



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:23 AM GMT

PDB ID : 2WV0
Title : CRYSTAL STRUCTURE OF THE GNTR-HUTC FAMILY MEMBER
YVOA FROM BACILLUS SUBTILIS
Authors : Resch, M.; Schiltz, E.; Titgemeyer, F.; Muller, Y.A.
Deposited on : 2009-10-12
Resolution : 2.40 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

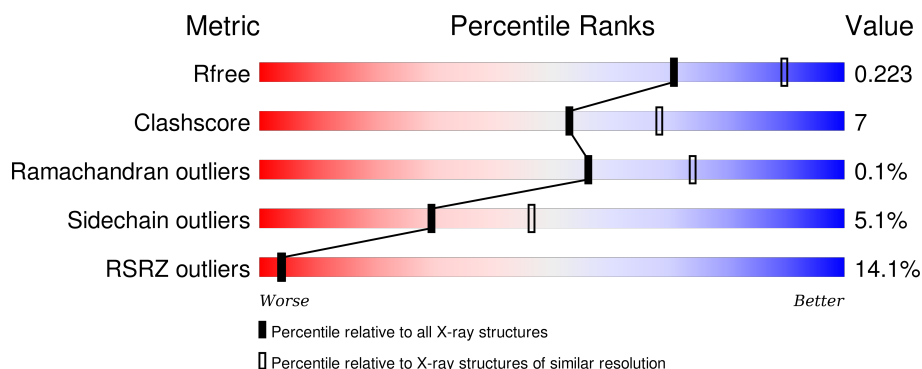
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	243	<div> <div>8%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>
1	B	243	<div> <div>9%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	C	243	<div> <div>2%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	D	243	<div> <div>7%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
1	E	243	<div> <div>12%</div> <div>79%</div> <div>15%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	243	<div><div></div><div>6%</div><div>80%</div><div>16%</div><div></div><div></div></div>
1	G	243	<div><div></div><div>12%</div><div>81%</div><div>14%</div><div></div><div></div></div>
1	H	243	<div><div></div><div>38%</div><div>72%</div><div>16%</div><div></div><div>8%</div></div>
1	I	243	<div><div></div><div>9%</div><div>85%</div><div>14%</div><div></div><div></div></div>
1	J	243	<div><div></div><div>36%</div><div>85%</div><div>10%</div><div></div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18689 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 HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	3	0
			1911	1207	330	364	10			
1	B	242	Total	C	N	O	S	0	3	0
			1872	1185	321	355	11			
1	C	242	Total	C	N	O	S	0	0	0
			1871	1180	323	358	10			
1	D	242	Total	C	N	O	S	0	5	0
			1913	1211	330	361	11			
1	E	234	Total	C	N	O	S	0	0	0
			1777	1119	306	343	9			
1	F	237	Total	C	N	O	S	0	2	0
			1853	1171	316	355	11			
1	G	237	Total	C	N	O	S	0	0	0
			1779	1123	302	345	9			
1	H	224	Total	C	N	O	S	0	0	0
			1485	922	267	291	5			
1	I	242	Total	C	N	O	S	0	0	0
			1842	1164	314	354	10			
1	J	235	Total	C	N	O	S	0	0	0
			1542	960	278	296	8			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	O	S	0	0
			5	4	1		

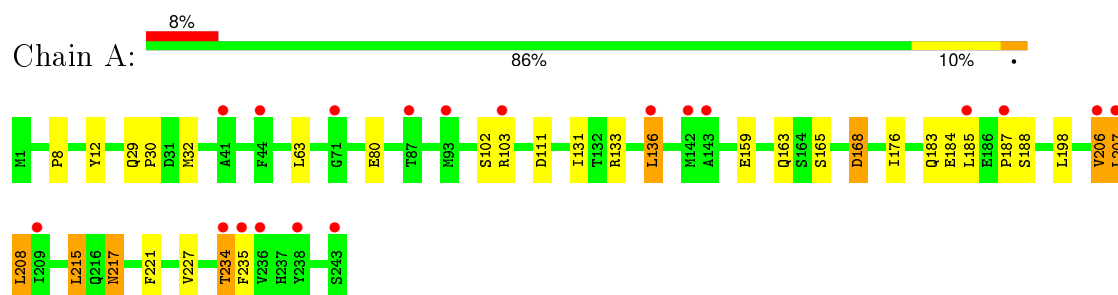
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	132	Total	O		0	0
			132	132			
3	B	109	Total	O		0	0
			109	109			
3	C	103	Total	O		0	0
			103	103			
3	D	113	Total	O		0	0
			113	113			
3	E	50	Total	O		0	0
			50	50			
3	F	93	Total	O		0	0
			93	93			
3	G	38	Total	O		0	0
			38	38			
3	H	24	Total	O		0	0
			24	24			
3	I	80	Total	O		0	0
			80	80			
3	J	27	Total	O		0	0
			27	27			

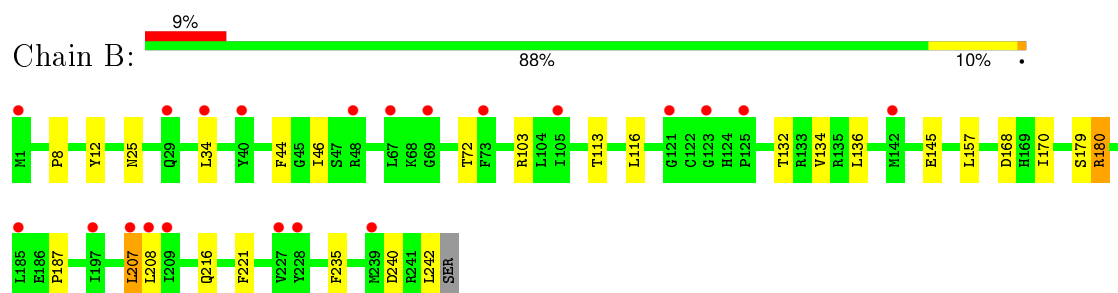
3 Residue-property plots

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.

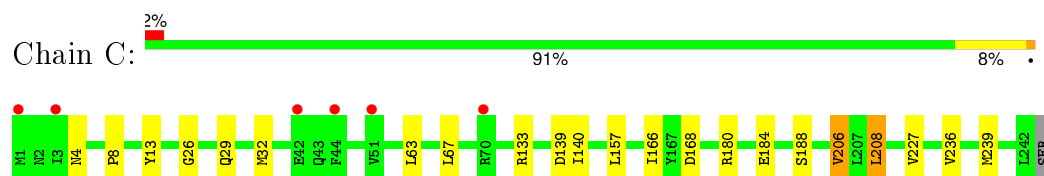
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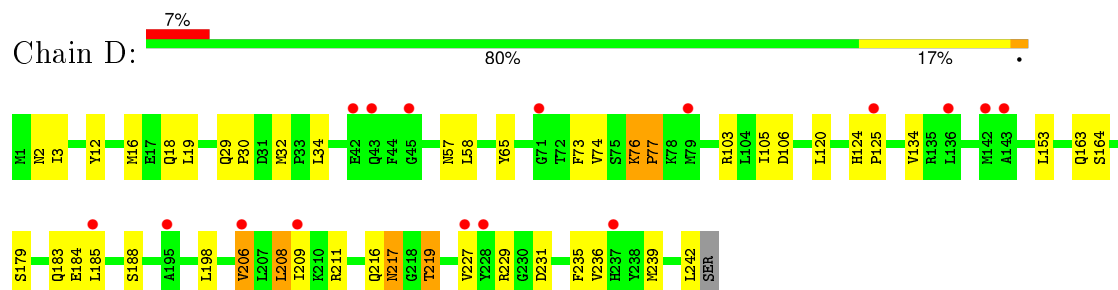
• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA



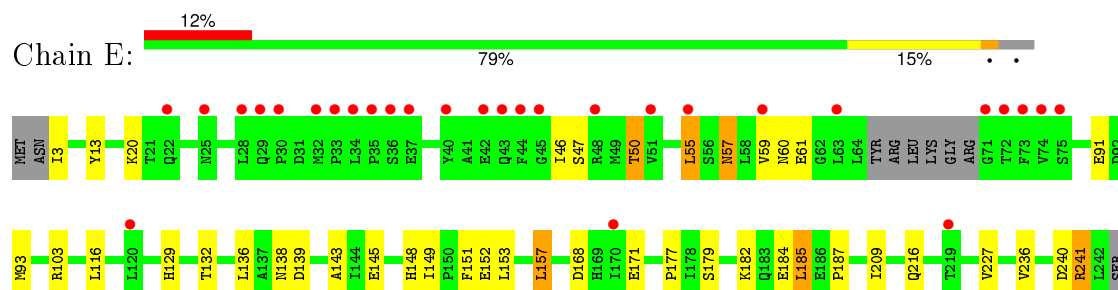
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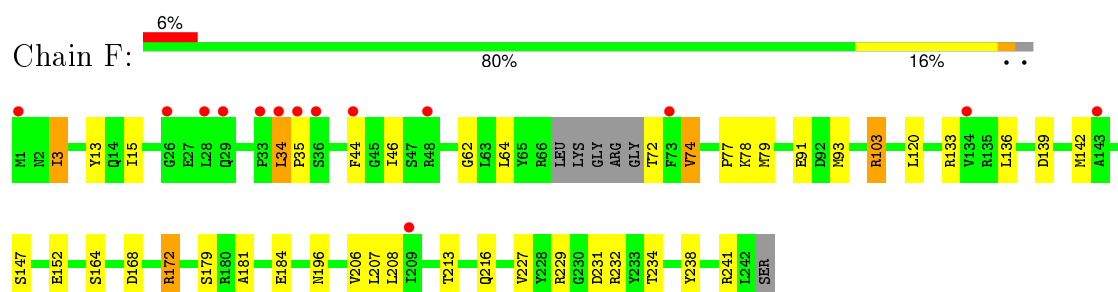
• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA



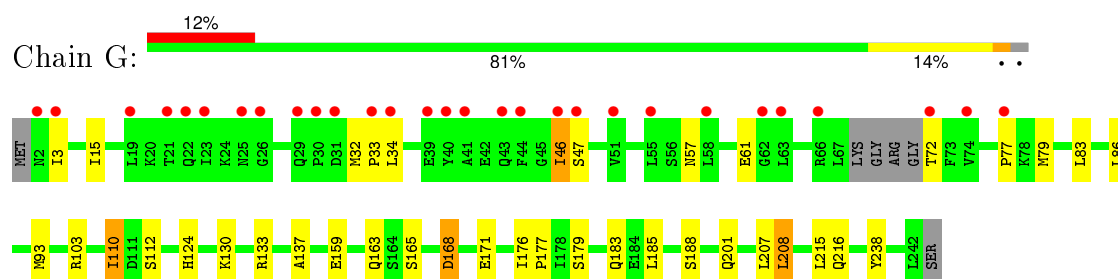
• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA



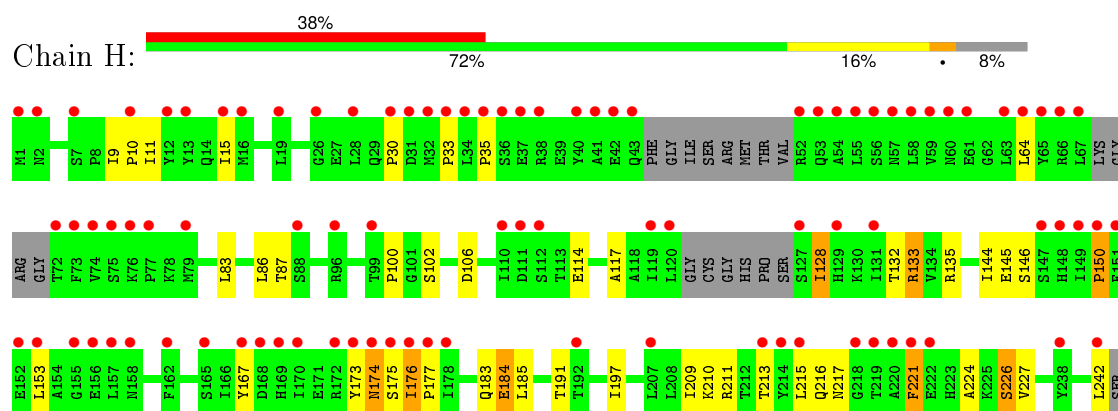
• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA



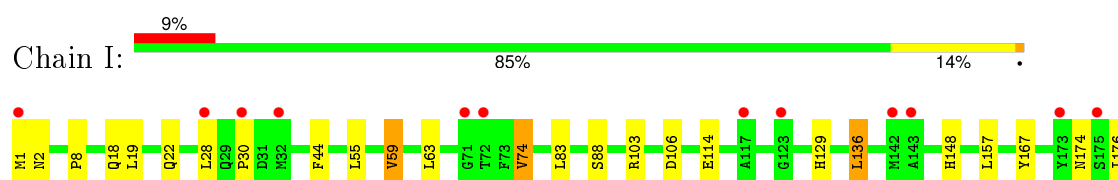
• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA

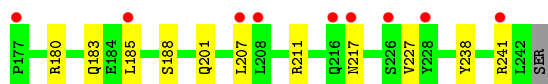


• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA



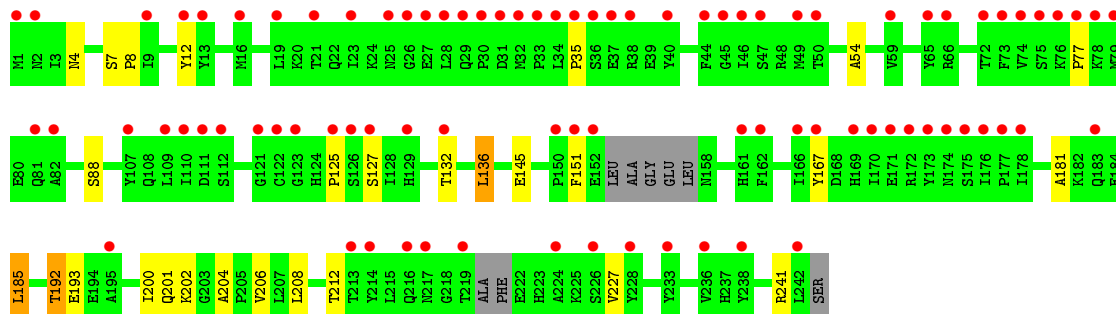
• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA





● Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA

Chain J: 36% 85% 10% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.41Å 137.08Å 120.19Å 90.00° 94.97° 90.00°	Depositor
Resolution (Å)	114.00 – 2.40 45.09 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (114.00-2.40) 99.3 (45.09-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.255 0.224 , 0.223	Depositor DCC
R_{free} test set	6241 reflections (4.79%)	DCC
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 130350 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18689	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.49	0/1957	0.64	1/2650 (0.0%)
1	B	0.46	0/1918	0.61	1/2601 (0.0%)
1	C	0.48	0/1908	0.63	0/2586
1	D	0.52	0/1966	0.70	0/2661
1	E	0.40	0/1812	0.61	1/2460 (0.0%)
1	F	0.45	0/1895	0.61	1/2566 (0.0%)
1	G	0.38	0/1813	0.54	0/2463
1	H	1.50	25/1504 (1.7%)	0.92	14/2057 (0.7%)
1	I	0.66	3/1879 (0.2%)	0.66	3/2549 (0.1%)
1	J	0.51	1/1567 (0.1%)	0.58	4/2144 (0.2%)
All	All	0.64	29/18219 (0.2%)	0.65	25/24737 (0.1%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	133	ARG	CZ-NH1	21.03	1.60	1.33
1	H	215	LEU	C-O	16.61	1.54	1.23
1	H	226	SER	CB-OG	15.30	1.62	1.42
1	H	102	SER	CB-OG	14.95	1.61	1.42
1	I	217	ASN	CG-OD1	13.10	1.52	1.24
1	H	87	THR	C-N	11.66	1.60	1.34
1	H	221	PHE	CG-CD2	11.60	1.56	1.38
1	H	128	ILE	C-N	11.31	1.60	1.34
1	H	167	TYR	CG-CD2	11.11	1.53	1.39
1	H	221	PHE	CE2-CZ	10.45	1.57	1.37
1	J	7	SER	CB-OG	10.08	1.55	1.42
1	I	180	ARG	CZ-NH1	10.07	1.46	1.33
1	H	215	LEU	C-N	9.29	1.55	1.34
1	H	128	ILE	C-O	9.22	1.40	1.23
1	H	216	GLN	C-N	8.19	1.52	1.34
1	I	241	ARG	C-O	8.07	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	100	PRO	N-CD	7.30	1.58	1.47
1	H	150	PRO	C-N	6.44	1.48	1.34
1	H	145	GLU	CG-CD	5.80	1.60	1.51
1	H	167	TYR	CE1-CZ	5.77	1.46	1.38
1	H	145	GLU	CB-CG	5.63	1.62	1.52
1	H	173	TYR	C-O	5.54	1.33	1.23
1	H	167	TYR	CG-CD1	5.53	1.46	1.39
1	H	217	ASN	C-O	5.52	1.33	1.23
1	H	175	SER	CA-CB	5.49	1.61	1.52
1	H	174	ASN	C-O	5.39	1.33	1.23
1	H	133	ARG	CD-NE	5.26	1.55	1.46
1	H	217	ASN	N-CA	5.26	1.56	1.46
1	H	175	SER	C-O	5.08	1.33	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	221	PHE	CB-CG-CD2	-13.12	111.61	120.80
1	I	180	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	H	221	PHE	CG-CD2-CE2	-8.52	111.43	120.80
1	H	167	TYR	CB-CG-CD1	-7.92	116.25	121.00
1	J	136	LEU	CA-CB-CG	7.51	132.58	115.30
1	F	136	LEU	CA-CB-CG	7.18	131.81	115.30
1	H	128	ILE	O-C-N	7.07	134.02	122.70
1	E	136	LEU	CA-CB-CG	6.65	130.59	115.30
1	H	167	TYR	CG-CD2-CE2	-6.38	116.19	121.30
1	H	221	PHE	CB-CG-CD1	6.23	125.16	120.80
1	B	136	LEU	CA-CB-CG	6.13	129.40	115.30
1	H	35	PRO	N-CA-CB	6.05	110.56	103.30
1	I	136	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	136	LEU	CA-CB-CG	5.89	128.84	115.30
1	H	133	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	J	35	PRO	N-CA-CB	5.83	110.30	103.30
1	I	180	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	H	33	PRO	N-CA-CB	5.75	110.20	103.30
1	J	125	PRO	N-CA-CB	5.70	110.14	103.30
1	J	77	PRO	N-CA-CB	5.69	110.13	103.30
1	H	30	PRO	N-CA-CB	5.68	110.11	103.30
1	H	128	ILE	CA-C-N	-5.59	104.90	117.20
1	H	167	TYR	CG-CD1-CE1	-5.40	116.98	121.30
1	H	87	THR	CA-C-N	-5.12	105.95	117.20
1	H	215	LEU	O-C-N	5.03	130.75	122.70

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	1911	0	1895	39	0
1	B	1872	0	1829	18	0
1	C	1871	0	1831	15	0
1	D	1913	0	1904	37	0
1	E	1777	0	1699	23	0
1	F	1853	0	1818	31	0
1	G	1779	0	1690	27	0
1	H	1485	0	1220	36	0
1	I	1842	0	1780	22	0
1	J	1542	0	1222	14	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	5	0	0	0	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	I	10	0	0	0	0
3	A	132	0	0	3	0
3	B	109	0	0	0	0
3	C	103	0	0	2	0
3	D	113	0	0	1	0
3	E	50	0	0	0	0
3	F	93	0	0	2	0
3	G	38	0	0	3	0
3	H	24	0	0	0	0
3	I	80	0	0	5	0
3	J	27	0	0	0	0
All	All	18689	0	16888	228	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 7.

All (228) 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:G:93:MET:CE	1:G:137:ALA:HB2	1.63	1.27
1:F:103:ARG:HG2	1:F:103:ARG:HH11	1.03	1.17
1:H:176:ILE:HG22	1:H:177:PRO:HD2	1.15	1.14
1:G:93:MET:HE3	1:G:137:ALA:HB2	1.10	1.08
1:H:176:ILE:CG2	1:H:177:PRO:HD2	1.86	1.05
1:D:16:MET:HE1	1:D:57:ASN:HD22	1.23	1.00
1:G:93:MET:CE	1:G:137:ALA:CB	2.42	0.97
1:H:176:ILE:HG22	1:H:177:PRO:CD	1.94	0.96
1:G:93:MET:HE3	1:G:137:ALA:CB	1.97	0.95
1:D:30:PRO:HB3	1:D:76:LYS:HD3	1.45	0.95
1:D:16:MET:HE2	1:D:57:ASN:HB2	1.50	0.94
1:F:103:ARG:HH11	1:F:103:ARG:CG	1.81	0.92
1:H:133:ARG:NH1	1:H:135:ARG:HH22	1.68	0.92
1:F:103:ARG:HG2	1:F:103:ARG:NH1	1.77	0.88
1:H:150:PRO:HB2	1:H:153:LEU:HD13	1.56	0.87
1:C:139:ASP:OD1	1:F:103:ARG:NH2	2.08	0.86
1:A:103[B]:ARG:HH11	1:I:103:ARG:HH21	1.24	0.83
1:C:13:TYR:OH	1:C:139:ASP:OD2	1.98	0.81
1:H:86:LEU:CD1	1:H:211:ARG:NH2	2.45	0.79
1:A:103[B]:ARG:HE	1:I:103:ARG:HE	1.31	0.79
1:C:180:ARG:HB2	1:D:239:MET:O	1.81	0.79
1:I:183:GLN:OE1	1:I:211:ARG:HD3	1.83	0.78
1:A:80:GLU:HG2	1:B:242:LEU:HD23	1.65	0.77
1:G:93:MET:HE1	1:G:137:ALA:CB	2.16	0.76
1:A:80:GLU:HG2	1:B:242:LEU:CD2	2.17	0.75
1:D:76:LYS:NZ	1:D:77:PRO:HD3	2.01	0.75
1:D:185:LEU:HD22	1:D:209:ILE:HG12	1.68	0.74
1:A:103[B]:ARG:NH1	1:I:103:ARG:HH21	1.86	0.73
1:B:113:THR:HG22	1:B:116:LEU:HB2	1.73	0.71
1:F:34:LEU:HD11	1:F:72:THR:OG1	1.91	0.70
1:E:13:TYR:OH	1:E:139:ASP:OD2	2.10	0.70
1:G:3:ILE:HD11	1:G:15:ILE:HG13	1.73	0.70
1:I:83:LEU:HD23	1:I:238:TYR:HE2	1.57	0.70
1:C:184:GLU:HG2	1:D:236:VAL:HG22	1.72	0.70
1:A:103[A]:ARG:HD2	3:I:2054:HOH:O	1.92	0.70
1:A:29[A]:GLN:HG2	1:A:32:MET:HG3	1.74	0.70
1:D:16:MET:CE	1:D:57:ASN:HD22	2.04	0.68
1:A:103[B]:ARG:HH11	1:I:103:ARG:NH2	1.92	0.67
1:D:12:TYR:HD1	1:D:16:MET:HE3	1.60	0.67
1:H:174:ASN:HB3	1:H:176:ILE:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176[A]:ILE:HG23	1:A:215:LEU:HG	1.79	0.65
1:H:144:ILE:HG12	1:H:197:ILE:HD11	1.80	0.64
1:C:26:GLY:O	1:C:29:GLN:NE2	2.31	0.64
1:B:12:TYR:OH	1:D:106:ASP:OD1	2.10	0.63
1:G:201:GLN:HG3	3:G:2032:HOH:O	1.98	0.62
1:D:217:ASN:HB3	1:D:219:THR:HG23	1.82	0.62
1:A:183:GLN:HE21	1:A:185:LEU:HD11	1.65	0.62
1:I:201:GLN:HG3	3:I:2069:HOH:O	1.99	0.61
1:A:103[A]:ARG:NH2	3:A:2054:HOH:O	2.33	0.61
1:F:179:SER:OG	1:F:216:GLN:HA	2.01	0.61
1:A:207:LEU:HG	1:B:187:PRO:HD3	1.82	0.60
1:F:64:LEU:HD23	1:F:74:VAL:HA	1.84	0.60
1:A:176[A]:ILE:CG2	1:A:215:LEU:HG	2.31	0.60
1:C:236:VAL:HG22	1:D:184:GLU:HG2	1.84	0.59
1:H:11:ILE:O	1:H:15:ILE:HG12	2.02	0.59
1:D:183:GLN:NE2	1:D:235:PHE:CE2	2.71	0.59
1:H:174:ASN:CB	1:H:176:ILE:CD1	2.80	0.59
1:H:183:GLN:HE21	1:H:185:LEU:HD21	1.68	0.59
1:G:79:MET:HB3	1:G:83:LEU:HD13	1.84	0.59
1:A:159:GLU:O	1:A:163:GLN:HG2	2.03	0.58
1:A:227:VAL:HG23	1:I:8:PRO:HG3	1.85	0.58
1:H:176:ILE:H	1:H:176:ILE:HD12	1.69	0.58
1:H:174:ASN:CB	1:H:176:ILE:HD11	2.33	0.58
1:D:76:LYS:HZ3	1:D:77:PRO:HD3	1.66	0.58
1:D:179:SER:HB2	1:D:216:GLN:HA	1.86	0.58
1:H:146:SER:O	1:H:224:ALA:HA	2.04	0.57
1:G:83:LEU:HD23	1:G:238:TYR:HE2	1.69	0.57
1:A:206:VAL:CG1	1:A:227:VAL:HG13	2.34	0.57
1:J:192:THR:HB	1:J:202:LYS:HD2	1.87	0.57
1:H:176:ILE:N	1:H:176:ILE:HD12	2.20	0.56
1:J:206:VAL:CG1	1:J:227:VAL:HG13	2.35	0.56
1:I:185:LEU:HD23	1:I:207:LEU:HD13	1.86	0.56
1:E:116:LEU:HD21	1:E:148:HIS:CD2	2.41	0.56
1:E:47:SER:HB3	1:E:50:THR:HG22	1.87	0.56
1:D:76:LYS:HZ2	1:D:77:PRO:HD3	1.70	0.56
1:D:30:PRO:HA	1:D:74:VAL:HB	1.87	0.56
1:F:93:MET:HA	1:F:93:MET:HE3	1.88	0.55
1:G:34:LEU:HD13	1:G:72:THR:HG22	1.88	0.55
1:C:140:ILE:HD11	1:F:196:ASN:HB3	1.89	0.55
1:G:159:GLU:HG3	1:G:163:GLN:NE2	2.21	0.55
1:B:179:SER:HB2	1:B:216:GLN:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:THR:HG22	3:A:2121:HOH:O	2.07	0.54
1:A:103[B]:ARG:NE	1:I:103:ARG:HE	2.01	0.54
1:H:144:ILE:CG1	1:H:197:ILE:HD11	2.38	0.54
1:A:206:VAL:HG13	1:A:227:VAL:HG13	1.89	0.53
1:E:20:LYS:HE3	1:E:138:ASN:OD1	2.09	0.53
1:A:103[B]:ARG:HE	1:I:103:ARG:NE	2.03	0.53
1:A:29[B]:GLN:HG3	1:A:30:PRO:HD2	1.91	0.53
1:G:165:SER:HB3	1:G:168:ASP:HB2	1.90	0.53
1:C:180:ARG:NH1	3:C:2066:HOH:O	2.42	0.52
1:A:8:PRO:HG2	1:I:227:VAL:HG23	1.91	0.52
1:A:12:TYR:OH	1:I:106:ASP:OD1	2.27	0.52
1:E:103:ARG:HD2	1:G:103:ARG:HB2	1.91	0.52
1:H:174:ASN:HB2	1:H:176:ILE:CD1	2.40	0.52
1:J:200:ILE:HD12	1:J:204:ALA:HB3	1.92	0.52
1:F:44:PHE:HB2	1:F:46:ILE:HG12	1.92	0.52
1:D:16:MET:CE	1:D:57:ASN:HB2	2.30	0.51
1:H:209:ILE:HB	1:H:226:SER:HB2	1.92	0.51
1:F:152:GLU:HG2	3:F:2045:HOH:O	2.10	0.51
1:J:181:ALA:HA	1:J:212:THR:O	2.11	0.51
1:D:183:GLN:HE22	1:D:235:PHE:HE2	1.59	0.51
1:A:183:GLN:NE2	1:A:235:PHE:CE2	2.80	0.50
1:J:206:VAL:HG13	1:J:227:VAL:HG13	1.92	0.50
1:H:176:ILE:CG2	1:H:177:PRO:CD	2.71	0.50
1:H:185:LEU:HD22	1:H:209:ILE:HG12	1.93	0.50
1:I:55:LEU:O	1:I:59:VAL:HG13	2.12	0.50
1:H:184:GLU:HG2	1:H:210:LYS:HB3	1.93	0.50
1:I:129:HIS:O	1:I:148:HIS:HA	2.12	0.49
1:A:133:ARG:HD3	3:A:2071:HOH:O	2.13	0.49
1:A:188:SER:HB2	1:A:208:LEU:HD22	1.95	0.49
1:E:93:MET:HE3	1:E:93:MET:HA	1.93	0.49
1:D:12:TYR:CD1	1:D:16:MET:HE3	2.45	0.48
1:D:65:TYR:CZ	1:D:73:PHE:HB2	2.47	0.48
1:B:180:ARG:HB2	1:B:180:ARG:HH21	1.78	0.48
1:J:132:THR:HA	1:J:145:GLU:O	2.13	0.48
1:H:174:ASN:O	1:H:176:ILE:HD11	2.13	0.48
1:F:168:ASP:HB3	1:F:172:ARG:NH2	2.28	0.48
1:B:103:ARG:HD2	1:D:103:ARG:HD3	1.95	0.48
1:A:131:ILE:HG22	1:A:133:ARG:HD2	1.94	0.48
1:B:44:PHE:HB2	1:B:46:ILE:HG12	1.95	0.48
1:H:174:ASN:C	1:H:176:ILE:CD1	2.82	0.48
1:D:105:ILE:HD11	1:D:134:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:TYR:OH	1:F:139:ASP:OD2	2.18	0.47
1:E:171:GLU:HG2	1:E:177:PRO:HA	1.97	0.47
1:E:185:LEU:HD12	1:E:209:ILE:HG12	1.97	0.47
1:B:103:ARG:HB3	1:B:134:VAL:HG13	1.97	0.47
1:H:106:ASP:CB	1:J:12:TYR:OH	2.62	0.47
1:G:176:ILE:HG13	1:G:177:PRO:HD2	1.97	0.47
1:F:34:LEU:HB2	1:F:35:PRO:HD2	1.98	0.46
1:H:114:GLU:HA	1:H:117:ALA:HB3	1.98	0.46
1:A:215:LEU:HD13	1:A:221:PHE:CD1	2.50	0.46
1:G:179:SER:HB2	1:G:216:GLN:HA	1.98	0.46
1:D:76:LYS:HZ2	1:D:77:PRO:CD	2.27	0.46
1:A:217:ASN:HA	1:A:217:ASN:HD22	1.53	0.46
1:A:187:PRO:HD3	1:B:207:LEU:HG	1.98	0.46
1:D:29:GLN:HB2	1:D:32:MET:HG3	1.98	0.46
1:D:188:SER:HB2	1:D:208:LEU:HD22	1.98	0.45
1:E:129:HIS:HB2	1:E:149:ILE:HB	1.99	0.45
1:A:102:SER:O	1:A:103[A]:ARG:NE	2.50	0.45
1:A:183:GLN:HE22	1:A:235:PHE:HE2	1.63	0.45
1:B:34:LEU:HD13	1:B:72:THR:HG23	1.98	0.45
1:E:187:PRO:HD3	1:F:207:LEU:HG	1.98	0.45
1:F:133:ARG:NH1	1:F:164:SER:O	2.49	0.45
1:G:32:MET:HG2	1:G:33:PRO:HD2	1.98	0.45
1:G:171:GLU:HG2	1:G:177:PRO:HA	1.97	0.45
1:C:29:GLN:HB3	1:C:32:MET:HG3	1.98	0.45
1:E:132:THR:HA	1:E:145:GLU:O	2.17	0.45
1:H:86:LEU:CD1	1:H:211:ARG:HH21	2.27	0.45
1:H:191:THR:HG21	1:J:4:ASN:ND2	2.33	0.44
1:E:179:SER:HB2	1:E:216:GLN:HA	1.99	0.44
1:C:133:ARG:CZ	1:C:166:ILE:HD12	2.47	0.44
1:H:153:LEU:HD23	1:H:221:PHE:HA	1.99	0.44
1:H:86:LEU:HD11	1:H:211:ARG:NH2	2.27	0.44
1:J:12:TYR:HB2	1:J:54:ALA:HB2	1.99	0.44
1:J:185:LEU:HA	1:J:208:LEU:O	2.18	0.44
1:E:55:LEU:O	1:E:59:VAL:HG23	2.18	0.44
1:G:103:ARG:NH1	3:G:2012:HOH:O	2.49	0.44
1:F:3:ILE:HD11	1:F:15:ILE:HG13	1.98	0.44
1:D:105:ILE:HD11	1:D:134:VAL:CG2	2.46	0.44
1:F:77:PRO:HB2	1:F:79:MET:HE3	1.99	0.44
1:F:229:ARG:HB3	1:F:231:ASP:OD1	2.17	0.44
1:F:103:ARG:NH1	1:F:103:ARG:CG	2.52	0.44
1:I:174:ASN:HB3	1:I:176:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2:ASN:C	1:I:18:GLN:HE22	2.20	0.44
1:E:91:GLU:CD	1:F:241:ARG:HH22	2.21	0.44
1:B:170:ILE:HD13	1:B:221:PHE:CD2	2.53	0.44
1:I:88:SER:HB3	1:I:167:TYR:CD1	2.52	0.43
1:B:132:THR:HA	1:B:145:GLU:O	2.18	0.43
1:E:185:LEU:CD1	1:E:209:ILE:HG12	2.48	0.43
1:I:30:PRO:HA	1:I:74:VAL:HG22	1.99	0.43
1:C:206:VAL:CG1	1:C:227:VAL:HG13	2.49	0.43
1:E:182:LYS:HD3	1:F:238:TYR:CZ	2.54	0.43
1:G:176:ILE:HG23	1:G:215:LEU:HD22	1.99	0.43
1:I:1:MET:N	3:I:2001:HOH:O	2.52	0.43
1:G:183:GLN:HE21	1:G:185:LEU:HD11	1.84	0.43
1:D:16:MET:HE1	1:D:57:ASN:ND2	2.08	0.43
1:F:181:ALA:HB2	1:F:213:THR:HG23	1.99	0.43
1:J:88:SER:HB2	1:J:167:TYR:CD2	2.54	0.43
1:H:227:VAL:HG23	1:J:8:PRO:HG2	2.01	0.43
1:J:206:VAL:HG11	1:J:227:VAL:HG13	2.00	0.42
1:E:129:HIS:CE1	1:E:157:LEU:HD22	2.54	0.42
1:J:127:SER:O	1:J:151:PHE:HB2	2.19	0.42
1:A:80:GLU:CG	1:B:242:LEU:HD23	2.43	0.42
1:C:133:ARG:NH1	1:C:166:ILE:HD12	2.34	0.42
1:C:188:SER:HB2	1:C:208:LEU:HD22	2.00	0.42
1:H:86:LEU:HD12	1:H:211:ARG:NH2	2.28	0.42
1:I:18:GLN:O	1:I:22:GLN:HG3	2.20	0.42
1:E:143:ALA:HA	1:E:227:VAL:O	2.19	0.42
1:I:1:MET:SD	1:I:44:PHE:HZ	2.43	0.42
1:C:8:PRO:HG3	1:F:227:VAL:HG23	2.02	0.42
1:D:183:GLN:HE21	1:D:185:LEU:HD21	1.85	0.42
1:B:34:LEU:HB2	1:B:72:THR:HG23	2.00	0.42
1:G:185:LEU:HD23	1:G:207:LEU:HD13	2.02	0.42
1:E:241:ARG:NH1	1:F:91:GLU:OE1	2.52	0.42
1:F:62:GLY:HA2	3:F:2016:HOH:O	2.19	0.41
1:F:34:LEU:HB2	1:F:35:PRO:CD	2.50	0.41
1:F:142:MET:HE1	1:F:232:ARG:CZ	2.50	0.41
1:H:174:ASN:C	1:H:176:ILE:HD11	2.41	0.41
1:H:211:ARG:HG2	1:H:213:THR:HG22	2.03	0.41
1:C:133:ARG:CD	3:C:2054:HOH:O	2.68	0.41
1:E:236:VAL:HG22	1:F:184:GLU:HG2	2.02	0.41
1:G:188:SER:HB2	1:G:208:LEU:HD22	2.01	0.41
1:H:174:ASN:HB3	1:H:176:ILE:CD1	2.45	0.41
1:A:206:VAL:HG11	1:A:227:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:HB3	1:A:217:ASN:HB2	2.03	0.41
1:G:57:ASN:O	1:G:61:GLU:HB2	2.20	0.41
1:A:184:GLU:HA	1:B:235:PHE:O	2.21	0.41
1:D:29:GLN:HA	1:D:30:PRO:HD3	1.97	0.41
1:G:110:ILE:CD1	1:G:130:LYS:HD2	2.51	0.41
1:E:184:GLU:HG3	1:F:234:THR:CG2	2.51	0.41
1:D:229:ARG:HB3	1:D:231:ASP:OD1	2.20	0.41
1:E:129:HIS:NE2	1:E:151:PHE:HD2	2.18	0.41
1:D:206:VAL:HG13	1:D:227:VAL:HG13	2.02	0.41
1:D:124:HIS:HA	1:D:125:PRO:HA	1.92	0.41
1:G:46:ILE:HG23	1:G:47:SER:N	2.35	0.41
1:G:133:ARG:HD3	3:G:2019:HOH:O	2.20	0.41
1:D:2:ASN:O	1:D:18:GLN:NE2	2.41	0.41
1:H:174:ASN:C	1:H:176:ILE:HD12	2.42	0.41
1:A:103[A]:ARG:CD	3:I:2054:HOH:O	2.60	0.41
1:E:57:ASN:O	1:E:61:GLU:HB2	2.21	0.41
1:A:103[B]:ARG:HD3	3:I:2039:HOH:O	2.20	0.40
1:B:8:PRO:HG3	1:D:227:VAL:HG23	2.04	0.40
1:G:112:SER:HB3	1:G:124:HIS:ND1	2.37	0.40
1:D:76:LYS:HA	1:D:77:PRO:HD3	1.83	0.40
1:D:77:PRO:HG3	3:D:2035:HOH:O	2.22	0.40
1:H:9:ILE:HA	1:H:10:PRO:HD3	1.96	0.40
1:F:77:PRO:HB2	1:F:79:MET:CE	2.51	0.40
1:A:165:SER:HB3	1:A:168:ASP:HB2	2.04	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	244/243 (100%)	240 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	243/243 (100%)	239 (98%)	4 (2%)	0	100	100
1	C	240/243 (99%)	238 (99%)	2 (1%)	0	100	100
1	D	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	39	56
1	E	230/243 (95%)	223 (97%)	7 (3%)	0	100	100
1	F	235/243 (97%)	230 (98%)	5 (2%)	0	100	100
1	G	233/243 (96%)	230 (99%)	3 (1%)	0	100	100
1	H	216/243 (89%)	202 (94%)	13 (6%)	1 (0%)	34	48
1	I	240/243 (99%)	236 (98%)	4 (2%)	0	100	100
1	J	229/243 (94%)	214 (93%)	15 (7%)	0	100	100
All	All	2355/2430 (97%)	2289 (97%)	64 (3%)	2 (0%)	56	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	128	ILE
1	D	77	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	207/213 (97%)	196 (95%)	11 (5%)	28	44
1	B	198/213 (93%)	191 (96%)	7 (4%)	43	64
1	C	200/213 (94%)	192 (96%)	8 (4%)	38	58
1	D	208/213 (98%)	192 (92%)	16 (8%)	16	24
1	E	186/213 (87%)	173 (93%)	13 (7%)	19	29
1	F	200/213 (94%)	190 (95%)	10 (5%)	30	48
1	G	183/213 (86%)	177 (97%)	6 (3%)	45	66
1	H	114/213 (54%)	108 (95%)	6 (5%)	28	44
1	I	193/213 (91%)	184 (95%)	9 (5%)	32	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	111/213 (52%)	105 (95%)	6 (5%)	27	43
All	All	1800/2130 (84%)	1708 (95%)	92 (5%)	29	46

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LEU
1	A	111	ASP
1	A	136	LEU
1	A	168	ASP
1	A	198	LEU
1	A	206	VAL
1	A	207	LEU
1	A	208	LEU
1	A	215	LEU
1	A	217	ASN
1	A	234	THR
1	B	25	ASN
1	B	157	LEU
1	B	168	ASP
1	B	180	ARG
1	B	207	LEU
1	B	208	LEU
1	B	240	ASP
1	C	4	ASN
1	C	63	LEU
1	C	67	LEU
1	C	157	LEU
1	C	168	ASP
1	C	206	VAL
1	C	208	LEU
1	C	239	MET
1	D	3	ILE
1	D	19	LEU
1	D	34	LEU
1	D	58	LEU
1	D	76	LYS
1	D	120	LEU
1	D	153	LEU
1	D	163	GLN
1	D	164	SER
1	D	198	LEU

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Mol	Chain	Res	Type
1	D	206	VAL
1	D	208	LEU
1	D	211	ARG
1	D	217	ASN
1	D	219	THR
1	D	242	LEU
1	E	3	ILE
1	E	46	ILE
1	E	50	THR
1	E	55	LEU
1	E	57	ASN
1	E	60	ASN
1	E	152	GLU
1	E	153	LEU
1	E	157	LEU
1	E	168	ASP
1	E	185	LEU
1	E	240	ASP
1	E	241	ARG
1	F	3	ILE
1	F	34	LEU
1	F	74	VAL
1	F	78	LYS
1	F	103	ARG
1	F	120	LEU
1	F	147	SER
1	F	172	ARG
1	F	206	VAL
1	F	208	LEU
1	G	46	ILE
1	G	77	PRO
1	G	86	LEU
1	G	110	ILE
1	G	168	ASP
1	G	208	LEU
1	H	64	LEU
1	H	83	LEU
1	H	132	THR
1	H	176	ILE
1	H	184	GLU
1	H	242	LEU
1	I	19	LEU

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Mol	Chain	Res	Type
1	I	28	LEU
1	I	59	VAL
1	I	63	LEU
1	I	74	VAL
1	I	114	GLU
1	I	136	LEU
1	I	157	LEU
1	I	188	SER
1	J	136	LEU
1	J	185	LEU
1	J	192	THR
1	J	193	GLU
1	J	201	GLN
1	J	241	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	B	25	ASN
1	B	223	HIS
1	C	84	GLN
1	D	57	ASN
1	D	148	HIS
1	D	217	ASN
1	E	22	GLN
1	E	25	ASN
1	E	60	ASN
1	E	108	GLN
1	E	148	HIS
1	E	163	GLN
1	F	53	GLN
1	F	60	ASN
1	G	163	GLN
1	G	196	ASN
1	H	161	HIS
1	H	183	GLN
1	H	196	ASN
1	I	22	GLN
1	I	57	ASN
1	J	4	ASN
1	J	14	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

15 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	$\# Z > 2$
2	SO4	A	1244	-	4,4,4	0.41	0	6,6,6	0.36	0
2	SO4	A	1245	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	B	1243	-	4,4,4	0.09	0	6,6,6	0.19	0
2	SO4	B	1244	-	4,4,4	0.31	0	6,6,6	0.17	0
2	SO4	C	1243	-	4,4,4	0.10	0	6,6,6	0.37	0
2	SO4	C	1244	-	4,4,4	0.41	0	6,6,6	0.22	0
2	SO4	D	1243	-	4,4,4	0.09	0	6,6,6	0.13	0
2	SO4	D	1244	-	4,4,4	0.41	0	6,6,6	0.62	0
2	SO4	E	1243	-	4,4,4	0.26	0	6,6,6	0.35	0
2	SO4	F	1243	-	4,4,4	0.17	0	6,6,6	0.38	0
2	SO4	F	1244	-	4,4,4	0.38	0	6,6,6	0.27	0
2	SO4	G	1243	-	4,4,4	0.20	0	6,6,6	0.25	0
2	SO4	G	1244	-	4,4,4	0.18	0	6,6,6	0.37	0
2	SO4	I	1243	-	4,4,4	0.20	0	6,6,6	0.17	0
2	SO4	I	1244	-	4,4,4	0.20	0	6,6,6	0.39	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
2	SO4	A	1244	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1245	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1243	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1244	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1243	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1244	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1243	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1244	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1243	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1243	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1244	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1243	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1244	-	-	0/0/0/0	0/0/0/0
2	SO4	I	1243	-	-	0/0/0/0	0/0/0/0
2	SO4	I	1244	-	-	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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	243/243 (100%)	0.68	19 (7%)	16 15	48, 60, 79, 87	0
1	B	242/243 (99%)	0.76	21 (8%)	13 12	44, 61, 76, 80	0
1	C	242/243 (99%)	0.43	6 (2%)	61 60	45, 58, 71, 82	0
1	D	242/243 (99%)	0.66	16 (6%)	22 22	42, 56, 72, 76	0
1	E	234/243 (96%)	0.68	29 (12%)	5 5	54, 67, 87, 95	0
1	F	237/243 (97%)	0.55	14 (5%)	26 26	48, 63, 79, 85	0
1	G	237/243 (97%)	0.66	29 (12%)	5 5	57, 69, 83, 89	0
1	H	224/243 (92%)	1.94	93 (41%)	0 0	62, 74, 86, 93	0
1	I	242/243 (99%)	0.62	21 (8%)	13 12	49, 63, 79, 93	0
1	J	235/243 (96%)	1.76	87 (37%)	0 0	62, 74, 87, 91	0
All	All	2378/2430 (97%)	0.86	335 (14%)	4 4	42, 65, 83, 95	0

All (335) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	67	LEU	9.1
1	J	1	MET	7.6
1	J	35	PRO	7.3
1	B	67	LEU	6.8
1	H	36	SER	6.4
1	J	32	MET	6.3
1	H	178	ILE	6.3
1	H	172	ARG	6.3
1	J	111	ASP	6.3
1	H	40	TYR	6.2
1	H	65	TYR	6.1
1	J	28	LEU	6.0
1	B	1	MET	6.0

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Mol	Chain	Res	Type	RSRZ
1	H	72	THR	5.9
1	J	73	PHE	5.9
1	J	178	ILE	5.9
1	H	66	ARG	5.7
1	J	214	TYR	5.7
1	J	38	ARG	5.7
1	F	36	SER	5.7
1	H	34	LEU	5.6
1	H	157	LEU	5.5
1	H	73	PHE	5.5
1	H	119	ILE	5.5
1	H	35	PRO	5.4
1	J	167	TYR	5.4
1	H	167	TYR	5.3
1	H	177	PRO	5.3
1	J	44	PHE	5.1
1	F	1	MET	5.1
1	H	127	SER	5.0
1	J	236	VAL	4.8
1	H	221	PHE	4.8
1	J	217	ASN	4.8
1	G	55	LEU	4.8
1	J	36	SER	4.7
1	H	176	ILE	4.7
1	H	19	LEU	4.7
1	H	59	VAL	4.6
1	H	63	LEU	4.6
1	E	44	PHE	4.4
1	H	52	ARG	4.4
1	G	44	PHE	4.4
1	F	34	LEU	4.4
1	H	111	ASP	4.4
1	J	152	GLU	4.3
1	E	40	TYR	4.3
1	I	71	GLY	4.3
1	J	19	LEU	4.3
1	J	122	CYS	4.3
1	J	121	GLY	4.2
1	H	152	GLU	4.2
1	J	77	PRO	4.2
1	H	156	GLU	4.1
1	H	169	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	173	TYR	4.1
1	H	222	GLU	4.0
1	H	1	MET	4.0
1	E	37	GLU	4.0
1	J	176	ILE	4.0
1	G	63	LEU	4.0
1	G	40	TYR	4.0
1	H	214	TYR	4.0
1	H	147	SER	4.0
1	H	96	ARG	4.0
1	E	33	PRO	4.0
1	G	43	GLN	4.0
1	J	177	PRO	3.9
1	H	215	LEU	3.9
1	J	34	LEU	3.9
1	G	26	GLY	3.8
1	G	33	PRO	3.8
1	J	30	PRO	3.8
1	H	2	ASN	3.8
1	B	69	GLY	3.8
1	J	40	TYR	3.8
1	E	73	PHE	3.8
1	J	25	ASN	3.7
1	J	76	LYS	3.7
1	J	110	ILE	3.7
1	J	175	SER	3.7
1	H	149	ILE	3.7
1	H	165	SER	3.7
1	H	53	GLN	3.6
1	H	120	LEU	3.6
1	J	47	SER	3.6
1	G	30	PRO	3.6
1	J	126	SER	3.6
1	G	31	ASP	3.6
1	I	177	PRO	3.5
1	J	162	PHE	3.5
1	F	33	PRO	3.5
1	H	15	ILE	3.5
1	H	175	SER	3.5
1	J	109	LEU	3.5
1	H	54	ALA	3.5
1	J	33	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	J	74	VAL	3.5
1	E	63	LEU	3.5
1	J	173	TYR	3.5
1	H	56	SER	3.5
1	H	60	ASN	3.4
1	J	170	ILE	3.4
1	B	239[A]	MET	3.4
1	J	238	TYR	3.4
1	H	79	MET	3.4
1	H	110	ILE	3.4
1	H	162	PHE	3.4
1	I	123	GLY	3.4
1	H	74	VAL	3.3
1	J	27	GLU	3.3
1	F	44	PHE	3.3
1	J	172	ARG	3.3
1	E	32	MET	3.3
1	J	242	LEU	3.3
1	E	59	VAL	3.3
1	J	29	GLN	3.3
1	A	209	ILE	3.3
1	E	34	LEU	3.3
1	H	77	PRO	3.3
1	H	168	ASP	3.2
1	J	79	MET	3.2
1	H	31	ASP	3.2
1	G	72	THR	3.2
1	H	13	TYR	3.2
1	J	123	GLY	3.2
1	B	29	GLN	3.2
1	H	28	LEU	3.1
1	B	40	TYR	3.1
1	J	31	ASP	3.1
1	H	61	GLU	3.1
1	G	29	GLN	3.1
1	A	236	VAL	3.1
1	J	13	TYR	3.1
1	E	30	PRO	3.1
1	H	41	ALA	3.1
1	A	41	ALA	3.1
1	G	66	ARG	3.0
1	E	74	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	30	PRO	3.0
1	H	38	ARG	3.0
1	I	32	MET	3.0
1	H	55	LEU	3.0
1	H	151	PHE	3.0
1	I	216	GLN	3.0
1	J	23	ILE	3.0
1	H	129	HIS	3.0
1	F	28	LEU	2.9
1	H	7	SER	2.9
1	J	226	SER	2.9
1	D	237[A]	HIS	2.9
1	H	57	ASN	2.9
1	J	65	TYR	2.9
1	F	26	GLY	2.9
1	H	155	GLY	2.9
1	J	26	GLY	2.9
1	I	173	TYR	2.9
1	B	207	LEU	2.9
1	H	33	PRO	2.9
1	H	174	ASN	2.9
1	E	42	GLU	2.8
1	G	25	ASN	2.8
1	H	32	MET	2.8
1	I	142	MET	2.8
1	I	30	PRO	2.8
1	H	158	ASN	2.8
1	B	227	VAL	2.8
1	B	73	PHE	2.8
1	C	44	PHE	2.8
1	E	72	THR	2.8
1	J	21	THR	2.8
1	E	55	LEU	2.8
1	J	233	TYR	2.8
1	J	213	THR	2.8
1	I	217	ASN	2.8
1	J	224	ALA	2.8
1	B	228	TYR	2.7
1	J	132	THR	2.7
1	E	28	LEU	2.7
1	D	79[A]	MET	2.7
1	E	35	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	228	TYR	2.7
1	J	127	SER	2.7
1	I	208	LEU	2.7
1	C	1	MET	2.7
1	D	228	TYR	2.7
1	H	64	LEU	2.7
1	J	49	MET	2.7
1	D	45	GLY	2.7
1	D	42	GLU	2.7
1	E	45	GLY	2.7
1	F	143	ALA	2.7
1	J	129	HIS	2.6
1	A	185	LEU	2.6
1	G	34	LEU	2.6
1	J	166	ILE	2.6
1	J	125	PRO	2.6
1	E	36	SER	2.6
1	H	170	ILE	2.6
1	B	142	MET	2.6
1	G	39	GLU	2.6
1	A	187	PRO	2.6
1	I	28	LEU	2.6
1	J	72	THR	2.6
1	H	148	HIS	2.6
1	A	207	LEU	2.6
1	G	3	ILE	2.6
1	H	219	THR	2.6
1	J	2	ASN	2.6
1	D	142	MET	2.6
1	J	16	MET	2.6
1	J	37	GLU	2.6
1	G	22	GLN	2.6
1	J	75	SER	2.5
1	H	58	LEU	2.5
1	C	51	VAL	2.5
1	H	112	SER	2.5
1	J	46	ILE	2.5
1	J	50	THR	2.5
1	E	29	GLN	2.5
1	J	150	PRO	2.5
1	A	234	THR	2.5
1	G	23	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	9	ILE	2.5
1	H	150	PRO	2.5
1	I	185	LEU	2.5
1	I	207	LEU	2.5
1	J	12	TYR	2.5
1	F	48	ARG	2.5
1	J	216	GLN	2.5
1	F	209	ILE	2.5
1	H	99	THR	2.5
1	C	70	ARG	2.5
1	H	10	PRO	2.5
1	H	76	LYS	2.5
1	E	120	LEU	2.5
1	A	206	VAL	2.4
1	J	183	GLN	2.4
1	E	43	GLN	2.4
1	E	219	THR	2.4
1	H	220	ALA	2.4
1	J	107	TYR	2.4
1	A	44	PHE	2.4
1	B	121	GLY	2.4
1	G	74	VAL	2.4
1	J	112	SER	2.4
1	I	72	THR	2.4
1	D	209	ILE	2.4
1	F	29	GLN	2.4
1	B	105	ILE	2.4
1	D	143	ALA	2.4
1	E	71	GLY	2.3
1	H	43	GLN	2.3
1	C	3	ILE	2.3
1	G	21	THR	2.3
1	I	1	MET	2.3
1	J	59	VAL	2.3
1	J	45	GLY	2.3
1	G	46	ILE	2.3
1	H	42	GLU	2.3
1	G	58	LEU	2.3
1	E	25	ASN	2.3
1	J	81	GLN	2.3
1	J	171	GLU	2.3
1	F	73	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	47	SER	2.3
1	I	175	SER	2.3
1	A	71	GLY	2.3
1	J	78	LYS	2.3
1	I	241	ARG	2.3
1	H	192	THR	2.3
1	B	209	ILE	2.2
1	E	75	SER	2.2
1	B	208	LEU	2.2
1	D	227	VAL	2.2
1	G	77	PRO	2.2
1	J	161	HIS	2.2
1	D	136	LEU	2.2
1	F	134	VAL	2.2
1	H	153	LEU	2.2
1	J	82	ALA	2.2
1	J	169	HIS	2.2
1	G	41	ALA	2.2
1	J	174	ASN	2.2
1	A	93	MET	2.2
1	H	88	SER	2.2
1	H	26	GLY	2.2
1	H	213	THR	2.2
1	A	103[A]	ARG	2.2
1	D	206	VAL	2.2
1	A	136	LEU	2.2
1	H	242	LEU	2.2
1	J	219	THR	2.2
1	D	71	GLY	2.1
1	I	228	TYR	2.1
1	A	235	PHE	2.1
1	D	185	LEU	2.1
1	B	125	PRO	2.1
1	B	123	GLY	2.1
1	I	117	ALA	2.1
1	I	143	ALA	2.1
1	A	142	MET	2.1
1	J	151	PHE	2.1
1	G	2	ASN	2.1
1	E	22	GLN	2.1
1	E	51	VAL	2.1
1	B	34	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	185	LEU	2.1
1	G	19	LEU	2.1
1	D	125	PRO	2.1
1	A	143	ALA	2.1
1	D	195	ALA	2.1
1	J	195	ALA	2.1
1	H	238	TYR	2.1
1	E	48	ARG	2.1
1	H	218	GLY	2.1
1	G	51	VAL	2.1
1	H	131	ILE	2.1
1	C	42	GLU	2.1
1	A	243	SER	2.1
1	B	48	ARG	2.1
1	J	66	ARG	2.1
1	G	62	GLY	2.1
1	H	37	GLU	2.1
1	A	87	THR	2.1
1	D	43	GLN	2.0
1	F	35	PRO	2.0
1	H	16	MET	2.0
1	B	197	ILE	2.0
1	E	170	ILE	2.0
1	H	12	TYR	2.0
1	H	75	SER	2.0
1	H	207	LEU	2.0
1	I	226	SER	2.0
1	A	238	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	I	1244	5/5	0.95	0.18	-0.11	55,57,60,60	0
2	SO4	F	1244	5/5	0.98	0.20	-0.41	43,44,45,46	0
2	SO4	E	1243	5/5	0.98	0.14	-0.57	59,59,60,60	0
2	SO4	C	1244	5/5	0.99	0.17	-0.61	40,41,42,42	0
2	SO4	D	1244	5/5	0.99	0.16	-0.88	36,37,38,39	0
2	SO4	B	1244	5/5	0.98	0.16	-0.94	47,48,48,49	0
2	SO4	G	1244	5/5	0.98	0.13	-1.21	54,55,56,57	0
2	SO4	F	1243	5/5	0.95	0.13	-1.42	61,63,64,64	0
2	SO4	I	1243	5/5	0.98	0.15	-1.47	47,48,50,51	0
2	SO4	G	1243	5/5	0.97	0.10	-1.63	77,77,78,78	0
2	SO4	C	1243	5/5	0.98	0.11	-2.64	50,53,55,56	0
2	SO4	A	1244	5/5	0.99	0.15	-2.74	38,39,40,41	0
2	SO4	B	1243	5/5	0.96	0.11	-3.34	67,68,68,69	0
2	SO4	D	1243	5/5	0.99	0.08	-3.84	54,54,56,56	0
2	SO4	A	1245	5/5	0.99	0.10	-5.11	55,55,56,58	0

6.5 Other polymers

There are no such residues in this entry.