



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 06:56 AM UTC

PDB ID : 7P49 / pdb_00007p49
Title : HLA-E*01:03 in complex with Mtb14
Authors : Walters, L.C.; Gillespie, G.M.
Deposited on : 2021-07-10
Resolution : 2.05 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

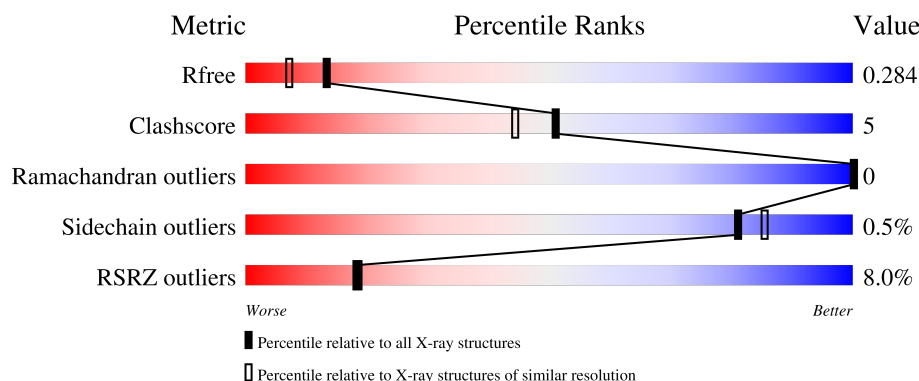
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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 $\leq 5\%$. 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	276	4% 89% 11%
1	C	276	8% 86% 14%
1	E	276	17% 84% 12% .
1	G	276	7% 88% 12%
2	B	100	9% 90% 9% .

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Mol	Chain	Length	Quality of chain
2	D	100	9% 84% 16%
2	F	100	2% 87% 13%
2	H	100	% 89% 10%
3	P	9	89% 11%
3	Q	9	11% 100%
3	R	9	100%
3	Z	9	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13373 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 HLA class I histocompatibility antigen, alpha chain E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	1	0
			2253	1410	403	433	7			
1	C	275	Total	C	N	O	S	0	0	0
			2239	1400	401	431	7			
1	E	266	Total	C	N	O	S	0	0	0
			2170	1361	387	415	7			
1	G	276	Total	C	N	O	S	0	0	0
			2246	1405	402	432	7			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	D	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	F	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	H	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

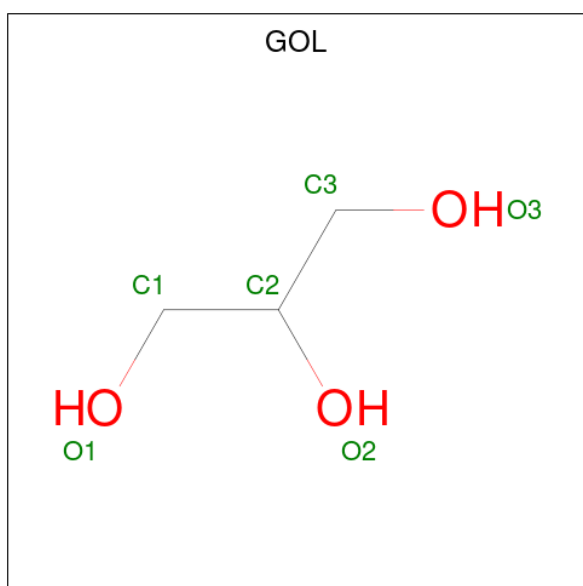
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P61769
D	1	MET	-	initiating methionine	UNP P61769
F	1	MET	-	initiating methionine	UNP P61769
H	1	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Phenolphthiocerol/phthiocerol polyketide synthase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	S	0	0	0
			66	40	13	12	1			
3	Q	9	Total	C	N	O	S	0	0	0
			66	40	13	12	1			
3	R	9	Total	C	N	O	S	0	0	0
			66	40	13	12	1			
3	Z	9	Total	C	N	O	S	0	0	0
			66	40	13	12	1			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



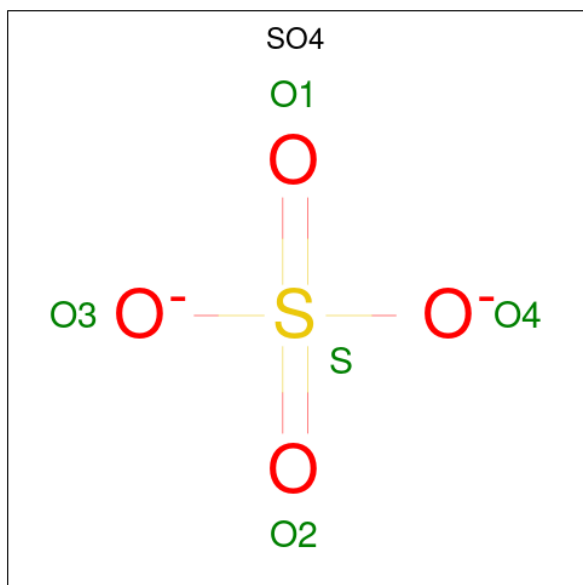
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	P	1	Total	O	S	0	0
			5	4	1		
5	Q	1	Total	O	S	0	0
			5	4	1		
5	R	1	Total	O	S	0	0
			5	4	1		
5	Z	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total 1	Zn 1	0	0
6	G	1	Total 1	Zn 1	0	0

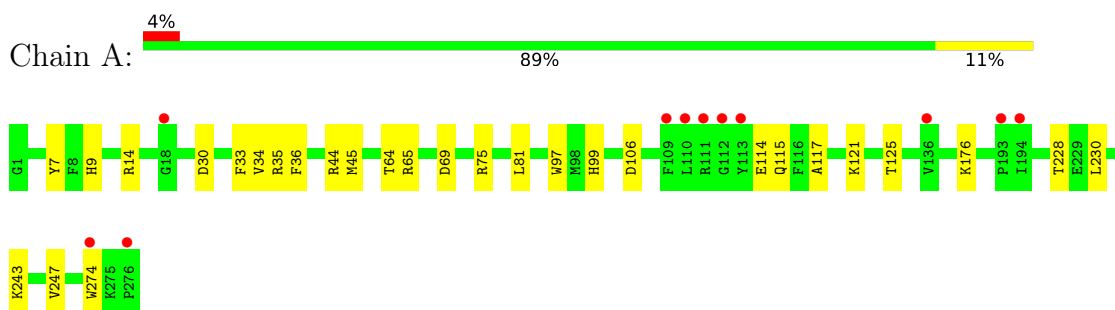
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	127	Total 127	O 127	0	0
7	B	45	Total 45	O 45	0	0
7	C	91	Total 91	O 91	0	0
7	D	45	Total 45	O 45	0	0
7	E	102	Total 102	O 102	0	0
7	F	61	Total 61	O 61	0	0
7	G	110	Total 110	O 110	0	0
7	H	48	Total 48	O 48	0	0
7	P	6	Total 6	O 6	0	0
7	Q	6	Total 6	O 6	0	0
7	R	6	Total 6	O 6	0	0
7	Z	3	Total 3	O 3	0	0

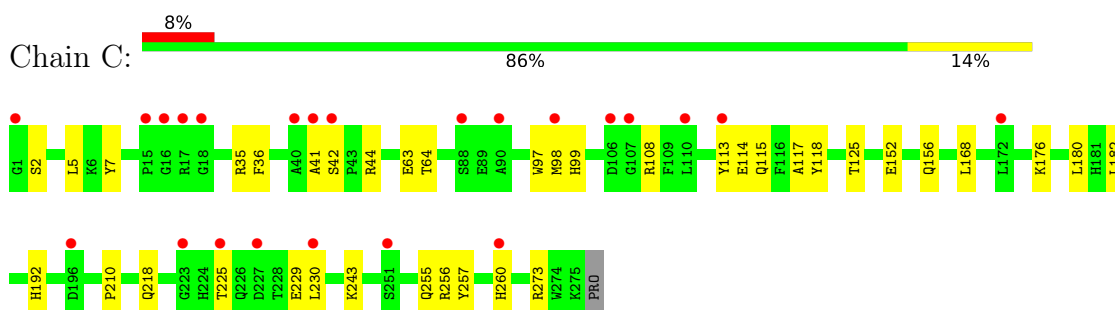
3 Residue-property plots [i](#)

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.

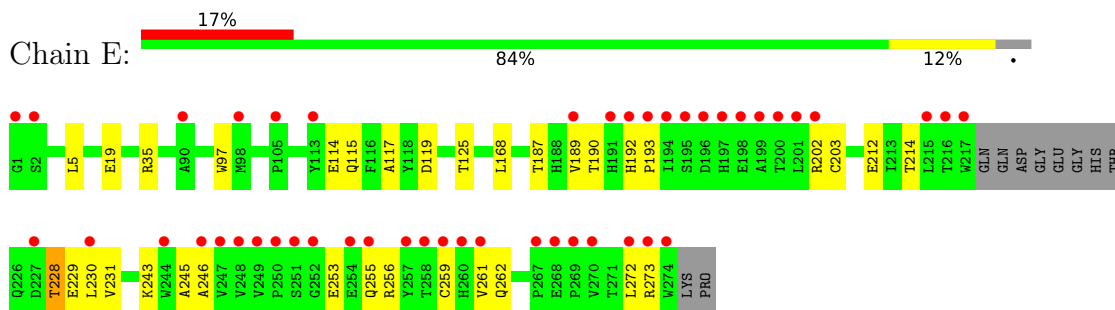
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E



- Molecule 1: HLA class I histocompatibility antigen, alpha chain E

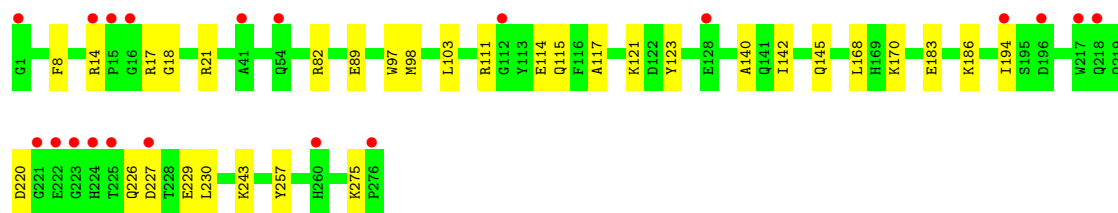


- Molecule 1: HLA class I histocompatibility antigen, alpha chain E

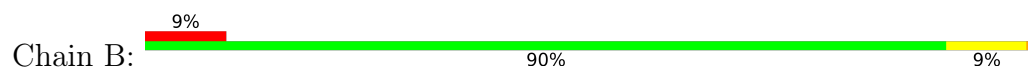


- Molecule 1: HLA class I histocompatibility antigen, alpha chain E

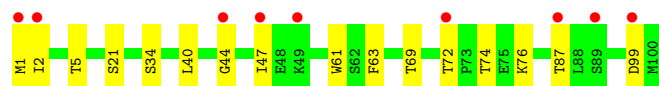
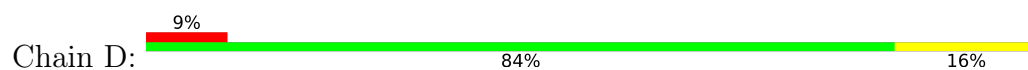




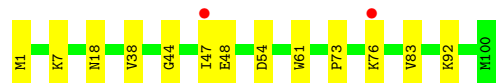
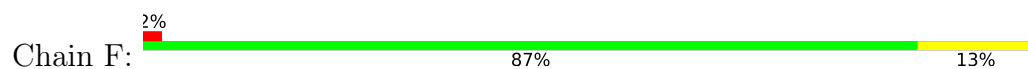
● Molecule 2: Beta-2-microglobulin



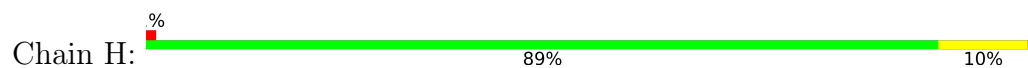
● Molecule 2: Beta-2-microglobulin



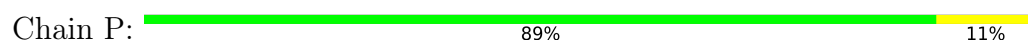
● Molecule 2: Beta-2-microglobulin



● Molecule 2: Beta-2-microglobulin

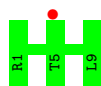


● Molecule 3: Phenolphthiocerol/phthiocerol polyketide synthase subunit B



● Molecule 3: Phenolphthiocerol/phthiocerol polyketide synthase subunit B





- Molecule 3: Phenolphthiocerol/phthiocerol polyketide synthase subunit B

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Phenolphthiocerol/phthiocerol polyketide synthase subunit B

Chain Z:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	245.15Å 47.93Å 152.44Å 90.00° 117.45° 90.00°	Depositor
Resolution (Å)	57.16 – 2.05 57.16 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.0 (57.16-2.05) 99.4 (57.16-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.05Å)	Xtriage
Refinement program	REFMAC 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.237 , 0.279 0.245 , 0.284	Depositor DCC
R_{free} test set	5007 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13373	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0172e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/2320	0.34	0/3156
1	C	0.16	0/2305	0.35	0/3134
1	E	0.17	0/2234	0.35	0/3038
1	G	0.15	0/2313	0.33	0/3146
2	B	0.14	0/860	0.34	0/1162
2	D	0.15	0/860	0.36	0/1162
2	F	0.15	0/860	0.33	0/1162
2	H	0.14	0/860	0.33	0/1162
3	P	0.22	0/65	0.47	0/85
3	Q	0.18	0/65	0.32	0/85
3	R	0.17	0/65	0.38	0/85
3	Z	0.14	0/65	0.35	0/85
All	All	0.15	0/12872	0.34	0/17462

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2253	0	2096	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2239	0	2081	29	0
1	E	2170	0	2021	24	0
1	G	2246	0	2088	26	0
2	B	837	0	803	6	0
2	D	837	0	803	11	0
2	F	837	0	803	10	0
2	H	837	0	803	11	0
3	P	66	0	74	3	0
3	Q	66	0	74	0	0
3	R	66	0	74	0	0
3	Z	66	0	74	0	0
4	A	12	0	16	3	0
4	B	12	0	16	1	0
4	C	18	0	24	1	0
4	D	12	0	16	0	0
4	E	6	0	8	0	0
4	G	6	0	8	0	0
5	A	25	0	0	0	0
5	B	10	0	0	0	0
5	C	20	0	0	0	0
5	D	10	0	0	0	0
5	E	10	0	0	0	0
5	F	15	0	0	0	0
5	G	10	0	0	0	0
5	H	15	0	0	0	0
5	P	5	0	0	0	0
5	Q	5	0	0	0	0
5	R	5	0	0	0	0
5	Z	5	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
7	A	127	0	0	6	0
7	B	45	0	0	0	0
7	C	91	0	0	10	0
7	D	45	0	0	2	0
7	E	102	0	0	8	0
7	F	61	0	0	2	2
7	G	110	0	0	13	2
7	H	48	0	0	5	1
7	P	6	0	0	0	0
7	Q	6	0	0	0	1
7	R	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Z	3	0	0	0	0
All	All	13373	0	11882	128	3

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 5.

All (128) 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:E:259:CYS:SG	7:E:496:HOH:O	2.27	0.93
1:G:257:TYR:O	7:G:401:HOH:O	1.89	0.91
1:E:203:CYS:SG	7:E:496:HOH:O	2.29	0.88
1:G:111:ARG:NH1	7:G:402:HOH:O	2.07	0.86
2:H:48:GLU:OE2	7:H:301:HOH:O	1.96	0.84
1:A:75:ARG:HE	4:A:302:GOL:H12	1.43	0.83
1:G:18:GLY:N	7:G:404:HOH:O	2.15	0.80
1:E:190:THR:O	7:E:401:HOH:O	1.99	0.80
1:C:98:MET:HG2	1:C:113:TYR:HE2	1.48	0.77
2:D:5:THR:HA	2:D:87:THR:HG21	1.67	0.75
2:H:21:SER:O	7:H:302:HOH:O	2.07	0.72
1:C:97:TRP:HE1	1:C:114:GLU:HG3	1.54	0.71
1:E:202:ARG:NH2	7:E:404:HOH:O	2.23	0.71
1:C:2:SER:O	7:C:401:HOH:O	2.09	0.70
1:E:19:GLU:OE1	7:E:402:HOH:O	2.09	0.69
1:C:115:GLN:NE2	7:C:410:HOH:O	2.26	0.68
2:H:90:GLN:OE1	7:H:304:HOH:O	2.11	0.67
1:C:118:TYR:OH	7:C:402:HOH:O	2.11	0.67
1:G:229:GLU:OE1	7:G:403:HOH:O	2.13	0.66
2:D:44:GLY:O	7:D:301:HOH:O	2.12	0.66
1:G:142:ILE:O	7:G:405:HOH:O	2.15	0.64
1:C:115:GLN:HG2	1:C:125:THR:HG23	1.80	0.64
1:E:212:GLU:O	7:E:403:HOH:O	2.16	0.63
1:C:192:HIS:NE2	2:D:99:ASP:OD2	2.31	0.62
1:E:187:THR:HG21	1:E:261:VAL:HG21	1.80	0.62
1:G:170:LYS:NZ	7:G:413:HOH:O	2.33	0.62
1:A:97:TRP:HE1	1:A:114:GLU:HG3	1.66	0.61
4:C:303:GOL:O3	7:C:403:HOH:O	2.16	0.61
1:E:253:GLU:HB3	1:E:256:ARG:HD3	1.83	0.60
1:G:142:ILE:C	7:G:405:HOH:O	2.43	0.60
1:G:183:GLU:OE2	7:G:406:HOH:O	2.17	0.59
1:E:230:LEU:HD22	1:E:243:LYS:HE3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:ILE:HG22	7:D:303:HOH:O	2.01	0.59
4:A:302:GOL:O1	7:A:401:HOH:O	2.17	0.58
1:G:14:ARG:HE	1:G:17:ARG:HD3	1.68	0.57
1:A:230:LEU:HD11	1:A:243:LYS:HE3	1.85	0.57
1:E:119:ASP:HB3	2:F:1:MET:HG3	1.87	0.57
1:C:44:ARG:HD2	1:C:64:THR:HG21	1.87	0.57
2:B:59:LYS:H	4:B:201:GOL:H11	1.70	0.56
1:G:183:GLU:OE1	7:G:407:HOH:O	2.18	0.56
1:C:229:GLU:OE1	7:C:404:HOH:O	2.18	0.56
2:F:92:LYS:NZ	7:F:302:HOH:O	2.38	0.56
1:A:30:ASP:HA	4:A:301:GOL:H11	1.86	0.56
2:D:74:THR:HG22	2:D:76:LYS:H	1.70	0.56
1:G:97:TRP:HE1	1:G:114:GLU:HG3	1.69	0.56
1:A:228:THR:HG22	1:A:247:VAL:HG12	1.88	0.55
2:D:1:MET:HG3	2:D:2:ILE:HG12	1.88	0.55
1:A:117:ALA:HB2	2:B:61:TRP:CE2	2.41	0.55
1:A:69:ASP:OD2	7:A:402:HOH:O	2.18	0.55
1:E:214:THR:HB	1:E:262:GLN:HB3	1.87	0.55
1:E:97:TRP:HE1	1:E:114:GLU:HG2	1.72	0.55
1:A:45:MET:HE1	3:P:2:MET:HE3	1.88	0.54
1:C:176:LYS:HB2	1:C:180:LEU:HD12	1.87	0.54
1:C:255:GLN:HB3	1:C:273:ARG:HH21	1.71	0.54
1:G:121:LYS:HB2	2:H:2:ILE:HD12	1.89	0.54
1:G:117:ALA:HB2	2:H:61:TRP:CE2	2.42	0.54
1:A:9:HIS:HE1	3:P:2:MET:HE2	1.72	0.54
2:D:21:SER:HA	2:D:72:THR:HG22	1.90	0.54
1:G:230:LEU:HD22	1:G:243:LYS:HE3	1.89	0.54
1:E:35:ARG:HD3	2:F:54:ASP:CG	2.33	0.53
1:C:230:LEU:HD22	1:C:243:LYS:HE3	1.90	0.53
1:E:115:GLN:HG2	1:E:125:THR:HG23	1.89	0.53
1:C:42:SER:N	7:C:408:HOH:O	2.24	0.53
1:A:75:ARG:NH1	7:A:404:HOH:O	2.21	0.52
1:C:117:ALA:HB2	2:D:61:TRP:CE2	2.44	0.52
2:H:90:GLN:HB3	7:H:304:HOH:O	2.08	0.52
1:G:227:ASP:O	7:G:408:HOH:O	2.19	0.52
1:E:273:ARG:NH1	7:E:410:HOH:O	2.42	0.51
1:C:5:LEU:HB2	1:C:168:LEU:HD13	1.93	0.51
1:C:108:ARG:HB2	7:C:471:HOH:O	2.11	0.50
1:E:117:ALA:HB2	2:F:61:TRP:CE2	2.47	0.49
1:G:14:ARG:HH11	1:G:21:ARG:HB2	1.77	0.49
1:A:65:ARG:HH11	1:G:226:GLN:HE22	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:HG2	7:A:505:HOH:O	2.12	0.49
2:H:48:GLU:H	2:H:48:GLU:CD	2.21	0.48
2:B:22:ASN:HB3	2:B:71:PHE:CE1	2.48	0.48
1:E:228:THR:HG22	1:E:245:ALA:HB1	1.95	0.48
1:A:9:HIS:CE1	3:P:2:MET:HE2	2.49	0.48
1:E:5:LEU:HB2	1:E:168:LEU:HD13	1.95	0.48
2:D:40:LEU:HD23	2:D:69:THR:HG22	1.94	0.47
1:G:82:ARG:NH1	1:G:89:GLU:HG2	2.29	0.47
1:G:103:LEU:HG	1:G:168:LEU:HD23	1.96	0.47
1:A:14:ARG:NH1	7:A:408:HOH:O	2.31	0.47
1:A:115:GLN:HG2	1:A:125:THR:HG23	1.97	0.47
2:F:47:ILE:HG22	2:F:48:GLU:O	2.15	0.47
1:E:229:GLU:HB3	1:E:246:ALA:HB3	1.97	0.46
1:A:7:TYR:HB2	1:A:99:HIS:CE1	2.51	0.46
1:C:225:THR:HG21	1:C:257:TYR:HE2	1.81	0.45
1:C:152:GLU:OE1	1:C:156:GLN:NE2	2.49	0.45
1:C:256:ARG:HD3	7:C:473:HOH:O	2.17	0.45
2:F:76:LYS:HE2	2:F:76:LYS:HB3	1.79	0.45
1:C:97:TRP:HE1	1:C:114:GLU:CG	2.24	0.44
1:A:121:LYS:HB2	2:B:2:ILE:HD12	1.99	0.44
1:C:41:ALA:N	7:C:408:HOH:O	2.51	0.44
1:C:35:ARG:HG2	1:C:36:PHE:N	2.33	0.44
1:C:176:LYS:HB2	1:C:176:LYS:HE3	1.74	0.44
1:A:274:TRP:O	7:A:403:HOH:O	2.21	0.44
1:A:44:ARG:HD2	1:A:64:THR:HG21	2.00	0.43
1:G:123:TYR:CZ	1:G:140:ALA:HA	2.53	0.43
1:C:7:TYR:HB2	1:C:99:HIS:CE1	2.54	0.43
1:G:186:LYS:N	1:G:186:LYS:HD2	2.34	0.43
1:E:189:VAL:HG12	7:E:401:HOH:O	2.18	0.43
1:G:98:MET:HE3	1:G:115:GLN:OE1	2.19	0.43
1:C:182:LEU:HD22	1:C:210:PRO:HD3	2.01	0.43
2:F:18:ASN:HA	2:F:73:PRO:O	2.19	0.43
1:E:255:GLN:H	1:E:255:GLN:CD	2.27	0.42
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.54	0.42
1:A:35:ARG:HG2	1:A:36:PHE:N	2.34	0.42
2:B:74:THR:HG22	2:B:75:GLU:H	1.84	0.42
1:G:8:PHE:HB3	2:H:57:PHE:CE2	2.53	0.42
1:G:220:ASP:HA	7:G:415:HOH:O	2.19	0.42
1:C:218:GLN:O	1:C:257:TYR:HA	2.20	0.42
1:G:145:GLN:N	7:G:405:HOH:O	2.51	0.42
1:C:192:HIS:HE2	2:D:99:ASP:CG	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:98:ARG:NH2	7:H:303:HOH:O	2.11	0.42
1:C:218:GLN:OE1	1:C:260:HIS:NE2	2.51	0.42
1:E:189:VAL:HG23	1:E:272:LEU:HD12	2.01	0.42
2:F:38:VAL:HG22	2:F:83:VAL:HG22	2.01	0.42
2:B:78:GLU:HB3	2:B:95:LYS:HE2	2.02	0.42
1:E:192:HIS:HA	1:E:193:PRO:HD3	1.89	0.41
1:E:231:VAL:O	1:E:243:LYS:NZ	2.29	0.41
1:G:275:LYS:HG3	7:G:439:HOH:O	2.20	0.41
2:D:34:SER:HB3	2:D:63:PHE:CE2	2.56	0.41
2:F:7:LYS:HE2	2:F:7:LYS:HB3	1.98	0.41
2:F:44:GLY:N	7:F:301:HOH:O	2.35	0.41
2:H:7:LYS:O	2:H:28:VAL:HA	2.22	0.40
2:H:38:VAL:HG22	2:H:83:VAL:HG22	2.02	0.40
1:C:63:GLU:OE1	7:C:405:HOH:O	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:324:HOH:O	7:H:339:HOH:O[4_546]	1.95	0.25
7:G:435:HOH:O	7:Q:201:HOH:O[3_455]	2.08	0.12
7:F:326:HOH:O	7:G:450:HOH:O[4_546]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	275/276 (100%)	268 (98%)	7 (2%)	0	100	100
1	C	273/276 (99%)	267 (98%)	6 (2%)	0	100	100
1	E	262/276 (95%)	256 (98%)	6 (2%)	0	100	100
1	G	274/276 (99%)	269 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	D	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	F	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	H	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	P	7/9 (78%)	7 (100%)	0	0	100	100
3	Q	7/9 (78%)	7 (100%)	0	0	100	100
3	R	7/9 (78%)	7 (100%)	0	0	100	100
3	Z	7/9 (78%)	7 (100%)	0	0	100	100
All	All	1504/1540 (98%)	1475 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	238/237 (100%)	236 (99%)	2 (1%)	73	77
1	C	236/237 (100%)	236 (100%)	0	100	100
1	E	229/237 (97%)	228 (100%)	1 (0%)	84	88
1	G	237/237 (100%)	236 (100%)	1 (0%)	84	88
2	B	95/95 (100%)	93 (98%)	2 (2%)	47	46
2	D	95/95 (100%)	95 (100%)	0	100	100
2	F	95/95 (100%)	95 (100%)	0	100	100
2	H	95/95 (100%)	94 (99%)	1 (1%)	65	68
3	P	6/6 (100%)	6 (100%)	0	100	100
3	Q	6/6 (100%)	6 (100%)	0	100	100
3	R	6/6 (100%)	6 (100%)	0	100	100
3	Z	6/6 (100%)	6 (100%)	0	100	100
All	All	1344/1352 (99%)	1337 (100%)	7 (0%)	81	85

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LEU
1	A	106	ASP
2	B	5	THR
2	B	74	THR
1	E	228	THR
1	G	194	ILE
2	H	90	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	E	72	GLN
1	E	155	HIS
1	E	188	HIS
2	F	14	HIS
1	G	145	GLN
1	G	148	ASN
1	G	224	HIS
3	P	7	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 2 are monoatomic - leaving 38 for Mogul analysis.

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	GOL	G	301	-	5,5,5	0.90	0	5,5,5	1.11	0
4	GOL	D	202	-	5,5,5	0.87	0	5,5,5	1.05	0
5	SO4	H	201	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	H	202	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	A	304	-	4,4,4	0.24	0	6,6,6	0.14	0
5	SO4	F	201	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	C	304	-	4,4,4	0.24	0	6,6,6	0.05	0
4	GOL	D	201	-	5,5,5	0.97	0	5,5,5	1.11	0
5	SO4	G	304	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	C	306	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	A	306	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	D	203	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	D	204	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	Q	101	-	4,4,4	0.28	0	6,6,6	0.14	0
4	GOL	C	301	-	5,5,5	0.96	0	5,5,5	0.96	0
4	GOL	C	302	-	5,5,5	0.87	0	5,5,5	1.16	1 (20%)
4	GOL	E	301	-	5,5,5	0.88	0	5,5,5	1.09	0
5	SO4	E	304	-	4,4,4	0.24	0	6,6,6	0.11	0
4	GOL	A	302	-	5,5,5	0.92	0	5,5,5	1.14	1 (20%)
4	GOL	A	301	-	5,5,5	0.88	0	5,5,5	0.98	0
4	GOL	B	204	-	5,5,5	0.86	0	5,5,5	1.15	0
5	SO4	P	101	-	4,4,4	0.25	0	6,6,6	0.08	0
5	SO4	B	203	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	E	303	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	F	203	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	A	303	-	4,4,4	0.25	0	6,6,6	0.14	0
5	SO4	R	101	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	G	303	-	4,4,4	0.25	0	6,6,6	0.10	0
5	SO4	H	203	-	4,4,4	0.23	0	6,6,6	0.11	0
4	GOL	B	201	-	5,5,5	0.92	0	5,5,5	1.10	0
5	SO4	Z	101	-	4,4,4	0.22	0	6,6,6	0.14	0
5	SO4	A	307	-	4,4,4	0.21	0	6,6,6	0.12	0
5	SO4	F	202	-	4,4,4	0.23	0	6,6,6	0.05	0
5	SO4	C	307	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	C	305	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	B	202	-	4,4,4	0.24	0	6,6,6	0.12	0
5	SO4	A	305	-	4,4,4	0.23	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	C	303	-	5,5,5	0.93	0	5,5,5	1.04	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
4	GOL	D	201	-	-	2/4/4/4	-
4	GOL	B	201	-	-	2/4/4/4	-
4	GOL	G	301	-	-	2/4/4/4	-
4	GOL	D	202	-	-	0/4/4/4	-
4	GOL	A	302	-	-	3/4/4/4	-
4	GOL	C	301	-	-	4/4/4/4	-
4	GOL	C	302	-	-	2/4/4/4	-
4	GOL	E	301	-	-	0/4/4/4	-
4	GOL	C	303	-	-	2/4/4/4	-
4	GOL	A	301	-	-	3/4/4/4	-
4	GOL	B	204	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	302	GOL	C3-C2-C1	-2.16	103.88	111.80
4	C	302	GOL	C3-C2-C1	-2.02	104.40	111.80

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GOL	O1-C1-C2-C3
4	B	201	GOL	C1-C2-C3-O3
4	C	301	GOL	C1-C2-C3-O3
4	D	201	GOL	O1-C1-C2-C3
4	A	302	GOL	C1-C2-C3-O3
4	B	204	GOL	O1-C1-C2-C3
4	C	301	GOL	O1-C1-C2-C3
4	C	302	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	C	303	GOL	O1-C1-C2-C3
4	B	201	GOL	O2-C2-C3-O3
4	C	301	GOL	O1-C1-C2-O2
4	C	301	GOL	O2-C2-C3-O3
4	C	303	GOL	O1-C1-C2-O2
4	D	201	GOL	O1-C1-C2-O2
4	A	301	GOL	O1-C1-C2-O2
4	A	301	GOL	O2-C2-C3-O3
4	G	301	GOL	C1-C2-C3-O3
4	A	302	GOL	O2-C2-C3-O3
4	B	204	GOL	O1-C1-C2-O2
4	A	302	GOL	O1-C1-C2-O2
4	C	302	GOL	O1-C1-C2-O2
4	G	301	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	GOL	2	0
4	A	301	GOL	1	0
4	B	201	GOL	1	0
4	C	303	GOL	1	0

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	276/276 (100%)	0.48	11 (3%)	42 42	21, 36, 57, 67	1 (0%)
1	C	275/276 (99%)	0.83	23 (8%)	17 17	26, 40, 63, 87	0
1	E	266/276 (96%)	0.96	46 (17%)	4 3	24, 39, 77, 101	0
1	G	276/276 (100%)	0.78	20 (7%)	21 21	27, 40, 62, 78	0
2	B	100/100 (100%)	0.84	9 (9%)	15 15	25, 43, 60, 71	0
2	D	100/100 (100%)	0.85	9 (9%)	15 15	29, 40, 59, 71	0
2	F	100/100 (100%)	0.61	2 (2%)	65 67	26, 38, 56, 64	0
2	H	100/100 (100%)	0.78	1 (1%)	79 81	29, 45, 64, 70	0
3	P	9/9 (100%)	0.52	0	100 100	30, 35, 40, 43	0
3	Q	9/9 (100%)	0.87	1 (11%)	10 10	36, 40, 46, 49	0
3	R	9/9 (100%)	0.34	0	100 100	30, 35, 40, 44	0
3	Z	9/9 (100%)	0.78	0	100 100	33, 40, 48, 49	0
All	All	1529/1540 (99%)	0.76	122 (7%)	18 18	21, 39, 64, 101	1 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	249	VAL	4.7
1	E	258	THR	4.5
1	E	274	TRP	4.3
1	E	250	PRO	4.3
2	D	1	MET	4.2
1	A	109	PHE	4.1
1	E	248	VAL	4.1
1	E	217	TRP	4.1
1	C	16	GLY	4.0
1	A	111	ARG	3.8
1	E	200	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	197	HIS	3.8
2	B	49	LYS	3.7
1	E	216	THR	3.7
1	E	247	VAL	3.6
1	A	136[A]	VAL	3.6
1	E	260	HIS	3.6
1	E	193	PRO	3.5
1	E	113	TYR	3.5
1	A	112	GLY	3.4
1	A	276	PRO	3.4
1	E	194	ILE	3.4
1	C	40	ALA	3.3
1	E	272	LEU	3.3
1	E	257	TYR	3.2
1	E	201	LEU	3.2
1	E	255	GLN	3.2
1	C	18	GLY	3.1
1	E	189	VAL	3.1
1	E	230	LEU	3.1
2	D	2	ILE	3.1
1	C	41	ALA	3.0
1	A	194	ILE	3.0
2	D	89	SER	3.0
1	C	227	ASP	3.0
1	E	196	ASP	3.0
1	E	191	HIS	3.0
1	G	15	PRO	3.0
1	E	246	ALA	3.0
1	A	110	LEU	3.0
1	E	198	GLU	2.9
1	C	15	PRO	2.9
1	C	1	GLY	2.9
1	E	261	VAL	2.9
1	E	251	SER	2.9
1	G	223	GLY	2.9
1	E	267	PRO	2.9
1	A	113	TYR	2.9
1	E	252	GLY	2.9
1	G	16	GLY	2.9
1	C	196	ASP	2.8
1	E	259	CYS	2.8
1	E	244	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	195	SER	2.7
1	E	215	LEU	2.7
1	E	199	ALA	2.7
1	E	192	HIS	2.7
1	E	269	PRO	2.6
2	B	18	ASN	2.6
1	C	113	TYR	2.6
1	G	14	ARG	2.6
1	C	90	ALA	2.6
3	Q	5	THR	2.6
1	G	276	PRO	2.5
2	F	47	ILE	2.5
2	B	50	VAL	2.5
1	C	172	LEU	2.5
1	E	270	VAL	2.4
1	C	223	GLY	2.4
1	G	221	GLY	2.4
1	G	225	THR	2.4
2	B	95	LYS	2.4
1	E	268	GLU	2.4
1	G	222	GLU	2.4
1	E	273	ARG	2.3
1	G	194	ILE	2.3
1	G	112	GLY	2.3
1	C	17	ARG	2.3
1	E	202	ARG	2.3
2	D	87	THR	2.3
1	C	110	LEU	2.3
2	B	99	ASP	2.3
1	E	98	MET	2.3
1	G	224	HIS	2.3
2	D	44	GLY	2.3
1	C	251	SER	2.2
1	C	42	SER	2.2
1	C	225	THR	2.2
1	C	98	MET	2.2
1	G	54	GLN	2.2
2	F	76	LYS	2.2
1	G	217	TRP	2.2
1	G	227	ASP	2.2
1	G	218	GLN	2.1
2	B	88	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	196	ASP	2.1
1	E	105	PRO	2.1
2	D	72	THR	2.1
2	B	19	GLY	2.1
1	E	2	SER	2.1
1	C	106	ASP	2.1
1	C	260	HIS	2.1
1	A	18	GLY	2.1
1	C	107	GLY	2.1
1	G	1	GLY	2.1
1	A	274	TRP	2.1
1	E	90	ALA	2.1
1	G	41	ALA	2.1
1	C	230	LEU	2.1
1	E	254	GLU	2.1
2	D	99	ASP	2.1
1	A	193	PRO	2.1
1	E	1	GLY	2.1
2	B	44	GLY	2.1
1	E	227	ASP	2.0
2	B	81	CYS	2.0
1	G	260	HIS	2.0
2	D	49	LYS	2.0
2	D	47	ILE	2.0
1	G	128	GLU	2.0
1	C	88	SER	2.0
2	H	88	LEU	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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
5	SO4	B	203	5/5	0.45	0.12	90,91,96,115	0
5	SO4	C	306	5/5	0.57	0.15	62,64,74,76	0
4	GOL	B	201	6/6	0.64	0.20	41,45,46,46	0
4	GOL	E	301	6/6	0.68	0.16	52,53,56,57	0
4	GOL	D	201	6/6	0.72	0.15	46,50,53,53	0
5	SO4	B	202	5/5	0.72	0.11	66,74,79,105	0
4	GOL	C	301	6/6	0.74	0.17	38,39,45,46	0
5	SO4	F	201	5/5	0.74	0.12	59,60,74,80	0
5	SO4	H	201	5/5	0.74	0.11	59,66,70,78	0
5	SO4	A	304	5/5	0.75	0.10	60,63,77,84	0
4	GOL	B	204	6/6	0.76	0.14	49,52,53,55	0
5	SO4	F	202	5/5	0.76	0.11	67,73,83,88	0
5	SO4	C	307	5/5	0.76	0.10	61,64,64,70	0
4	GOL	A	302	6/6	0.77	0.17	41,42,46,48	0
5	SO4	C	305	5/5	0.79	0.09	62,68,73,82	0
5	SO4	A	306	5/5	0.82	0.10	58,66,74,80	0
5	SO4	Q	101	5/5	0.82	0.12	52,52,61,64	0
5	SO4	R	101	5/5	0.82	0.10	47,50,57,70	0
5	SO4	H	202	5/5	0.83	0.08	63,66,76,76	0
5	SO4	E	304	5/5	0.84	0.09	53,60,69,82	0
4	GOL	C	302	6/6	0.85	0.12	35,41,43,50	0
5	SO4	H	203	5/5	0.86	0.09	50,55,63,66	0
5	SO4	A	307	5/5	0.86	0.10	47,62,71,74	0
5	SO4	C	304	5/5	0.86	0.08	56,59,67,73	0
5	SO4	A	303	5/5	0.87	0.13	41,43,49,56	0
4	GOL	C	303	6/6	0.87	0.15	37,41,44,48	0
5	SO4	D	203	5/5	0.87	0.08	51,63,72,72	0
5	SO4	D	204	5/5	0.87	0.09	53,57,63,69	0
4	GOL	A	301	6/6	0.88	0.11	35,36,38,40	0
5	SO4	G	304	5/5	0.89	0.08	50,53,62,66	0
5	SO4	E	303	5/5	0.89	0.09	49,51,64,66	0
5	SO4	A	305	5/5	0.89	0.08	54,59,64,64	0
5	SO4	Z	101	5/5	0.89	0.12	48,51,57,59	0
4	GOL	G	301	6/6	0.90	0.10	37,40,40,45	0
5	SO4	F	203	5/5	0.90	0.08	52,55,63,64	0
5	SO4	P	101	5/5	0.90	0.10	47,47,52,61	0
4	GOL	D	202	6/6	0.91	0.12	31,33,34,36	0
5	SO4	G	303	5/5	0.92	0.12	47,51,53,54	0
6	ZN	E	302	1/1	0.94	0.07	45,45,45,45	1
6	ZN	G	302	1/1	0.98	0.03	39,39,39,39	1

6.5 Other polymers [i](#)

There are no such residues in this entry.