	:	6WH9
Title	:	Ketoreductase from module 1 of the 6-deoxyerythronolide B synthase (KR1) in complex with antibody fragment (Fab) 1D10
Authors	:	Cogan, D.P.; Mathews, I.I.; Khosla, C.
Deposited on	:	2020-04-07
Resolution	:	2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

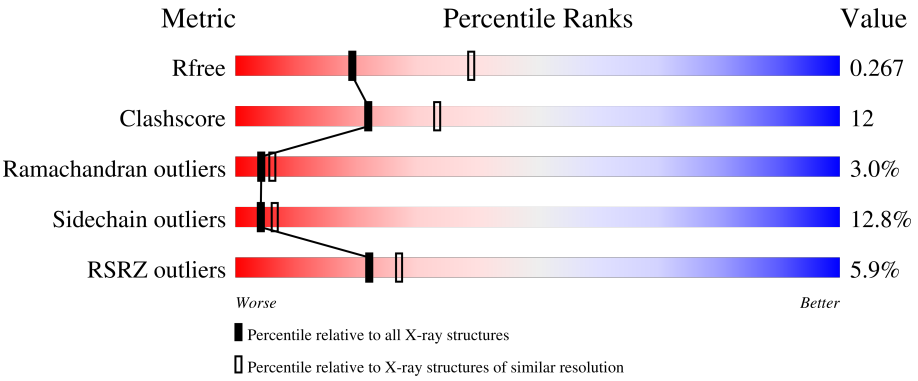
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	485	12% 65% 20% · 11%
1	D	485	6% 70% 19% · 7%
1	G	485	6% 66% 23% · 9%
2	B	246	2% 70% 17% · 9%
2	E	246	7% 54% 30% 7% 9%

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Mol	Chain	Length	Quality of chain
2	H	246	2% 63% 23% 11%
3	C	231	2% 64% 23% 6% 7%
3	F	231	2% 66% 22% 5% 6%
3	I	231	2% 66% 20% 7% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19434 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 KR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	439	Total	C	N	O	S	0	0	0
			3237	2023	590	617	7			
1	D	450	Total	C	N	O	S	0	0	0
			3283	2049	593	635	6			
1	A	431	Total	C	N	O	S	0	0	0
			3104	1940	558	599	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1444	GLY	-	expression tag	UNP Q5UNP6
G	1445	SER	-	expression tag	UNP Q5UNP6
G	1446	HIS	-	expression tag	UNP Q5UNP6
G	1447	MET	-	expression tag	UNP Q5UNP6
D	1444	GLY	-	expression tag	UNP Q5UNP6
D	1445	SER	-	expression tag	UNP Q5UNP6
D	1446	HIS	-	expression tag	UNP Q5UNP6
D	1447	MET	-	expression tag	UNP Q5UNP6
A	1444	GLY	-	expression tag	UNP Q5UNP6
A	1445	SER	-	expression tag	UNP Q5UNP6
A	1446	HIS	-	expression tag	UNP Q5UNP6
A	1447	MET	-	expression tag	UNP Q5UNP6

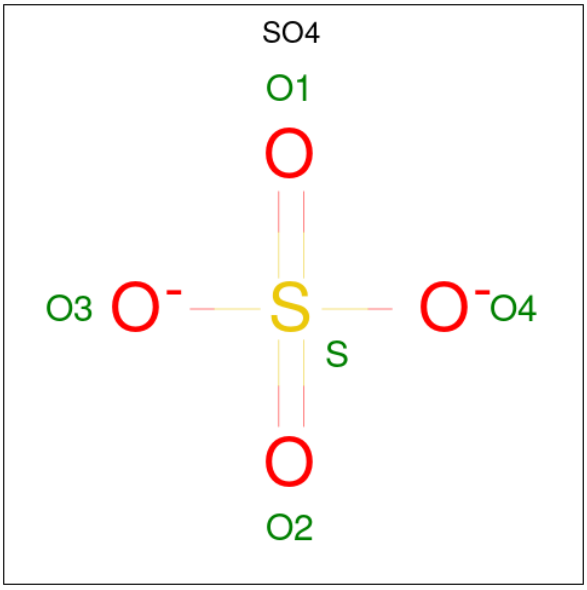
- Molecule 2 is a protein called 1D10 (Fab heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	224	Total	C	N	O	S	0	0	0
			1640	1027	275	330	8			
2	B	225	Total	C	N	O	S	0	0	0
			1633	1022	270	333	8			
2	H	219	Total	C	N	O	S	0	0	0
			1613	1013	271	322	7			

- Molecule 3 is a protein called 1D10 (Fab light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	216	Total	C	N	O	S	0	0	0
			1573	997	258	313	5			
3	C	215	Total	C	N	O	S	0	0	0
			1577	999	257	316	5			
3	I	216	Total	C	N	O	S	0	1	0
			1593	1009	259	320	5			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	O	S		0	0
			5	4	1			
4	E	1	Total	O	S		0	0
			5	4	1			
4	F	1	Total	O	S		0	0
			5	4	1			
4	B	1	Total	O	S		0	0
			5	4	1			
4	C	1	Total	O	S		0	0
			5	4	1			
4	D	1	Total	O	S		0	0
			5	4	1			
4	A	1	Total	O	S		0	0
			5	4	1			

- Molecule 5 is water.

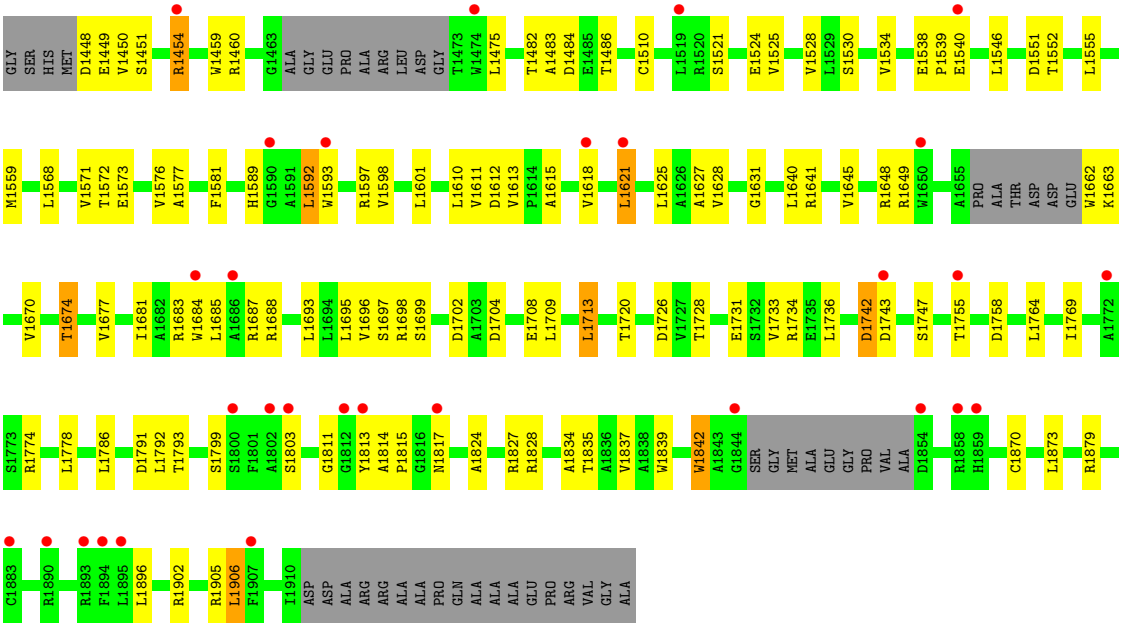
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	14	Total O 14 14	0	0
5	E	14	Total O 14 14	0	0
5	F	20	Total O 20 20	0	0
5	B	13	Total O 13 13	0	0
5	C	26	Total O 26 26	0	0
5	H	16	Total O 16 16	0	0
5	I	23	Total O 23 23	0	0
5	D	9	Total O 9 9	0	0
5	A	11	Total O 11 11	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

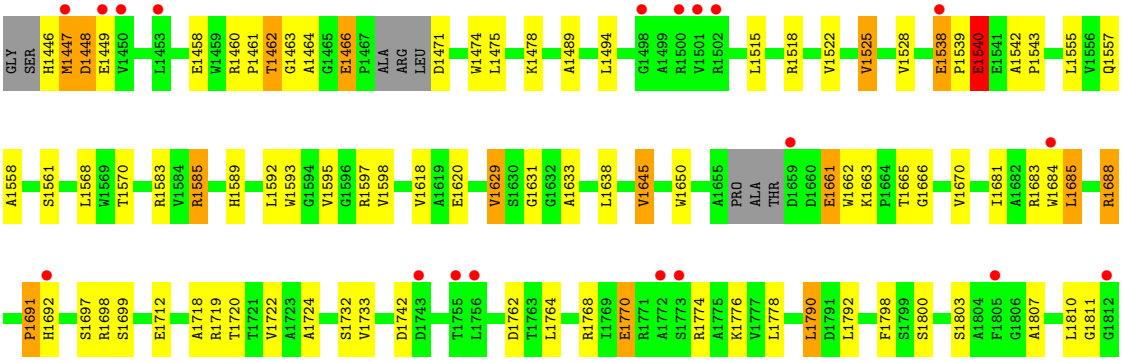
• Molecule 1: KR1

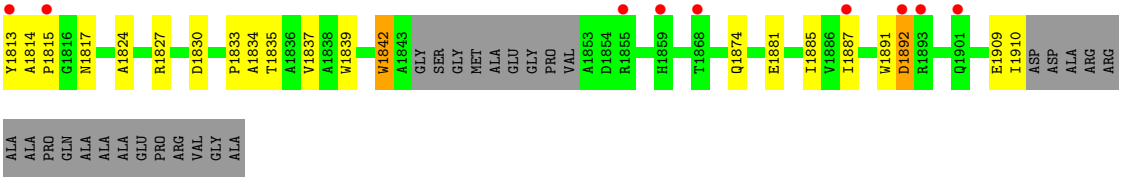
Chain G:



• Molecule 1: KR1

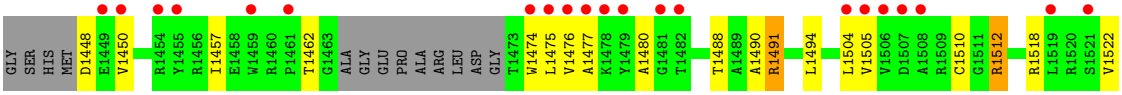
Chain D:

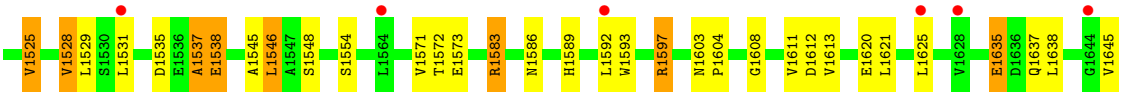


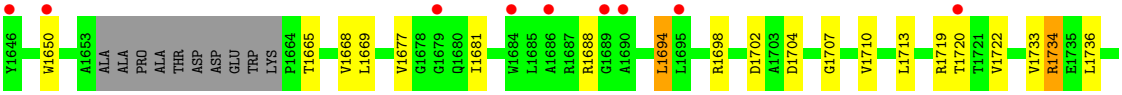


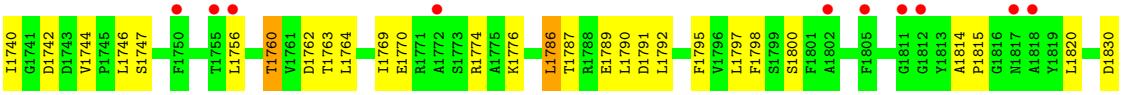
• Molecule 1: KR1

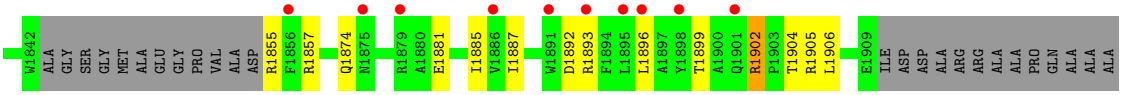
Chain A:





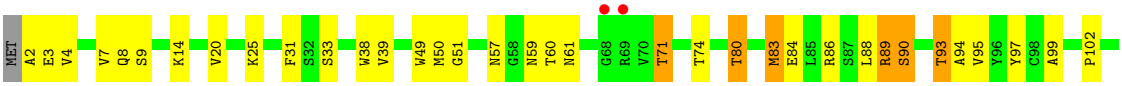


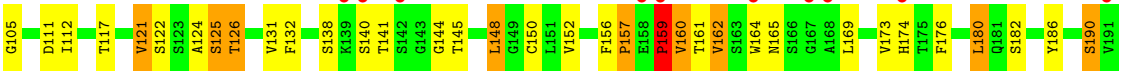


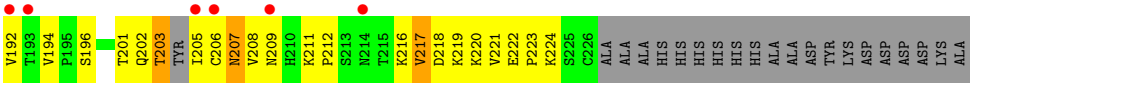


• Molecule 2: 1D10 (Fab heavy chain)

Chain E:

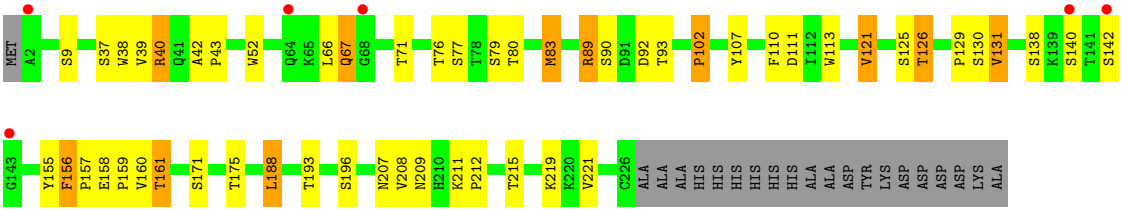




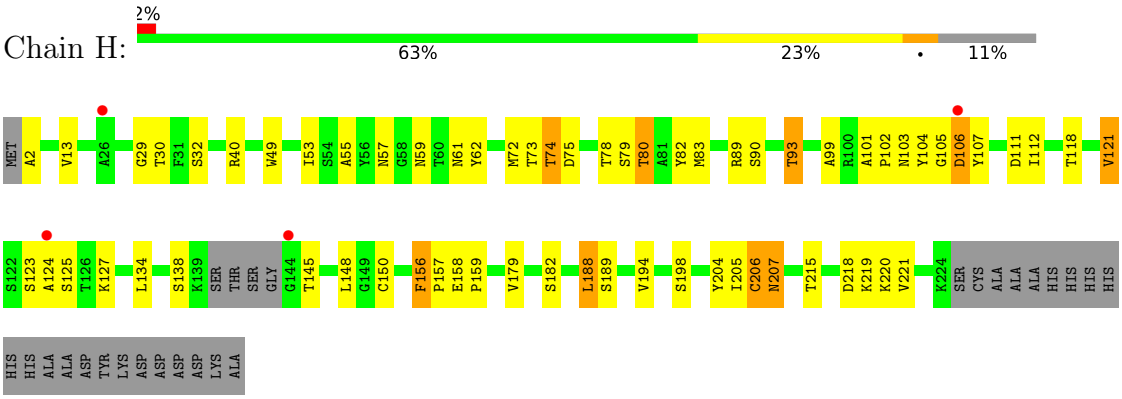


• Molecule 2: 1D10 (Fab heavy chain)

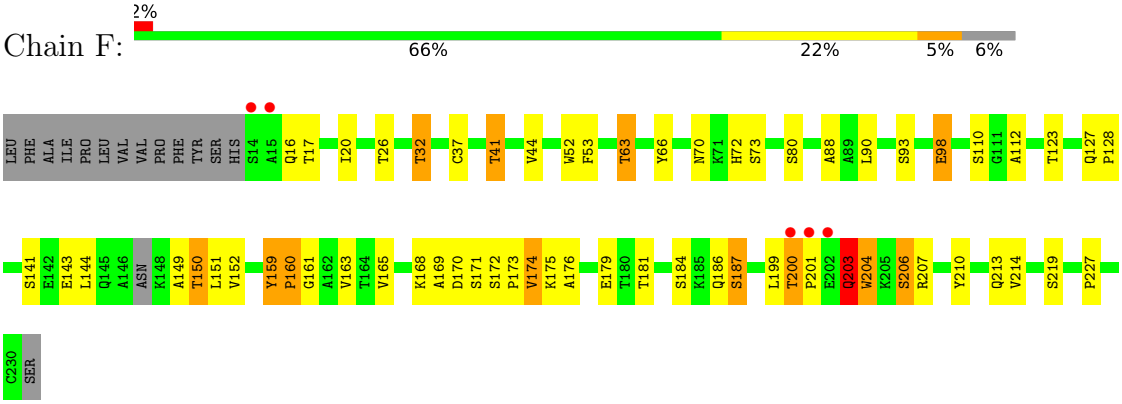
Chain B:



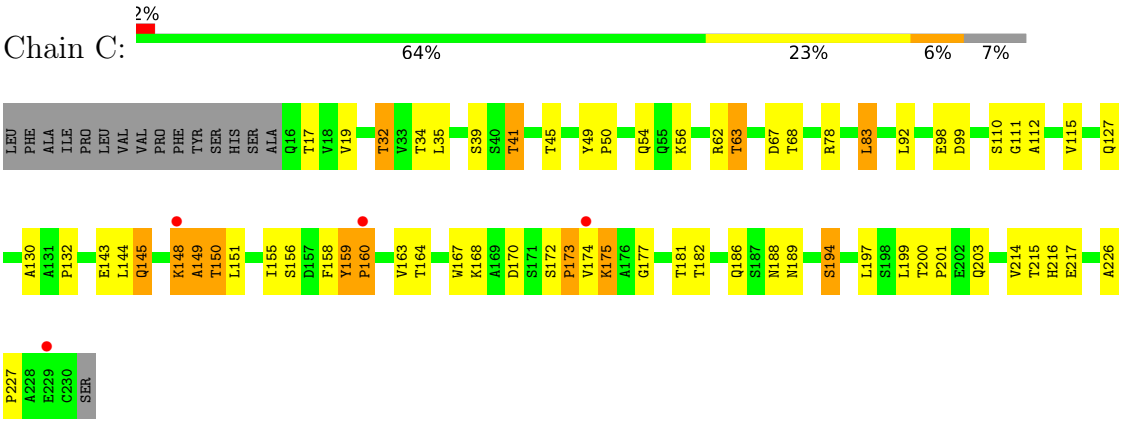
• Molecule 2: 1D10 (Fab heavy chain)



• Molecule 3: 1D10 (Fab light chain)

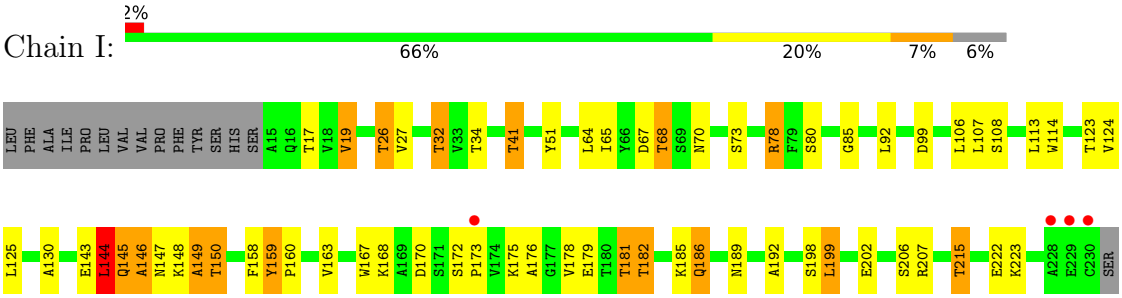


• Molecule 3: 1D10 (Fab light chain)



• Molecule 3: 1D10 (Fab light chain)

Chain I:


2%
66%
20%
7%
6%
LEU PHE ALA ILE PRO LEU VAL VAL PRO PHE TYR SER HIS SER A15 Q16 T17 V18 V19 T26 V27 T32 V33 T34 T41 Y51 L64 I65 Y66 D67 T68 S69 N70 S73 R78 F79 S80 G85 L92 D99 L106 L107 S108 L113 W114 T123 V124
L125 A130 E143 L144 Q145 A146 N147 K148 A149 T150 F158 Y159 P160 V163 W167 K168 A169 D170 S171 S172 P173 V174 K175 A176 G177 V178 E179 T180 T181 T182 K185 Q186 N189 A192 S198 L199 E202 S206 R207 T215 E222 K223 A228 E229 C230 SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	186.03Å 114.81Å 186.14Å 90.00° 96.53° 90.00°	Depositor
Resolution (Å)	39.59 – 2.75 39.59 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.59-2.75) 99.6 (39.59-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.228 , 0.271 0.229 , 0.267	Depositor DCC
R_{free} test set	5043 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	83.7	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19434	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.69	0/3156	0.81	0/4311
1	D	0.68	0/3340	0.81	0/4558
1	G	0.67	0/3294	0.80	0/4490
2	B	0.69	0/1672	0.88	0/2291
2	E	0.70	0/1676	0.87	0/2286
2	H	0.70	0/1650	0.89	0/2253
3	C	0.74	1/1620 (0.1%)	0.95	1/2223 (0.0%)
3	F	0.69	0/1615	0.91	0/2215
3	I	0.72	0/1636	0.92	0/2244
All	All	0.69	1/19659 (0.0%)	0.86	1/26871 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	159	TYR	C-N	8.23	1.49	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	159	TYR	N-CA-CB	5.98	121.37	110.60

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	3104	0	3008	54	0
1	D	3283	0	3191	59	0
1	G	3237	0	3184	65	0
2	B	1633	0	1543	32	0
2	E	1640	0	1589	78	0
2	H	1613	0	1561	49	0
3	C	1577	0	1506	60	0
3	F	1573	0	1500	36	0
3	I	1593	0	1525	37	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
5	A	11	0	0	1	0
5	B	13	0	0	0	0
5	C	26	0	0	2	0
5	D	9	0	0	0	0
5	E	14	0	0	0	0
5	F	20	0	0	3	0
5	G	14	0	0	3	0
5	H	16	0	0	0	0
5	I	23	0	0	1	0
All	All	19434	0	18607	446	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 12.

All (446) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1760:THR:HB	1:A:1762:ASP:OD1	1.60	1.00
2:E:90:SER:O	2:E:93:THR:HG23	1.66	0.96
2:B:89:ARG:HD2	2:B:90:SER:H	1.38	0.89
2:E:20:VAL:HG23	2:E:88:LEU:HD11	1.53	0.89
3:C:186:GLN:NE2	3:C:188:ASN:HD22	1.75	0.83
2:H:101:ALA:HB1	2:H:105:GLY:HA3	1.60	0.82
1:A:1764:LEU:HD21	1:A:1769:ILE:HD11	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:PRO:HB2	3:C:216:HIS:NE2	1.93	0.82
3:F:110:SER:HB3	1:D:1699:SER:HB2	1.62	0.81
3:C:159:TYR:HB3	3:C:160:PRO:HD3	1.61	0.80
3:F:168:LYS:HA	3:F:173:PRO:HD2	1.65	0.78
3:F:149:ALA:O	3:F:150:THR:OG1	2.04	0.76
3:C:160:PRO:HG2	3:C:216:HIS:CE1	2.20	0.76
2:B:156:PHE:HB3	2:B:157:PRO:HD3	1.67	0.75
2:H:78:THR:HG23	2:H:80:THR:HG23	1.66	0.75
3:I:168:LYS:HA	3:I:173:PRO:HD2	1.69	0.75
2:H:102:PRO:HD3	2:H:111:ASP:HB2	1.73	0.71
2:H:89:ARG:O	2:H:121:VAL:HG21	1.91	0.70
3:I:159:TYR:O	3:I:160:PRO:C	2.30	0.70
3:C:173:PRO:O	3:C:175:LYS:N	2.24	0.70
1:G:1451:SER:HA	1:G:1454:ARG:HD3	1.74	0.70
3:F:159:TYR:O	3:F:160:PRO:C	2.30	0.70
1:D:1597:ARG:NH1	1:D:1803:SER:O	2.25	0.70
1:G:1755:THR:HG22	5:G:2108:HOH:O	1.91	0.70
3:C:181:THR:HG22	3:C:182:THR:O	1.92	0.69
1:G:1713:LEU:HD13	1:G:1720:THR:HG21	1.72	0.69
2:E:89:ARG:HD3	2:E:90:SER:H	1.58	0.69
2:E:162:VAL:HG23	2:E:208:VAL:HG22	1.75	0.69
1:G:1699:SER:OG	3:C:110:SER:HB3	1.94	0.68
3:I:146:ALA:O	3:I:148:LYS:N	2.25	0.68
2:H:62:TYR:HE1	2:H:72:MET:HG2	1.59	0.68
1:G:1726:ASP:OD2	3:C:45:THR:HG23	1.94	0.68
3:C:144:LEU:CD2	3:C:148:LYS:CB	2.72	0.67
3:C:17:THR:OG1	3:C:41:THR:HG21	1.95	0.67
2:H:90:SER:HA	2:H:121:VAL:CG2	2.25	0.67
1:G:1764:LEU:HD21	1:G:1769:ILE:HD11	1.76	0.66
2:B:126:THR:HA	2:B:156:PHE:HB3	1.77	0.66
2:E:173:VAL:HG22	2:E:192:VAL:HG22	1.78	0.66
3:C:110:SER:OG	3:C:111:GLY:N	2.25	0.66
3:I:167:TRP:O	3:I:173:PRO:HD2	1.96	0.65
1:G:1552:THR:HG22	5:G:2101:HOH:O	1.96	0.65
3:C:167:TRP:O	3:C:173:PRO:HD2	1.96	0.65
3:F:53:PHE:CE1	3:F:63:THR:HB	2.32	0.65
3:C:186:GLN:HE22	3:C:188:ASN:HD22	1.44	0.65
2:B:93:THR:HG22	2:B:121:VAL:H	1.62	0.65
2:H:90:SER:O	2:H:93:THR:HG23	1.97	0.64
1:D:1583:ARG:NH1	1:D:1830:ASP:OD1	2.26	0.64
2:B:161:THR:HG22	2:B:209:ASN:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:143:GLU:O	3:I:145:GLN:N	2.27	0.64
1:A:1583:ARG:NH1	1:A:1830:ASP:OD1	2.31	0.63
3:F:53:PHE:CD1	3:F:63:THR:HB	2.33	0.63
3:I:206:SER:OG	3:I:207:ARG:N	2.31	0.63
2:H:90:SER:HA	2:H:121:VAL:HG23	1.79	0.63
2:H:156:PHE:HB3	2:H:157:PRO:HD3	1.81	0.63
2:E:169:LEU:HD22	2:E:192:VAL:HG11	1.80	0.63
2:H:75:ASP:OD2	2:H:78:THR:HG22	1.98	0.63
1:G:1613:VAL:HG21	1:G:1621:LEU:HD22	1.81	0.62
1:A:1475:LEU:HD23	1:A:1525:VAL:HG21	1.81	0.62
2:H:101:ALA:CB	2:H:105:GLY:HA3	2.29	0.62
3:C:160:PRO:CB	3:C:216:HIS:NE2	2.62	0.62
1:A:1597:ARG:HD2	1:A:1637:GLN:OE1	2.00	0.62
2:E:211:LYS:HB2	2:E:212:PRO:HD3	1.83	0.61
3:I:144:LEU:HA	3:I:148:LYS:CB	2.31	0.61
3:I:67:ASP:OD2	1:A:1774:ARG:NH2	2.33	0.61
2:E:25:LYS:HG3	2:E:80:THR:HG22	1.84	0.60
2:E:202:GLN:HG2	2:E:203:THR:H	1.66	0.60
1:G:1839:TRP:CD2	1:G:1842:TRP:HZ3	2.19	0.60
2:E:93:THR:HG22	2:E:121:VAL:H	1.66	0.60
3:I:32:THR:HA	3:I:92:LEU:O	2.02	0.60
2:B:89:ARG:HD2	2:B:90:SER:N	2.12	0.60
2:H:55:ALA:HA	2:H:74:THR:HG21	1.83	0.60
1:D:1458:GLU:OE1	1:D:1460:ARG:NH1	2.35	0.60
1:G:1483:ALA:O	1:G:1486:THR:N	2.33	0.59
2:E:57:ASN:OD1	2:E:59:ASN:HB2	2.02	0.59
1:D:1684:TRP:CE3	1:D:1685:LEU:HD23	2.38	0.59
3:I:143:GLU:OE1	3:I:150:THR:HG23	2.02	0.59
2:E:164:TRP:CE2	2:E:192:VAL:HG23	2.37	0.59
2:H:2:ALA:CB	2:H:103:ASN:H	2.16	0.59
1:A:1572:THR:HG21	1:A:1593:TRP:HE1	1.67	0.59
2:B:188:LEU:C	2:B:188:LEU:HD12	2.23	0.58
1:G:1611:VAL:HG23	1:G:1640:LEU:HD13	1.85	0.58
3:C:155:ILE:HG22	3:C:158:PHE:CE1	2.38	0.58
2:E:71:THR:OG1	2:E:86:ARG:NH1	2.37	0.58
1:G:1813:TYR:O	1:G:1817:ASN:ND2	2.35	0.58
3:C:132:PRO:HB3	3:C:158:PHE:CD1	2.39	0.58
2:E:162:VAL:CG1	2:E:162:VAL:O	2.51	0.57
3:C:181:THR:CG2	3:C:182:THR:O	2.51	0.57
3:C:144:LEU:HD23	3:C:148:LYS:CB	2.34	0.57
3:F:168:LYS:CA	3:F:173:PRO:HD2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:168:LYS:HA	3:I:173:PRO:CD	2.35	0.57
1:D:1460:ARG:HG3	1:D:1909:GLU:OE1	2.04	0.57
1:D:1589:HIS:HA	1:D:1592:LEU:HD12	1.87	0.57
1:G:1683:ARG:O	1:G:1687:ARG:HG2	2.04	0.57
1:G:1581:PHE:HA	1:D:1462:THR:HG22	1.85	0.57
3:C:143:GLU:C	3:C:145:GLN:H	2.08	0.57
2:E:164:TRP:CD1	2:E:192:VAL:HG22	2.40	0.57
3:F:26:THR:HG22	3:F:123:THR:OG1	2.04	0.57
1:G:1731:GLU:OE1	1:G:1734:ARG:NH2	2.38	0.56
1:G:1814:ALA:HB3	1:G:1815:PRO:HD3	1.86	0.56
2:E:132:PHE:CE1	3:F:143:GLU:HA	2.40	0.56
1:D:1474:TRP:CZ2	1:D:1629:VAL:HG11	2.41	0.56
1:D:1539:PRO:O	1:D:1540:GLU:O	2.24	0.56
1:A:1764:LEU:HD21	1:A:1769:ILE:CD1	2.35	0.56
3:I:186[B]:GLN:HE21	3:I:192:ALA:HB2	1.71	0.56
1:D:1814:ALA:HB3	1:D:1815:PRO:HD3	1.87	0.56
2:E:8:GLN:NE2	2:E:117:THR:HG23	2.21	0.56
3:F:32:THR:HG21	5:F:418:HOH:O	2.05	0.56
1:D:1684:TRP:CE3	1:D:1685:LEU:CD2	2.89	0.56
3:C:160:PRO:CG	3:C:216:HIS:CE1	2.89	0.56
3:F:200:THR:CB	3:F:201:PRO:HD3	2.36	0.55
3:C:163:VAL:HG12	3:C:216:HIS:HB2	1.87	0.55
1:G:1693:LEU:HB2	1:G:1720:THR:HG22	1.88	0.55
1:G:1726:ASP:OD1	1:G:1728:THR:OG1	2.22	0.55
2:E:222:GLU:CB	2:E:223:PRO:CD	2.84	0.55
1:A:1740:ILE:HD12	1:A:1746:LEU:HB2	1.89	0.55
1:G:1625:LEU:O	1:G:1628:VAL:HG12	2.07	0.55
2:H:101:ALA:HB1	2:H:105:GLY:CA	2.35	0.55
1:D:1813:TYR:O	1:D:1817:ASN:ND2	2.39	0.55
2:E:160:VAL:HG13	2:E:208:VAL:HG13	1.88	0.55
1:A:1688:ARG:HH21	1:A:1874:GLN:NE2	2.04	0.55
3:I:143:GLU:C	3:I:145:GLN:H	2.10	0.54
3:F:159:TYR:HB3	3:F:160:PRO:HD3	1.89	0.54
1:G:1597:ARG:NH1	1:G:1803:SER:O	2.41	0.54
2:E:111:ASP:OD1	3:F:72:HIS:NE2	2.40	0.54
1:A:1635:GLU:HB3	1:A:1638:LEU:HD21	1.90	0.54
1:A:1650:TRP:CD1	1:A:1906:LEU:HD21	2.42	0.54
3:C:148:LYS:H	3:C:201:PRO:HD3	1.73	0.54
1:D:1770:GLU:OE2	1:D:1774:ARG:NH1	2.40	0.54
1:A:1688:ARG:NH2	1:A:1874:GLN:NE2	2.55	0.54
2:H:104:TYR:CB	1:A:1512:ARG:HH12	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:159:TYR:HB3	3:I:160:PRO:HD3	1.89	0.54
2:E:8:GLN:HE21	2:E:117:THR:HG23	1.72	0.54
2:B:83:MET:SD	2:B:83:MET:C	2.86	0.54
2:E:164:TRP:HE1	2:E:173:VAL:HG13	1.72	0.54
1:D:1474:TRP:CH2	1:D:1629:VAL:HG11	2.42	0.54
1:G:1528:VAL:HG11	1:G:1559:MET:SD	2.48	0.53
3:C:160:PRO:CG	3:C:216:HIS:NE2	2.71	0.53
1:A:1776:LYS:HG2	1:A:1820:LEU:HD11	1.90	0.53
2:E:9:SER:O	2:E:117:THR:HG22	2.08	0.53
3:F:204:TRP:CZ2	3:F:227:PRO:HA	2.43	0.53
1:A:1744:VAL:HG13	1:A:1744:VAL:O	2.08	0.53
1:D:1515:LEU:HD23	1:D:1558:ALA:CB	2.38	0.53
1:D:1466:GLU:HB2	1:D:1631:GLY:HA2	1.91	0.53
2:H:148:LEU:HD11	2:H:221:VAL:HG12	1.90	0.53
2:H:179:VAL:HG21	3:I:179:GLU:HB3	1.88	0.53
2:H:101:ALA:CB	2:H:106:ASP:H	2.21	0.53
2:E:157:PRO:HB3	2:E:212:PRO:HD2	1.89	0.53
3:C:78:ARG:NH1	3:C:99:ASP:OD1	2.42	0.53
2:B:113:TRP:HE1	3:C:63:THR:HG22	1.73	0.53
3:I:17:THR:OG1	3:I:41:THR:HG21	2.09	0.53
1:G:1459:TRP:CZ2	1:G:1576:VAL:HG11	2.44	0.53
2:E:162:VAL:HG11	2:E:190:SER:CB	2.38	0.52
2:E:180:LEU:HB3	2:E:186:TYR:CE1	2.45	0.52
3:C:130:ALA:HB3	3:C:159:TYR:H	1.74	0.52
1:G:1696:VAL:HG11	1:G:1736:LEU:HD21	1.91	0.52
1:G:1747:SER:O	1:G:1793:THR:N	2.38	0.52
3:C:56:LYS:HE2	3:C:98:GLU:O	2.09	0.52
3:F:110:SER:HB3	1:D:1699:SER:CB	2.34	0.52
3:I:108:SER:OG	1:A:1698:ARG:NH1	2.43	0.52
2:E:164:TRP:HB2	2:E:169:LEU:O	2.10	0.52
2:B:93:THR:CG2	2:B:121:VAL:H	2.22	0.52
2:H:62:TYR:CE1	2:H:72:MET:HG2	2.44	0.52
1:A:1620:GLU:CD	1:A:1620:GLU:H	2.13	0.52
1:A:1474:TRP:CB	5:A:2110:HOH:O	2.58	0.51
1:G:1839:TRP:CD2	1:G:1842:TRP:CZ3	2.97	0.51
2:E:169:LEU:CD2	2:E:192:VAL:HG11	2.40	0.51
1:D:1461:PRO:O	1:D:1462:THR:HG23	2.11	0.51
1:D:1557:GLN:NE2	1:D:1764:LEU:O	2.42	0.51
1:G:1551:ASP:O	1:G:1555:LEU:HB2	2.10	0.51
2:B:40:ARG:NH2	2:B:92:ASP:OD1	2.44	0.51
2:H:102:PRO:HD3	2:H:111:ASP:CB	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1505:VAL:O	1:A:1518:ARG:NH1	2.40	0.51
1:A:1734:ARG:HD3	1:A:1786:LEU:HD21	1.91	0.51
1:G:1538:GLU:O	1:G:1540:GLU:N	2.44	0.51
2:B:156:PHE:O	2:B:157:PRO:C	2.48	0.51
2:H:158:GLU:N	2:H:159:PRO:CD	2.74	0.51
1:D:1464:ALA:HA	1:D:1633:ALA:HB2	1.93	0.51
1:G:1681:ILE:O	1:G:1685:LEU:HB2	2.11	0.51
1:G:1482:THR:O	1:G:1483:ALA:HB3	2.11	0.50
2:H:194:VAL:HG11	2:H:204:TYR:CE1	2.46	0.50
2:H:2:ALA:HB2	2:H:102:PRO:HB2	1.92	0.50
1:A:1814:ALA:HB3	1:A:1815:PRO:HD3	1.93	0.50
2:H:124:ALA:HB1	2:H:156:PHE:CG	2.47	0.50
1:G:1555:LEU:HD13	1:G:1568:LEU:HD11	1.93	0.50
1:A:1573:GLU:HA	1:A:1613:VAL:O	2.11	0.50
1:G:1534:VAL:HG13	1:G:1573:GLU:CD	2.33	0.50
3:F:159:TYR:O	3:F:161:GLY:N	2.44	0.50
2:E:131:VAL:HG21	2:E:217:VAL:HG11	1.92	0.50
3:F:32:THR:HG22	5:F:403:HOH:O	2.11	0.50
3:C:155:ILE:HG22	3:C:158:PHE:HE1	1.77	0.50
3:C:181:THR:HB	3:C:194:SER:H	1.77	0.50
2:E:164:TRP:CD1	2:E:192:VAL:CG2	2.94	0.49
2:E:209:ASN:HA	2:E:216:LYS:HA	1.94	0.49
2:E:124:ALA:O	2:E:125:SER:HB2	2.12	0.49
2:E:148:LEU:HD21	2:E:194:VAL:HG13	1.94	0.49
1:A:1490:ALA:O	1:A:1494:LEU:HD23	2.12	0.49
2:E:20:VAL:O	2:E:84:GLU:HA	2.13	0.49
2:H:156:PHE:O	2:H:157:PRO:C	2.51	0.49
1:A:1635:GLU:OE1	1:A:1905:ARG:HB2	2.13	0.49
3:F:203:GLN:OE1	3:F:203:GLN:HA	2.10	0.49
3:I:19:VAL:CG1	3:I:107:LEU:HD12	2.43	0.49
1:G:1774:ARG:NH2	3:C:67:ASP:OD1	2.46	0.49
1:A:1707:GLY:O	1:A:1710:VAL:HG12	2.13	0.49
1:G:1530:SER:CB	5:G:2101:HOH:O	2.60	0.48
2:E:95:VAL:HG23	2:E:97:TYR:CE2	2.48	0.48
3:C:143:GLU:CB	5:C:409:HOH:O	2.61	0.48
3:C:159:TYR:O	3:C:159:TYR:CD1	2.66	0.48
1:D:1489:ALA:CB	1:D:1618:VAL:CG1	2.91	0.48
2:E:164:TRP:CE2	2:E:192:VAL:CG2	2.97	0.48
2:E:144:GLY:O	2:E:196:SER:OG	2.26	0.48
2:B:158:GLU:O	2:B:158:GLU:OE2	2.32	0.48
3:F:127:GLN:HB2	3:F:128:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:215:THR:HG23	5:I:311:HOH:O	2.13	0.48
1:D:1807:ALA:HB3	1:D:1810:LEU:HD12	1.95	0.48
2:E:131:VAL:HG12	2:E:219:LYS:HD3	1.96	0.48
3:F:17:THR:HG23	3:F:41:THR:CG2	2.44	0.48
1:D:1837:VAL:HG11	1:D:1839:TRP:CZ2	2.48	0.48
2:H:158:GLU:N	2:H:159:PRO:HD2	2.29	0.48
3:C:188:ASN:O	3:C:189:ASN:HB2	2.13	0.47
3:I:222:GLU:HG3	3:I:222:GLU:O	2.13	0.47
1:A:1694:LEU:HD21	1:A:1736:LEU:HD11	1.94	0.47
2:B:42:ALA:O	2:B:43:PRO:C	2.52	0.47
3:I:149:ALA:HB1	3:I:199:LEU:CD2	2.45	0.47
2:B:110:PHE:O	3:C:63:THR:HG21	2.14	0.47
1:D:1540:GLU:C	1:D:1540:GLU:OE1	2.52	0.47
2:H:2:ALA:CB	2:H:103:ASN:N	2.76	0.47
3:I:78:ARG:NH2	3:I:99:ASP:OD1	2.48	0.47
2:E:156:PHE:H	2:E:157:PRO:CD	2.27	0.47
2:B:89:ARG:O	2:B:121:VAL:HG21	2.14	0.47
2:E:132:PHE:CD1	3:F:143:GLU:HA	2.49	0.47
2:E:156:PHE:N	2:E:157:PRO:CD	2.78	0.47
2:H:62:TYR:HE1	2:H:72:MET:CG	2.25	0.47
2:H:205:ILE:HD12	2:H:207:ASN:HD21	1.78	0.47
3:F:174:VAL:O	3:F:176:ALA:O	2.32	0.47
3:C:19:VAL:HG21	3:C:115:VAL:HG13	1.97	0.47
3:C:78:ARG:HG3	3:C:92:LEU:CD1	2.45	0.47
2:H:134:LEU:HG	2:H:150:CYS:HA	1.96	0.47
3:I:130:ALA:O	3:I:158:PHE:HA	2.15	0.47
2:E:159:PRO:HG2	2:E:212:PRO:HD3	1.97	0.47
1:G:1799:SER:OG	1:G:1817:ASN:HB3	2.15	0.47
1:G:1837:VAL:HG11	1:G:1839:TRP:CZ2	2.49	0.47
2:E:162:VAL:HG11	2:E:190:SER:OG	2.15	0.47
2:B:102:PRO:HD3	2:B:111:ASP:HB2	1.95	0.47
3:F:17:THR:HG23	3:F:41:THR:HG23	1.96	0.46
3:I:168:LYS:CA	3:I:173:PRO:HD2	2.42	0.46
3:I:41:THR:HB	1:A:1702:ASP:OD2	2.16	0.46
3:I:149:ALA:HB1	3:I:199:LEU:HD23	1.97	0.46
3:F:186:GLN:HG3	3:F:187:SER:N	2.30	0.46
1:G:1839:TRP:CG	1:G:1842:TRP:HZ3	2.34	0.46
1:A:1529:LEU:HD11	1:A:1571:VAL:HG13	1.97	0.46
2:H:89:ARG:O	2:H:121:VAL:CG2	2.60	0.46
2:H:101:ALA:HB2	2:H:106:ASP:H	1.80	0.46
2:E:38:TRP:HB3	2:E:50:MET:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:ARG:HG3	3:C:92:LEU:HD12	1.98	0.46
1:D:1718:ALA:O	1:D:1720:THR:HG23	2.16	0.46
2:E:89:ARG:O	2:E:121:VAL:HG21	2.16	0.46
2:E:202:GLN:HG2	2:E:203:THR:N	2.31	0.46
1:A:1475:LEU:O	1:A:1528:VAL:HA	2.15	0.46
1:G:1552:THR:HG21	1:G:1592:LEU:CD1	2.45	0.46
2:E:206:CYS:O	2:E:218:ASP:HA	2.15	0.46
2:B:52:TRP:HE1	3:C:112:ALA:HB1	1.81	0.46
2:H:83:MET:SD	2:H:83:MET:C	2.94	0.46
1:D:1891:TRP:O	1:D:1892:ASP:C	2.54	0.46
1:G:1598:VAL:HG22	1:G:1598:VAL:O	2.16	0.45
2:H:205:ILE:HA	2:H:219:LYS:O	2.16	0.45
1:G:1459:TRP:CZ2	1:G:1576:VAL:CG1	2.99	0.45
1:G:1742:ASP:OD1	1:G:1742:ASP:N	2.50	0.45
2:E:207:ASN:OD1	2:E:207:ASN:N	2.50	0.45
2:B:90:SER:HA	2:B:121:VAL:HG23	1.98	0.45
2:H:93:THR:HG22	2:H:121:VAL:H	1.82	0.45
2:E:14:LYS:HG3	2:E:20:VAL:HG22	1.98	0.45
3:F:169:ALA:HB1	3:F:207:ARG:HG3	1.97	0.45
2:H:53:ILE:HD13	2:H:73:THR:CA	2.46	0.45
1:D:1464:ALA:HB2	1:D:1633:ALA:HB3	1.98	0.45
2:E:105:GLY:O	1:D:1768:ARG:HD2	2.17	0.45
3:F:199:LEU:HD11	3:F:210:TYR:CE2	2.51	0.45
3:C:32:THR:HG22	5:C:403:HOH:O	2.16	0.45
1:D:1839:TRP:HB3	1:D:1842:TRP:HZ3	1.82	0.45
1:A:1776:LYS:NZ	1:A:1798:PHE:O	2.49	0.45
2:E:152:VAL:HG11	2:E:160:VAL:HG11	1.98	0.45
2:H:2:ALA:CB	2:H:102:PRO:HB2	2.47	0.45
3:I:181:THR:HG23	3:I:182:THR:O	2.17	0.45
2:H:73:THR:HG22	2:H:82:TYR:HB2	1.98	0.45
2:H:124:ALA:HB1	2:H:156:PHE:CD1	2.52	0.45
3:I:26:THR:HA	3:I:123:THR:O	2.17	0.45
1:A:1457:ILE:HG12	1:A:1885:ILE:HD11	1.98	0.45
2:E:164:TRP:NE1	2:E:173:VAL:HG13	2.32	0.45
2:B:131:VAL:HG11	2:B:208:VAL:HG11	1.98	0.45
3:C:68:THR:HG23	3:C:83:LEU:HD13	1.99	0.45
2:E:83:MET:SD	2:E:83:MET:C	2.95	0.45
2:B:125:SER:O	2:B:126:THR:C	2.55	0.45
3:C:49:TYR:N	3:C:50:PRO:HD3	2.32	0.45
3:C:160:PRO:HD2	3:C:216:HIS:NE2	2.32	0.45
1:A:1770:GLU:OE1	1:A:1774:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1702:ASP:OD2	3:C:41:THR:HG22	2.16	0.44
1:A:1604:PRO:HB3	1:A:1902:ARG:HD2	1.98	0.44
2:E:162:VAL:O	2:E:162:VAL:HG12	2.17	0.44
2:B:126:THR:HA	2:B:157:PRO:HD3	1.99	0.44
1:G:1731:GLU:OE1	1:G:1731:GLU:HA	2.18	0.44
2:E:161:THR:O	2:E:208:VAL:HA	2.16	0.44
2:H:49:TRP:CZ3	3:I:113:LEU:HD12	2.53	0.44
1:G:1613:VAL:HG21	1:G:1621:LEU:CD2	2.45	0.44
1:A:1764:LEU:HD23	1:A:1764:LEU:C	2.38	0.44
1:A:1885:ILE:HG22	1:A:1887:ILE:HG22	2.00	0.44
1:D:1790:LEU:HB3	1:D:1792:LEU:HD21	2.00	0.44
1:G:1870:CYS:O	1:G:1873:LEU:HB3	2.18	0.44
3:C:149:ALA:HB2	3:C:199:LEU:O	2.18	0.44
2:E:20:VAL:CG2	2:E:88:LEU:HD11	2.38	0.44
3:I:185:LYS:CE	3:I:189:ASN:OD1	2.66	0.44
2:B:158:GLU:N	2:B:159:PRO:HD2	2.32	0.43
1:A:1480:ALA:HB2	1:A:1505:VAL:HG21	2.00	0.43
1:A:1613:VAL:HG21	1:A:1621:LEU:HD13	2.00	0.43
1:A:1776:LYS:CG	1:A:1820:LEU:HD11	2.48	0.43
3:C:168:LYS:HA	3:C:173:PRO:HD2	2.00	0.43
2:H:206:CYS:O	2:H:218:ASP:HA	2.17	0.43
1:A:1475:LEU:HD12	1:A:1504:LEU:HB2	1.99	0.43
1:A:1586:ASN:HB3	1:A:1589:HIS:CD2	2.53	0.43
2:E:164:TRP:NE1	2:E:192:VAL:HG22	2.33	0.43
3:C:143:GLU:C	3:C:145:GLN:N	2.71	0.43
2:H:57:ASN:OD1	2:H:59:ASN:HB2	2.18	0.43
3:I:27:VAL:O	3:I:124:VAL:HA	2.18	0.43
3:I:222:GLU:O	3:I:223:LYS:HD3	2.18	0.43
1:D:1620:GLU:CD	1:D:1620:GLU:H	2.21	0.43
1:G:1670:VAL:HG22	1:G:1695:LEU:HD23	1.99	0.43
3:F:123:THR:HG23	5:F:406:HOH:O	2.18	0.43
3:C:35:LEU:N	3:C:35:LEU:HD12	2.33	0.43
2:H:99:ALA:HA	2:H:112:ILE:O	2.18	0.43
1:D:1683:ARG:NH1	1:D:1712:GLU:OE1	2.51	0.43
1:D:1697:SER:O	1:D:1724:ALA:HA	2.19	0.43
1:D:1885:ILE:HG22	1:D:1887:ILE:HG22	2.00	0.43
1:D:1489:ALA:CB	1:D:1618:VAL:HG11	2.49	0.43
1:D:1650:TRP:CH2	1:D:1885:ILE:HG21	2.54	0.43
1:A:1491:ARG:HA	1:A:1494:LEU:HB2	2.00	0.43
2:E:2:ALA:HA	2:E:102:PRO:HB3	2.01	0.43
2:E:49:TRP:CZ2	2:E:51:GLY:HA2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:200:THR:O	3:C:203:GLN:HB2	2.19	0.43
1:D:1475:LEU:CD1	1:D:1525:VAL:HG21	2.47	0.43
2:E:125:SER:O	2:E:126:THR:HB	2.19	0.43
1:D:1447:MET:O	1:D:1449:GLU:N	2.50	0.43
1:G:1598:VAL:O	1:G:1598:VAL:CG2	2.66	0.43
1:G:1685:LEU:HD12	1:G:1685:LEU:HA	1.89	0.43
2:E:90:SER:HA	2:E:121:VAL:CG2	2.49	0.43
2:E:164:TRP:CD1	2:E:173:VAL:CG2	3.02	0.43
3:F:159:TYR:CD1	3:F:159:TYR:C	2.90	0.43
3:F:199:LEU:HD12	3:F:204:TRP:HB2	2.00	0.43
3:C:151:LEU:HB2	3:C:197:LEU:HB3	2.00	0.43
1:G:1662:TRP:HE1	1:G:1793:THR:HG22	1.83	0.43
2:E:160:VAL:HG13	2:E:208:VAL:CG1	2.49	0.43
2:E:174:HIS:O	2:E:176:PHE:CE1	2.71	0.43
3:I:143:GLU:O	3:I:148:LYS:CB	2.67	0.43
1:D:1688:ARG:CD	1:D:1874:GLN:HE22	2.32	0.43
1:D:1827:ARG:NH1	1:D:1833:PRO:O	2.51	0.43
1:G:1648:ARG:O	1:G:1906:LEU:HD23	2.19	0.42
2:B:38:TRP:CE2	2:B:83:MET:HB2	2.54	0.42
3:C:130:ALA:O	3:C:158:PHE:HA	2.19	0.42
3:C:160:PRO:HD2	3:C:216:HIS:CE1	2.54	0.42
3:C:160:PRO:HB3	3:C:217:GLU:OE2	2.19	0.42
1:D:1595:VAL:O	1:D:1598:VAL:HG22	2.18	0.42
1:G:1758:ASP:HB2	2:B:107:TYR:CZ	2.53	0.42
2:E:162:VAL:HA	2:E:207:ASN:O	2.19	0.42
2:H:188:LEU:C	2:H:188:LEU:HD23	2.40	0.42
1:A:1795:PHE:CE2	1:A:1797:LEU:HD21	2.53	0.42
2:E:61:ASN:ND2	3:F:112:ALA:HB3	2.34	0.42
3:I:51:TYR:HB2	3:I:106:LEU:HB3	2.01	0.42
3:I:144:LEU:HD12	3:I:148:LYS:CB	2.49	0.42
2:E:220:LYS:HD3	2:E:220:LYS:C	2.40	0.42
2:B:89:ARG:NH1	2:B:90:SER:OG	2.51	0.42
2:B:131:VAL:HG11	2:B:208:VAL:CG1	2.50	0.42
1:A:1611:VAL:HA	1:A:1638:LEU:O	2.18	0.42
2:E:164:TRP:HB3	2:E:169:LEU:HB3	2.01	0.42
3:F:163:VAL:CG2	3:F:214:VAL:HG13	2.49	0.42
1:D:1471:ASP:OD1	1:D:1471:ASP:C	2.57	0.42
1:D:1824:ALA:HA	1:D:1834:ALA:HB1	2.01	0.42
1:A:1545:ALA:O	1:A:1546:LEU:C	2.57	0.42
1:G:1674:THR:HG21	1:G:1697:SER:OG	2.20	0.42
3:C:148:LYS:H	3:C:201:PRO:HG3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1464:ALA:HB1	1:D:1631:GLY:HA3	2.01	0.42
1:D:1593:TRP:HB3	1:D:1597:ARG:NH2	2.35	0.42
2:E:165:ASN:HA	2:E:205:ILE:HG12	2.01	0.42
3:F:168:LYS:HD3	3:F:213:GLN:NE2	2.35	0.42
2:B:90:SER:HA	2:B:121:VAL:CG2	2.49	0.42
2:B:188:LEU:C	2:B:188:LEU:CD1	2.88	0.42
2:H:30:THR:HG21	1:A:1763:THR:HG21	2.02	0.42
1:G:1589:HIS:O	1:G:1592:LEU:HB2	2.20	0.42
2:B:211:LYS:N	2:B:212:PRO:CD	2.83	0.42
2:H:53:ILE:CD1	2:H:73:THR:HA	2.50	0.42
1:D:1474:TRP:CH2	1:D:1629:VAL:CG1	3.03	0.42
2:E:111:ASP:HA	3:F:63:THR:HG21	2.02	0.42
1:D:1463:GLY:HA3	1:D:1645:VAL:HG21	2.02	0.42
1:D:1538:GLU:CG	1:D:1538:GLU:O	2.68	0.41
1:D:1910:ILE:HD12	1:D:1910:ILE:O	2.20	0.41
1:A:1477:ALA:HA	1:A:1504:LEU:O	2.19	0.41
1:G:1593:TRP:HB3	1:G:1597:ARG:NH2	2.34	0.41
3:C:155:ILE:HG21	3:C:214:VAL:HG11	2.02	0.41
2:H:29:GLY:HA3	2:H:103:ASN:OD1	2.20	0.41
1:G:1627:ALA:O	1:G:1631:GLY:N	2.45	0.41
1:G:1684:TRP:CD1	1:G:1870:CYS:HB3	2.55	0.41
1:G:1774:ARG:O	1:G:1778:LEU:N	2.52	0.41
2:E:125:SER:O	2:E:126:THR:CB	2.69	0.41
2:E:148:LEU:O	2:E:148:LEU:HG	2.20	0.41
3:C:127:GLN:HG2	3:C:159:TYR:CG	2.56	0.41
2:H:205:ILE:HG22	2:H:220:LYS:HA	2.02	0.41
1:D:1661:GLU:O	1:D:1663:LYS:N	2.46	0.41
1:A:1572:THR:CG2	1:A:1612:ASP:HA	2.50	0.41
1:A:1604:PRO:CB	1:A:1902:ARG:HD2	2.50	0.41
1:G:1824:ALA:HA	1:G:1834:ALA:HB1	2.01	0.41
2:E:145:THR:HA	2:E:194:VAL:O	2.20	0.41
3:C:83:LEU:HD12	3:C:83:LEU:HA	1.93	0.41
1:D:1774:ARG:O	1:D:1778:LEU:HB2	2.20	0.41
1:A:1537:ALA:O	1:A:1538:GLU:CB	2.69	0.41
3:C:226:ALA:HA	3:C:227:PRO:HD2	1.89	0.41
1:A:1476:VAL:HG13	1:A:1476:VAL:O	2.20	0.41
1:G:1662:TRP:NE1	1:G:1793:THR:HG22	2.36	0.41
3:C:159:TYR:HB3	3:C:160:PRO:CD	2.42	0.41
2:H:53:ILE:HD13	2:H:73:THR:HA	2.02	0.41
1:D:1598:VAL:HG21	1:D:1811:GLY:HA2	2.02	0.41
3:C:159:TYR:CD1	3:C:159:TYR:C	2.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:64:LEU:O	3:I:65:ILE:HD13	2.21	0.41
1:D:1555:LEU:HD13	1:D:1568:LEU:HD11	2.02	0.41
1:D:1681:ILE:HG12	1:D:1798:PHE:HZ	1.86	0.41
3:F:66:TYR:CZ	3:F:70:ASN:HB3	2.56	0.41
2:B:129:PRO:HB3	2:B:155:TYR:HB3	2.02	0.41
3:C:54:GLN:OE1	3:C:62:ARG:NH2	2.50	0.41
1:G:1572:THR:OG1	1:G:1612:ASP:OD1	2.29	0.41
1:G:1597:ARG:O	1:G:1601:LEU:HD12	2.20	0.41
1:G:1598:VAL:HG11	1:G:1811:GLY:HA2	2.02	0.41
2:E:99:ALA:HA	2:E:112:ILE:O	2.21	0.41
2:B:66:LEU:O	2:B:67:GLN:C	2.59	0.41
3:I:106:LEU:HD11	3:I:114:TRP:HB3	2.03	0.41
1:A:1681:ILE:HD11	1:A:1798:PHE:CE2	2.55	0.41
2:E:156:PHE:H	2:E:157:PRO:HD2	1.86	0.41
1:D:1515:LEU:CD2	1:D:1558:ALA:CB	2.99	0.41
1:A:1572:THR:HG23	1:A:1612:ASP:HA	2.02	0.41
1:D:1542:ALA:HA	1:D:1543:PRO:HD3	1.94	0.40
2:E:164:TRP:CD1	2:E:173:VAL:CG1	3.05	0.40
1:A:1787:THR:HB	1:A:1792:LEU:HD11	2.03	0.40
1:G:1733:VAL:HG23	1:G:1786:LEU:HD13	2.02	0.40
3:F:37:CYS:HB3	3:F:88:ALA:HB3	2.03	0.40
1:D:1688:ARG:HG3	1:D:1874:GLN:HE22	1.85	0.40
1:G:1621:LEU:HD13	1:G:1621:LEU:HA	1.88	0.40
3:F:52:TRP:CD2	3:F:90:LEU:HB2	2.57	0.40
1:G:1662:TRP:NE1	1:G:1793:THR:CG2	2.84	0.40
1:G:1709:LEU:CD2	1:G:1713:LEU:HD21	2.52	0.40
2:E:14:LYS:O	2:E:121:VAL:HA	2.21	0.40
2:E:38:TRP:HB3	2:E:50:MET:CE	2.51	0.40
1:D:1691:PRO:HB2	1:D:1692:HIS:ND1	2.36	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	423/485 (87%)	376 (89%)	41 (10%)	6 (1%)	11 19
1	D	442/485 (91%)	402 (91%)	28 (6%)	12 (3%)	5 7
1	G	431/485 (89%)	380 (88%)	43 (10%)	8 (2%)	8 14
2	B	223/246 (91%)	200 (90%)	16 (7%)	7 (3%)	4 6
2	E	220/246 (89%)	181 (82%)	28 (13%)	11 (5%)	2 2
2	H	215/246 (87%)	193 (90%)	20 (9%)	2 (1%)	17 31
3	C	213/231 (92%)	186 (87%)	18 (8%)	9 (4%)	3 3
3	F	212/231 (92%)	183 (86%)	18 (8%)	11 (5%)	2 2
3	I	215/231 (93%)	185 (86%)	19 (9%)	11 (5%)	2 2
All	All	2594/2886 (90%)	2286 (88%)	231 (9%)	77 (3%)	4 6

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	1484	ASP
1	G	1539	PRO
1	G	1546	LEU
1	G	1615	ALA
2	E	125	SER
2	E	159	PRO
2	E	201	THR
2	E	221	VAL
3	F	171	SER
3	F	174	VAL
3	F	206	SER
2	B	140	SER
2	B	156	PHE
3	C	148	LYS
3	C	174	VAL
2	H	156	PHE
3	I	146	ALA
3	I	147	ASN
3	I	159	TYR
1	D	1540	GLU
1	G	1449	GLU
2	E	126	THR
2	E	160	VAL
2	E	190	SER
3	F	187	SER
3	F	203	GLN

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Mol	Chain	Res	Type
2	B	126	THR
3	C	177	GLY
3	I	85	GLY
3	I	149	ALA
3	I	170	ASP
3	I	176	ALA
1	D	1662	TRP
1	D	1892	ASP
1	A	1450	VAL
1	A	1537	ALA
1	A	1892	ASP
2	E	140	SER
3	F	98	GLU
3	F	150	THR
3	F	200	THR
3	C	145	GLN
3	C	149	ALA
3	I	144	LEU
1	D	1447	MET
1	D	1462	THR
1	A	1546	LEU
1	G	1577	ALA
2	E	94	ALA
2	B	142	SER
3	C	150	THR
3	C	172	SER
3	I	68	THR
3	I	125	LEU
1	D	1448	ASP
1	D	1585	ARG
1	G	1663	LYS
1	G	1677	VAL
2	E	157	PRO
3	F	172	SER
2	B	67	GLN
2	B	77	SER
2	B	102	PRO
1	D	1666	GLY
1	D	1691	PRO
1	A	1538	GLU
1	A	1608	GLY
2	E	141	THR

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Mol	Chain	Res	Type
3	F	16	GLN
3	F	159	TYR
2	H	107	TYR
1	D	1629	VAL
3	C	160	PRO
3	C	173	PRO
3	I	172	SER
1	D	1522	VAL
1	D	1466	GLU

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	295/348 (85%)	246 (83%)	49 (17%)	2 3
1	D	315/348 (90%)	282 (90%)	33 (10%)	7 11
1	G	314/348 (90%)	278 (88%)	36 (12%)	5 9
2	B	179/202 (89%)	154 (86%)	25 (14%)	3 5
2	E	182/202 (90%)	155 (85%)	27 (15%)	3 4
2	H	178/202 (88%)	155 (87%)	23 (13%)	4 6
3	C	170/191 (89%)	157 (92%)	13 (8%)	13 23
3	F	168/191 (88%)	144 (86%)	24 (14%)	3 4
3	I	172/191 (90%)	148 (86%)	24 (14%)	3 5
All	All	1973/2223 (89%)	1719 (87%)	254 (13%)	4 6

All (254) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	1448	ASP
1	G	1450	VAL
1	G	1454	ARG
1	G	1460	ARG
1	G	1475	LEU

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Mol	Chain	Res	Type
1	G	1510	CYS
1	G	1521	SER
1	G	1524	GLU
1	G	1525	VAL
1	G	1571	VAL
1	G	1592	LEU
1	G	1610	LEU
1	G	1618	VAL
1	G	1621	LEU
1	G	1641	ARG
1	G	1645	VAL
1	G	1649	ARG
1	G	1674	THR
1	G	1688	ARG
1	G	1698	ARG
1	G	1704	ASP
1	G	1708	GLU
1	G	1713	LEU
1	G	1742	ASP
1	G	1743	ASP
1	G	1791	ASP
1	G	1792	LEU
1	G	1827	ARG
1	G	1828	ARG
1	G	1835	THR
1	G	1842	TRP
1	G	1879	ARG
1	G	1896	LEU
1	G	1902	ARG
1	G	1905	ARG
1	G	1906	LEU
2	E	3	GLU
2	E	4	VAL
2	E	7	VAL
2	E	31	PHE
2	E	33	SER
2	E	39	VAL
2	E	60	THR
2	E	71	THR
2	E	74	THR
2	E	80	THR
2	E	83	MET

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Mol	Chain	Res	Type
2	E	89	ARG
2	E	90	SER
2	E	93	THR
2	E	121	VAL
2	E	122	SER
2	E	138	SER
2	E	148	LEU
2	E	150	CYS
2	E	159	PRO
2	E	162	VAL
2	E	180	LEU
2	E	182	SER
2	E	203	THR
2	E	207	ASN
2	E	217	VAL
2	E	224	LYS
3	F	20	ILE
3	F	32	THR
3	F	41	THR
3	F	44	VAL
3	F	63	THR
3	F	73	SER
3	F	80	SER
3	F	93	SER
3	F	98	GLU
3	F	141	SER
3	F	144	LEU
3	F	151	LEU
3	F	152	VAL
3	F	160	PRO
3	F	165	VAL
3	F	170	ASP
3	F	175	LYS
3	F	179	GLU
3	F	181	THR
3	F	184	SER
3	F	203	GLN
3	F	204	TRP
3	F	206	SER
3	F	219	SER
2	B	9	SER
2	B	37	SER

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Mol	Chain	Res	Type
2	B	39	VAL
2	B	40	ARG
2	B	71	THR
2	B	76	THR
2	B	79	SER
2	B	80	THR
2	B	83	MET
2	B	89	ARG
2	B	121	VAL
2	B	130	SER
2	B	131	VAL
2	B	138	SER
2	B	160	VAL
2	B	161	THR
2	B	171	SER
2	B	175	THR
2	B	188	LEU
2	B	193	THR
2	B	196	SER
2	B	207	ASN
2	B	215	THR
2	B	219	LYS
2	B	221	VAL
3	C	32	THR
3	C	34	THR
3	C	39	SER
3	C	41	THR
3	C	63	THR
3	C	83	LEU
3	C	150	THR
3	C	156	SER
3	C	164	THR
3	C	170	ASP
3	C	175	LYS
3	C	194	SER
3	C	215	THR
2	H	13	VAL
2	H	32	SER
2	H	40	ARG
2	H	61	ASN
2	H	74	THR
2	H	79	SER

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Mol	Chain	Res	Type
2	H	80	THR
2	H	93	THR
2	H	106	ASP
2	H	118	THR
2	H	121	VAL
2	H	123	SER
2	H	125	SER
2	H	127	LYS
2	H	138	SER
2	H	145	THR
2	H	182	SER
2	H	188	LEU
2	H	189	SER
2	H	198	SER
2	H	206	CYS
2	H	207	ASN
2	H	215	THR
3	I	19	VAL
3	I	26	THR
3	I	32	THR
3	I	34	THR
3	I	41	THR
3	I	68	THR
3	I	70	ASN
3	I	73	SER
3	I	78	ARG
3	I	80	SER
3	I	144	LEU
3	I	145	GLN
3	I	150	THR
3	I	163	VAL
3	I	175	LYS
3	I	178	VAL
3	I	181	THR
3	I	182	THR
3	I	186[A]	GLN
3	I	186[B]	GLN
3	I	198	SER
3	I	199	LEU
3	I	202	GLU
3	I	215	THR
1	D	1446	HIS

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Mol	Chain	Res	Type
1	D	1448	ASP
1	D	1478	LYS
1	D	1494	LEU
1	D	1518	ARG
1	D	1525	VAL
1	D	1528	VAL
1	D	1538	GLU
1	D	1540	GLU
1	D	1561	SER
1	D	1570	THR
1	D	1585	ARG
1	D	1638	LEU
1	D	1645	VAL
1	D	1661	GLU
1	D	1665	THR
1	D	1670	VAL
1	D	1685	LEU
1	D	1688	ARG
1	D	1698	ARG
1	D	1719	ARG
1	D	1722	VAL
1	D	1732	SER
1	D	1733	VAL
1	D	1742	ASP
1	D	1762	ASP
1	D	1770	GLU
1	D	1776	LYS
1	D	1790	LEU
1	D	1800	SER
1	D	1835	THR
1	D	1842	TRP
1	D	1881	GLU
1	A	1448	ASP
1	A	1462	THR
1	A	1488	THR
1	A	1491	ARG
1	A	1510	CYS
1	A	1512	ARG
1	A	1522	VAL
1	A	1525	VAL
1	A	1528	VAL
1	A	1531	LEU

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Mol	Chain	Res	Type
1	A	1535	ASP
1	A	1548	SER
1	A	1554	SER
1	A	1583	ARG
1	A	1592	LEU
1	A	1597	ARG
1	A	1603	ASN
1	A	1625	LEU
1	A	1635	GLU
1	A	1645	VAL
1	A	1665	THR
1	A	1668	VAL
1	A	1669	LEU
1	A	1677	VAL
1	A	1694	LEU
1	A	1704	ASP
1	A	1713	LEU
1	A	1719	ARG
1	A	1720	THR
1	A	1722	VAL
1	A	1733	VAL
1	A	1734	ARG
1	A	1742	ASP
1	A	1747	SER
1	A	1756	LEU
1	A	1760	THR
1	A	1786	LEU
1	A	1789	GLU
1	A	1790	LEU
1	A	1791	ASP
1	A	1800	SER
1	A	1855	ARG
1	A	1857	ARG
1	A	1881	GLU
1	A	1893	ARG
1	A	1896	LEU
1	A	1899	THR
1	A	1902	ARG
1	A	1904	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	1589	HIS
1	G	1826	GLN
2	E	61	ASN
2	E	67	GLN
2	E	181	GLN
2	E	202	GLN
3	F	96	GLN
2	B	59	ASN
2	B	174	HIS
2	B	181	GLN
3	C	70	ASN
3	C	186	GLN
1	D	1586	ASN
1	D	1784	HIS
1	D	1874	GLN
1	A	1557	GLN
1	A	1603	ASN
1	A	1874	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

7 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	$\#\|Z\| > 2$
4	SO4	G	2001	-	4,4,4	0.40	0	6,6,6	0.09	0
4	SO4	D	2001	-	4,4,4	0.38	0	6,6,6	0.07	0
4	SO4	C	301	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	F	301	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	E	301	-	4,4,4	0.37	0	6,6,6	0.09	0
4	SO4	B	301	-	4,4,4	0.37	0	6,6,6	0.08	0
4	SO4	A	2001	-	4,4,4	0.41	0	6,6,6	0.04	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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	431/485 (88%)	0.68	56 (12%) 3 4	89, 144, 181, 212	0
1	D	450/485 (92%)	0.40	28 (6%) 20 25	76, 121, 160, 211	0
1	G	439/485 (90%)	0.45	30 (6%) 17 20	76, 119, 164, 209	0
2	B	225/246 (91%)	0.00	6 (2%) 54 63	61, 86, 111, 162	0
2	E	224/246 (91%)	0.50	18 (8%) 12 15	75, 104, 159, 232	0
2	H	219/246 (89%)	0.02	4 (1%) 68 76	57, 83, 109, 149	0
3	C	215/231 (93%)	-0.23	4 (1%) 66 75	55, 69, 101, 152	0
3	F	216/231 (93%)	-0.03	5 (2%) 60 69	57, 76, 111, 153	0
3	I	216/231 (93%)	-0.10	4 (1%) 66 75	57, 75, 113, 142	0
All	All	2635/2886 (91%)	0.27	155 (5%) 22 27	55, 104, 164, 232	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	201	PRO	9.7
3	F	200	THR	4.8
1	A	1895	LEU	4.7
2	E	206	CYS	4.5
1	A	1650	TRP	4.5
2	E	139	LYS	4.5
1	A	1450	VAL	4.5
1	A	1478	LYS	4.2
2	E	140	SER	4.0
1	A	1505	VAL	4.0
1	D	1447	MET	4.0
2	E	205	ILE	3.9
3	I	229	GLU	3.9
1	A	1477	ALA	3.9
1	G	1519	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
2	E	214	ASN	3.8
1	G	1907	PHE	3.8
1	A	1564	LEU	3.7
1	A	1479	TYR	3.7
2	E	193	THR	3.7
3	I	230	CYS	3.7
1	A	1772	ALA	3.7
2	B	143	GLY	3.6
1	D	1502	ARG	3.6
2	E	164	TRP	3.6
1	D	1449	GLU	3.4
1	D	1772	ALA	3.4
1	A	1476	VAL	3.4
1	A	1504	LEU	3.4
1	A	1531	LEU	3.4
1	D	1500	ARG	3.4
1	A	1875	ASN	3.3
2	B	2	ALA	3.3
1	A	1474	TRP	3.2
1	A	1506	VAL	3.2
2	E	209	ASN	3.2
1	D	1450	VAL	3.1
2	E	174	HIS	3.1
1	A	1811	GLY	3.1
1	A	1508	ALA	3.1
1	G	1858	ARG	3.1
2	H	124	ALA	3.1
1	A	1628	VAL	3.1
1	G	1540	GLU	3.1
2	E	167	GLY	3.0
1	D	1805	PHE	3.0
1	D	1755	THR	3.0
1	D	1893	ARG	3.0
1	A	1521	SER	2.9
1	A	1646	TYR	2.9
1	G	1854	ASP	2.9
2	B	68	GLY	2.9
2	H	106	ASP	2.9
2	B	140	SER	2.9
3	F	14	SER	2.9
1	G	1894	PHE	2.9
2	E	68	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	1454	ARG	2.8
1	G	1474	TRP	2.8
1	A	1898	TYR	2.7
1	A	1812	GLY	2.7
1	G	1800	SER	2.7
3	C	148	LYS	2.7
1	G	1772	ALA	2.7
1	D	1498	GLY	2.7
1	G	1844	GLY	2.7
2	E	158	GLU	2.7
1	A	1686	ALA	2.7
1	G	1618	VAL	2.6
1	A	1459	TRP	2.6
1	A	1449	GLU	2.6
2	E	191	VAL	2.6
1	A	1592	LEU	2.6
1	A	1896	LEU	2.5
3	F	202	GLU	2.5
1	A	1679	GLY	2.5
2	E	192	VAL	2.5
1	A	1755	THR	2.5
1	D	1812	GLY	2.5
1	A	1901	GLN	2.5
1	G	1890	ARG	2.5
1	A	1802	ALA	2.5
1	A	1695	LEU	2.5
1	A	1684	TRP	2.5
1	A	1455	TYR	2.5
1	G	1755	THR	2.4
1	D	1692	HIS	2.4
1	G	1650	TRP	2.4
1	A	1817	ASN	2.4
1	G	1590	GLY	2.4
3	I	228	ALA	2.4
1	G	1684	TRP	2.4
1	G	1893	ARG	2.4
1	D	1743	ASP	2.4
1	A	1805	PHE	2.4
1	A	1750	PHE	2.4
1	A	1507	ASP	2.4
1	A	1454	ARG	2.4
1	G	1812	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	1895	LEU	2.3
1	G	1859	HIS	2.3
1	A	1690	ALA	2.3
1	A	1891	TRP	2.3
1	A	1893	ARG	2.3
1	D	1501	VAL	2.3
3	C	160	PRO	2.3
1	D	1855	ARG	2.3
1	D	1859	HIS	2.2
2	B	142	SER	2.2
1	A	1481	GLY	2.2
1	A	1886	VAL	2.2
1	D	1453	LEU	2.2
1	A	1475	LEU	2.2
1	A	1756	LEU	2.2
1	D	1684	TRP	2.2
1	D	1538	GLU	2.2
1	G	1813	TYR	2.2
1	D	1773	SER	2.2
1	A	1818	ALA	2.2
1	D	1887	ILE	2.2
1	D	1815	PRO	2.2
1	A	1519	LEU	2.2
1	G	1593	TRP	2.2
1	G	1686	ALA	2.2
1	G	1817	ASN	2.1
3	I	173	PRO	2.1
1	G	1802	ALA	2.1
2	E	69	ARG	2.1
1	A	1461	PRO	2.1
2	H	26	ALA	2.1
1	G	1883	CYS	2.1
1	A	1625	LEU	2.1
1	G	1743	ASP	2.1
1	A	1720	THR	2.1
1	D	1756	LEU	2.1
3	C	174	VAL	2.1
3	F	15	ALA	2.1
1	G	1621	LEU	2.1
2	B	64	GLN	2.1
1	D	1868	THR	2.1
1	A	1482	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	229	GLU	2.1
1	D	1659	ASP	2.1
1	A	1856	PHE	2.1
1	D	1901	GLN	2.0
2	E	159	PRO	2.0
1	D	1892	ASP	2.0
1	A	1689	GLY	2.0
1	A	1879	ARG	2.0
1	D	1813	TYR	2.0
1	G	1803	SER	2.0
1	A	1644	GLY	2.0
2	E	168	ALA	2.0
2	E	142	SER	2.0
2	H	144	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	B	301	5/5	0.86	0.19	109,116,127,128	0
4	SO4	E	301	5/5	0.87	0.19	118,123,130,136	0
4	SO4	F	301	5/5	0.93	0.10	123,128,132,135	0
4	SO4	C	301	5/5	0.94	0.09	127,129,132,132	0
4	SO4	G	2001	5/5	0.96	0.31	86,89,101,104	0
4	SO4	A	2001	5/5	0.96	0.24	88,94,101,105	0
4	SO4	D	2001	5/5	0.97	0.30	87,90,96,96	0

6.5 Other polymers (i)

There are no such residues in this entry.