



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:23 AM UTC

PDB ID : 7P4B / pdb_00007p4b
Title : HLA-E*01:03 in complex with IL9
Authors : Walters, L.C.; Gillespie, G.M.
Deposited on : 2021-07-10
Resolution : 1.72 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:

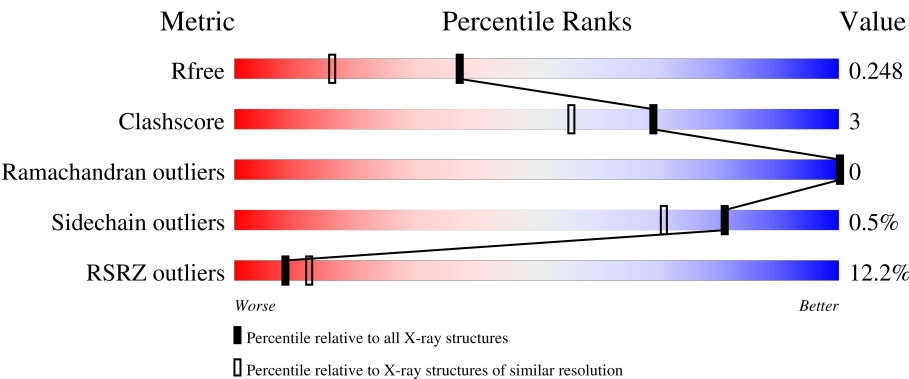
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	277	9% 90% 9%
1	C	277	5% 94% 5%
1	E	277	35% 81% 13% 6%
1	G	277	4% 92% 7%
2	B	100	12% 91% 8%

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Mol	Chain	Length	Quality of chain
2	D	100	3% 90% 10%
2	F	100	4% 95% 5%
2	H	100	12% 96%
3	P	9	22% 78% 11% 11%
3	Q	9	44% 89% 11%
3	R	9	33% 100%
3	Z	9	11% 89% 11%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13836 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
			2256	1411	405	433	7			
1	C	276	Total	C	N	O	S	0	2	0
			2264	1415	407	435	7			
1	E	260	Total	C	N	O	S	0	0	0
			2123	1331	377	408	7			
1	G	276	Total	C	N	O	S	0	4	0
			2281	1425	411	438	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	PRO	-	expression tag	UNP P13747
C	277	PRO	-	expression tag	UNP P13747
E	277	PRO	-	expression tag	UNP P13747
G	277	PRO	-	expression tag	UNP P13747

- 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			

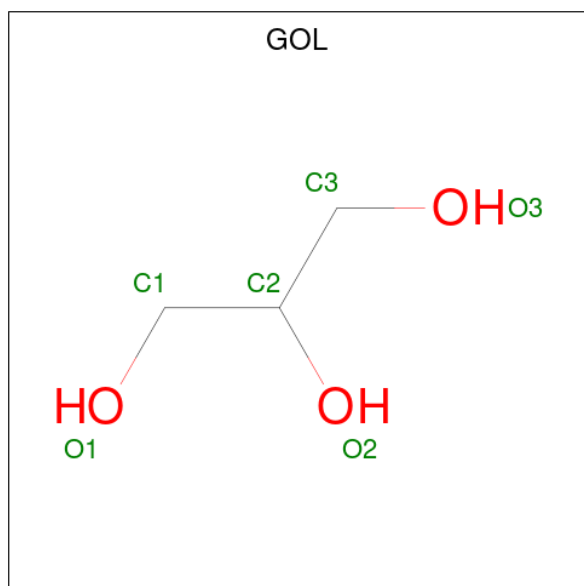
There are 4 discrepancies between the modelled and reference sequences:

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 ESAT-6-like protein EsxH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	S	0	0	0
			77	52	10	13	2			
3	Q	9	Total	C	N	O	S	0	0	0
			77	52	10	13	2			
3	R	9	Total	C	N	O	S	0	0	0
			77	52	10	13	2			
3	Z	9	Total	C	N	O	S	0	0	0
			77	52	10	13	2			

- 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	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		

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

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

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

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	167	Total	O	0	0
			167	167		
8	B	47	Total	O	0	0
			47	47		
8	C	250	Total	O	0	0
			250	250		
8	D	106	Total	O	0	0
			106	106		
8	E	118	Total	O	0	0
			118	118		
8	F	77	Total	O	0	0
			77	77		
8	G	249	Total	O	0	0
			249	249		
8	H	69	Total	O	0	0
			69	69		
8	P	8	Total	O	0	0
			8	8		
8	Q	5	Total	O	0	0
			5	5		
8	R	5	Total	O	0	0
			5	5		

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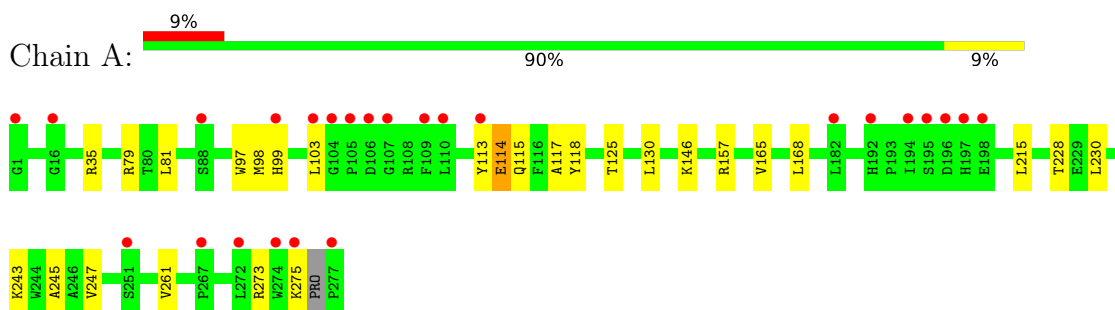
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	Z	8	Total	O	0	0
			8	8		

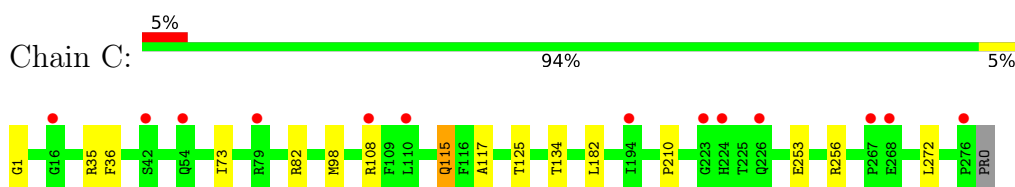
3 Residue-property plots [i](#)

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.

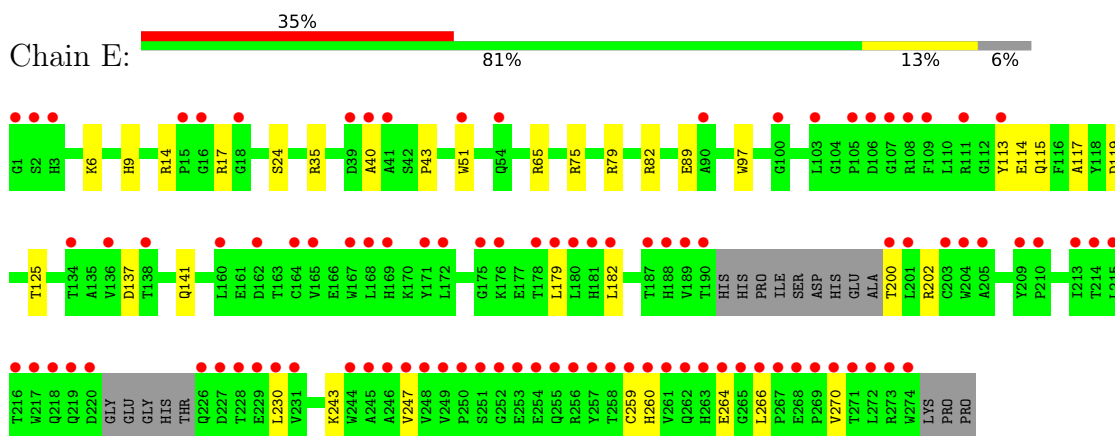
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E



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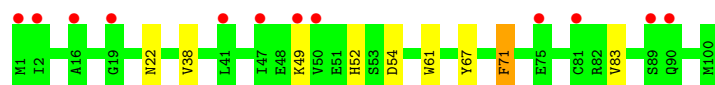
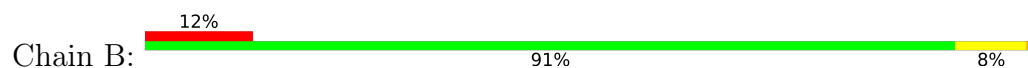


- Molecule 1: HLA class I histocompatibility antigen, alpha chain E

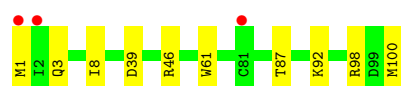
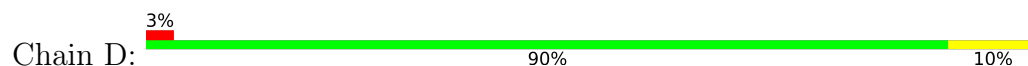




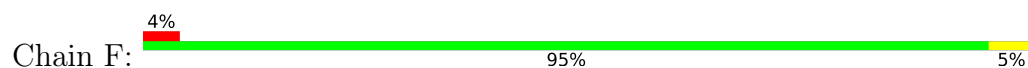
- Molecule 2: Beta-2-microglobulin



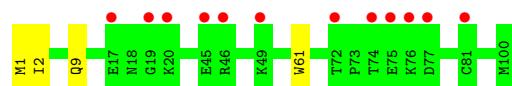
- Molecule 2: Beta-2-microglobulin



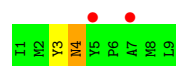
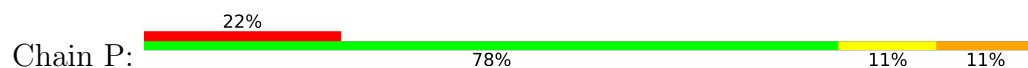
- Molecule 2: Beta-2-microglobulin



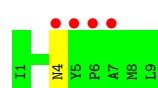
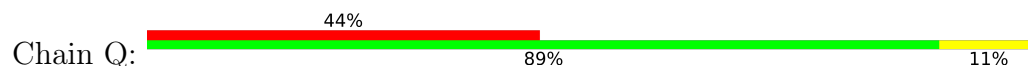
- Molecule 2: Beta-2-microglobulin



- Molecule 3: ESAT-6-like protein EsxH

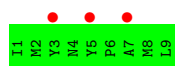


- Molecule 3: ESAT-6-like protein EsxH



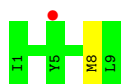
- Molecule 3: ESAT-6-like protein EsxH

Chain R:  33% 100%



- Molecule 3: ESAT-6-like protein EsxH

Chain Z:  11% 89% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	244.56Å 48.53Å 153.16Å 90.00° 116.95° 90.00°	Depositor
Resolution (Å)	75.18 – 1.72 75.18 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.8 (75.18-1.72) 100.0 (75.18-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 1.72Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.201 , 0.237 0.214 , 0.248	Depositor DCC
R_{free} test set	8637 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtrriage
Anisotropy	0.695	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13836	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.03 % 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 2.3675e-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: PO4, SO4, GOL, 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	0.14	0/2323	0.34	0/3157
1	C	0.17	0/2331	0.39	0/3170
1	E	0.13	0/2182	0.36	0/2964
1	G	0.17	0/2349	0.38	0/3195
2	B	0.12	0/860	0.34	0/1162
2	D	0.16	0/860	0.43	0/1162
2	F	0.13	0/860	0.36	0/1162
2	H	0.13	0/860	0.36	0/1162
3	P	0.11	0/79	0.42	0/105
3	Q	0.22	0/79	0.62	0/105
3	R	0.13	0/79	0.38	0/105
3	Z	0.13	0/79	0.47	0/105
All	All	0.15	0/12941	0.37	0/17554

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	2256	0	2094	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2264	0	2106	13	0
1	E	2123	0	1981	24	0
1	G	2281	0	2118	15	0
2	B	837	0	803	6	0
2	D	837	0	803	7	0
2	F	837	0	803	4	0
2	H	837	0	803	5	0
3	P	77	0	78	2	0
3	Q	77	0	78	1	0
3	R	77	0	78	0	0
3	Z	77	0	78	1	0
4	A	6	0	8	0	0
4	C	18	0	24	0	0
4	D	24	0	32	2	0
4	G	6	0	8	0	0
4	H	6	0	8	2	0
5	A	15	0	0	1	0
5	C	15	0	0	0	0
5	D	5	0	0	0	0
5	F	10	0	0	0	0
5	G	15	0	0	0	0
5	H	20	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
7	F	5	0	0	0	0
8	A	167	0	0	3	0
8	B	47	0	0	0	0
8	C	250	0	0	4	0
8	D	106	0	0	1	0
8	E	118	0	0	5	0
8	F	77	0	0	0	0
8	G	249	0	0	2	0
8	H	69	0	0	0	0
8	P	8	0	0	1	0
8	Q	5	0	0	0	0
8	R	5	0	0	0	0
8	Z	8	0	0	0	0
All	All	13836	0	11903	85	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 3.

All (85) 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	8:E:409:HOH:O	2.44	0.76
2:D:98:ARG:HE	4:D:203:GOL:H11	1.50	0.74
1:E:202:ARG:O	8:E:401:HOH:O	2.08	0.71
1:C:115:GLN:HB3	1:C:125[A]:THR:HG22	1.74	0.69
1:E:200:THR:N	8:E:403:HOH:O	2.27	0.68
1:A:115:GLN:HG2	1:A:125:THR:HG23	1.77	0.67
1:C:73:ILE:HD11	3:Z:8:MET:HE1	1.76	0.67
1:A:273:ARG:HD2	1:A:275:LYS:HE3	1.77	0.65
1:E:200:THR:OG1	1:E:247:VAL:O	2.15	0.65
1:A:98:MET:SD	8:A:567:HOH:O	2.55	0.65
1:A:228:THR:HG22	1:A:247:VAL:HG12	1.77	0.64
1:E:9:HIS:ND1	1:E:24:SER:OG	2.27	0.63
1:E:115:GLN:HG2	1:E:125:THR:HG23	1.81	0.63
1:E:200:THR:N	8:E:404:HOH:O	2.32	0.62
1:C:35:ARG:NH1	8:C:404:HOH:O	2.35	0.60
1:C:108:ARG:NH2	8:C:403:HOH:O	2.32	0.60
1:A:103:LEU:HD21	1:A:165:VAL:HG13	1.84	0.60
1:C:117:ALA:HB2	2:D:61:TRP:CE2	2.37	0.60
1:E:75:ARG:HE	1:E:79:ARG:HH22	1.48	0.59
1:A:103:LEU:HG	1:A:168:LEU:HD23	1.85	0.59
1:A:117:ALA:HB2	2:B:61:TRP:CE2	2.37	0.59
1:A:146:LYS:HG2	1:E:65:ARG:HD2	1.86	0.58
2:F:74:THR:OG1	2:F:77:ASP:OD1	2.20	0.57
1:C:253:GLU:HB3	1:C:256:ARG:HD3	1.85	0.57
1:E:117:ALA:HB2	2:F:61:TRP:CE2	2.40	0.56
1:G:115:GLN:HG2	1:G:125:THR:HG23	1.86	0.56
1:G:117:ALA:HB2	2:H:61:TRP:CE2	2.41	0.55
1:A:35:ARG:NH2	2:B:54:ASP:OD1	2.39	0.55
1:A:125:THR:OG1	8:A:401:HOH:O	2.18	0.54
1:G:226:GLN:H	1:G:226:GLN:CD	2.15	0.54
1:A:99[A]:HIS:NE2	8:A:402:HOH:O	2.23	0.54
1:G:119:ASP:HB3	2:H:1:MET:HG3	1.90	0.53
1:G:82:ARG:NH1	1:G:89:GLU:HG2	2.24	0.53
1:E:79:ARG:HG2	1:E:82:ARG:NH2	2.24	0.52
2:D:39:ASP:OD1	2:D:46:ARG:NH1	2.43	0.52
1:G:121:LYS:HB2	2:H:2:ILE:HD12	1.92	0.52
1:C:98:MET:SD	8:D:339:HOH:O	2.59	0.51
1:C:98:MET:HG3	1:C:115:GLN:HG3	1.92	0.51
1:C:1:GLY:N	8:C:415:HOH:O	2.44	0.50
1:E:260:HIS:N	8:E:409:HOH:O	2.44	0.50
1:C:82:ARG:NE	8:C:407:HOH:O	2.40	0.49
2:B:22:ASN:HB3	2:B:71:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:187:THR:HB	1:G:272:LEU:HD21	1.96	0.48
1:G:17:ARG:NH1	8:G:414:HOH:O	2.44	0.47
2:H:9:GLN:OE1	4:H:201:GOL:H11	2.14	0.47
1:E:119:ASP:HB3	2:F:1:MET:HG3	1.97	0.46
1:C:182:LEU:HD22	1:C:210:PRO:HD3	1.97	0.46
2:D:8:ILE:HD12	2:D:92:LYS:HD2	1.97	0.46
1:G:274:TRP:CH2	1:G:276:PRO:HB3	2.51	0.45
1:A:97:TRP:HE1	1:A:114:GLU:HG2	1.81	0.45
2:D:3:GLN:HB2	2:D:87:THR:HG22	1.97	0.45
1:E:182:LEU:HD21	1:E:264:GLU:HG2	1.97	0.45
1:A:230:LEU:HD11	1:A:243:LYS:HE3	1.99	0.45
1:C:35:ARG:HG2	1:C:36:PHE:N	2.33	0.44
1:A:130:LEU:HB3	1:A:157:ARG:HG2	1.99	0.44
1:E:35:ARG:HD3	2:F:54:ASP:CG	2.43	0.44
1:E:230:LEU:HG	1:E:243:LYS:HE3	2.00	0.44
2:H:9:GLN:HA	4:H:201:GOL:H32	2.00	0.44
1:A:99[B]:HIS:CD2	1:A:114:GLU:HG3	2.54	0.43
1:E:40:ALA:HB3	1:E:43:PRO:HB3	1.99	0.43
1:A:215:LEU:HD22	1:A:261:VAL:HG22	2.00	0.43
1:E:137:ASP:O	1:E:141:GLN:HG3	2.18	0.43
1:A:79:ARG:NH2	5:A:304:SO4:O3	2.52	0.43
1:E:266:LEU:HD13	1:E:270:VAL:HB	2.00	0.43
1:G:259:CYS:HB3	1:G:272:LEU:HD13	1.99	0.43
2:D:1:MET:SD	2:D:1:MET:N	2.88	0.43
1:E:6:LYS:HE2	1:E:113:TYR:HE2	1.83	0.42
1:G:103:LEU:HG	1:G:168:LEU:HD23	2.00	0.42
2:D:100:MET:HE2	4:D:201:GOL:H12	2.02	0.42
1:E:14:ARG:HD2	1:E:17:ARG:HH12	1.84	0.42
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.54	0.42
1:A:230:LEU:HD13	1:A:245:ALA:HB2	2.01	0.42
1:E:82:ARG:NH1	1:E:89:GLU:HB3	2.34	0.42
1:G:150:ALA:HA	3:Q:4:ASN:HD22	1.84	0.42
3:P:3:TYR:O	8:P:101:HOH:O	2.21	0.42
3:P:4:ASN:HD22	3:P:4:ASN:HA	1.56	0.42
1:E:97:TRP:HE1	1:E:114:GLU:CG	2.33	0.41
1:C:125[A]:THR:OG1	1:C:134:THR:HB	2.21	0.41
1:E:51:TRP:CZ2	1:E:179:LEU:HD11	2.56	0.41
1:G:5:LEU:HB2	1:G:168:LEU:HD13	2.01	0.41
1:G:133:TRP:HB2	1:G:144:GLU:HG3	2.02	0.41
2:B:38:VAL:HG22	2:B:83:VAL:HG22	2.02	0.41
2:B:52:HIS:HB3	2:B:67:TYR:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:LYS:HE3	2:B:49:LYS:HB2	1.86	0.40
1:G:218:GLN:NE2	8:G:404:HOH:O	2.33	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	274/277 (99%)	268 (98%)	6 (2%)	0	100	100
1	C	276/277 (100%)	270 (98%)	6 (2%)	0	100	100
1	E	254/277 (92%)	246 (97%)	8 (3%)	0	100	100
1	G	278/277 (100%)	276 (99%)	2 (1%)	0	100	100
2	B	98/100 (98%)	98 (100%)	0	0	100	100
2	D	98/100 (98%)	98 (100%)	0	0	100	100
2	F	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	H	98/100 (98%)	98 (100%)	0	0	100	100
3	P	7/9 (78%)	6 (86%)	1 (14%)	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%)	6 (86%)	1 (14%)	0	100	100
All	All	1502/1544 (97%)	1477 (98%)	25 (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	238/238 (100%)	236 (99%)	2 (1%)	73	61
1	C	239/238 (100%)	237 (99%)	2 (1%)	73	61
1	E	224/238 (94%)	224 (100%)	0	100	100
1	G	241/238 (101%)	240 (100%)	1 (0%)	84	76
2	B	95/95 (100%)	94 (99%)	1 (1%)	65	50
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%)	95 (100%)	0	100	100
3	P	8/8 (100%)	7 (88%)	1 (12%)	4	0
3	Q	8/8 (100%)	8 (100%)	0	100	100
3	R	8/8 (100%)	8 (100%)	0	100	100
3	Z	8/8 (100%)	8 (100%)	0	100	100
All	All	1354/1364 (99%)	1347 (100%)	7 (0%)	81	71

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

Mol	Chain	Res	Type
1	A	113	TYR
1	A	114	GLU
2	B	71	PHE
1	C	115	GLN
1	C	272	LEU
1	G	272	LEU
3	P	4	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	E	115	GLN

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Mol	Chain	Res	Type
2	F	14	HIS
1	G	218	GLN
3	P	4	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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	$\# Z > 2$
5	SO4	G	304	-	4,4,4	0.24	0	6,6,6	0.10	0
4	GOL	C	306	-	5,5,5	0.89	0	5,5,5	1.14	1 (20%)
5	SO4	G	303	-	4,4,4	0.21	0	6,6,6	0.09	0
5	SO4	H	202	-	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	0.07	0
5	SO4	H	203	-	4,4,4	0.23	0	6,6,6	0.22	0
5	SO4	A	302	-	4,4,4	0.23	0	6,6,6	0.13	0
5	SO4	C	303	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	H	204	-	4,4,4	0.25	0	6,6,6	0.10	0
5	SO4	F	201	-	4,4,4	0.23	0	6,6,6	0.07	0
4	GOL	C	301	-	5,5,5	0.95	0	5,5,5	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PO4	F	203	-	4,4,4	0.97	0	6,6,6	0.46	0
4	GOL	H	201	-	5,5,5	0.91	0	5,5,5	1.07	0
5	SO4	A	304	-	4,4,4	0.23	0	6,6,6	0.12	0
5	SO4	G	305	-	4,4,4	0.24	0	6,6,6	0.06	0
4	GOL	C	302	-	5,5,5	0.97	0	5,5,5	1.05	0
5	SO4	C	304	-	4,4,4	0.24	0	6,6,6	0.11	0
4	GOL	D	201	-	5,5,5	0.98	0	5,5,5	1.02	0
4	GOL	D	202	-	5,5,5	0.96	0	5,5,5	1.05	0
4	GOL	D	203	-	5,5,5	0.93	0	5,5,5	1.16	1 (20%)
5	SO4	A	303	-	4,4,4	0.24	0	6,6,6	0.08	0
4	GOL	D	204	-	5,5,5	0.88	0	5,5,5	1.06	0
5	SO4	F	202	-	4,4,4	0.23	0	6,6,6	0.12	0
5	SO4	H	205	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	D	205	-	4,4,4	0.23	0	6,6,6	0.08	0
4	GOL	A	301	-	5,5,5	0.90	0	5,5,5	1.09	0
4	GOL	G	301	-	5,5,5	1.18	0	5,5,5	0.92	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	204	-	-	2/4/4/4	-
4	GOL	C	306	-	-	0/4/4/4	-
4	GOL	H	201	-	-	0/4/4/4	-
4	GOL	C	302	-	-	0/4/4/4	-
4	GOL	A	301	-	-	1/4/4/4	-
4	GOL	D	201	-	-	0/4/4/4	-
4	GOL	D	202	-	-	1/4/4/4	-
4	GOL	C	301	-	-	1/4/4/4	-
4	GOL	D	203	-	-	0/4/4/4	-
4	GOL	G	301	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	306	GOL	C3-C2-C1	-2.06	104.24	111.80
4	D	203	GOL	C3-C2-C1	-2.06	104.25	111.80

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	204	GOL	O2-C2-C3-O3
4	A	301	GOL	O1-C1-C2-C3
4	C	301	GOL	C1-C2-C3-O3
4	D	202	GOL	C1-C2-C3-O3
4	D	204	GOL	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	201	GOL	2	0
5	A	304	SO4	1	0
4	D	201	GOL	1	0
4	D	203	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	276/277 (99%)	0.77	25 (9%)	15 20	16, 33, 54, 79	1 (0%)
1	C	276/277 (99%)	0.36	13 (4%)	36 42	10, 24, 46, 58	2 (0%)
1	E	260/277 (93%)	1.72	96 (36%)	1 1	20, 41, 69, 81	0
1	G	276/277 (99%)	0.30	11 (3%)	42 49	9, 24, 48, 76	4 (1%)
2	B	100/100 (100%)	0.95	12 (12%)	9 13	21, 38, 61, 70	0
2	D	100/100 (100%)	0.22	3 (3%)	52 61	14, 25, 42, 60	0
2	F	100/100 (100%)	0.74	4 (4%)	42 49	19, 33, 57, 72	0
2	H	100/100 (100%)	0.73	12 (12%)	9 13	15, 33, 57, 72	0
3	P	9/9 (100%)	1.39	2 (22%)	2 4	28, 32, 46, 51	0
3	Q	9/9 (100%)	1.62	4 (44%)	0 1	21, 26, 38, 42	0
3	R	9/9 (100%)	2.07	3 (33%)	1 2	29, 33, 46, 49	0
3	Z	9/9 (100%)	1.08	1 (11%)	10 14	19, 26, 36, 46	0
All	All	1524/1544 (98%)	0.76	186 (12%)	8 12	9, 30, 57, 81	7 (0%)

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	PRO	7.0
1	E	217	TRP	6.0
1	E	274	TRP	5.5
1	E	230	LEU	5.4
1	E	246	ALA	5.1
1	E	252	GLY	4.9
1	E	265	GLY	4.8
1	A	103	LEU	4.7
1	E	201	LEU	4.6
1	E	269	PRO	4.6
1	A	113	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	261	VAL	4.6
1	A	104	GLY	4.4
1	E	257	TYR	4.4
3	P	5	TYR	4.4
1	E	244	TRP	4.4
1	E	259	CYS	4.4
3	Z	5	TYR	4.3
1	E	215	LEU	4.3
3	Q	7	ALA	4.2
3	Q	5	TYR	4.2
1	E	182	LEU	4.2
1	C	16	GLY	4.1
2	D	1	MET	4.1
1	A	197	HIS	4.1
1	E	248	VAL	4.1
1	E	188	HIS	4.0
1	A	1	GLY	4.0
1	E	187	THR	4.0
1	E	165	VAL	3.9
1	E	267	PRO	3.9
1	E	168	LEU	3.9
3	R	7	ALA	3.9
1	E	189	VAL	3.8
1	C	79[A]	ARG	3.8
1	E	220	ASP	3.8
1	E	203	CYS	3.8
1	E	213	ILE	3.8
1	E	247	VAL	3.8
1	E	266	LEU	3.8
1	E	253	GLU	3.7
1	E	216	THR	3.6
1	G	194	ILE	3.6
2	B	19	GLY	3.6
1	E	113	TYR	3.6
1	E	200	THR	3.5
1	E	260	HIS	3.5
1	A	275	LYS	3.5
1	E	231	VAL	3.5
1	E	190	THR	3.5
3	R	5	TYR	3.5
1	E	180	LEU	3.4
1	E	258	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	105	PRO	3.4
1	C	42	SER	3.3
1	G	226	GLN	3.3
1	E	245	ALA	3.3
1	E	167	TRP	3.3
1	E	270	VAL	3.3
1	E	227	ASP	3.2
1	E	262	GLN	3.2
1	E	18	GLY	3.2
1	G	227	ASP	3.2
2	B	41	LEU	3.1
1	A	194	ILE	3.1
1	E	16	GLY	3.1
1	E	218	GLN	3.1
1	E	204	TRP	3.1
1	E	249	VAL	3.1
1	E	2	SER	3.1
1	E	254	GLU	3.1
1	E	107	GLY	3.0
2	B	16	ALA	3.0
2	D	81	CYS	3.0
1	E	105	PRO	3.0
2	H	76	LYS	3.0
1	E	136	VAL	3.0
1	E	40	ALA	3.0
1	A	274	TRP	3.0
1	E	39	ASP	3.0
1	E	214	THR	3.0
1	E	271	THR	3.0
2	F	75	GLU	3.0
1	E	175	GLY	3.0
2	H	72	THR	2.9
1	E	264	GLU	2.9
1	E	272	LEU	2.9
1	E	54	GLN	2.9
2	B	1	MET	2.9
1	C	224	HIS	2.9
1	E	263	HIS	2.9
1	E	219	GLN	2.9
1	E	172	LEU	2.8
1	E	205	ALA	2.8
1	E	273	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	179	LEU	2.8
1	E	108	ARG	2.7
1	A	110	LEU	2.7
1	E	250	PRO	2.7
1	E	103	LEU	2.7
1	E	229	GLU	2.7
2	H	75	GLU	2.7
1	E	111	ARG	2.7
1	E	228	THR	2.7
1	G	225	THR	2.7
1	E	1	GLY	2.6
2	H	17	GLU	2.6
1	E	251	SER	2.6
3	R	3	TYR	2.6
1	G	224	HIS	2.6
1	A	106	ASP	2.6
1	E	41	ALA	2.6
1	G	223	GLY	2.5
1	E	3	HIS	2.5
1	E	226	GLN	2.5
1	G	18	GLY	2.5
2	B	49	LYS	2.5
2	H	19	GLY	2.5
1	E	90	ALA	2.5
1	C	194	ILE	2.5
1	A	107	GLY	2.4
2	B	90	GLN	2.4
1	E	169	HIS	2.4
1	A	16	GLY	2.4
1	C	276	PRO	2.4
1	A	109	PHE	2.4
1	E	171	TYR	2.4
1	A	99[A]	HIS	2.4
1	E	164	CYS	2.4
2	B	81	CYS	2.4
1	E	15	PRO	2.4
1	E	210	PRO	2.4
1	A	182	LEU	2.4
2	H	77	ASP	2.4
2	F	2	ILE	2.4
3	Q	6	PRO	2.3
1	A	198	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	268	GLU	2.3
2	B	2	ILE	2.3
2	B	50	VAL	2.3
1	C	223	GLY	2.3
2	B	47	ILE	2.3
1	A	195	SER	2.3
1	E	51	TRP	2.3
2	B	89	SER	2.3
2	H	20	LYS	2.3
1	E	209	TYR	2.3
2	H	49	LYS	2.3
1	C	267	PRO	2.2
1	E	181	HIS	2.2
2	B	75	GLU	2.2
1	E	178	THR	2.2
2	H	81	CYS	2.2
1	E	109	PHE	2.2
1	C	108	ARG	2.2
2	F	46	ARG	2.2
1	E	176	LYS	2.2
1	A	196	ASP	2.2
3	P	7	ALA	2.2
1	G	222	GLU	2.2
1	E	256	ARG	2.2
1	E	134	THR	2.2
2	H	74	THR	2.2
1	C	54	GLN	2.1
1	E	100	GLY	2.1
3	Q	4	ASN	2.1
1	A	251	SER	2.1
1	G	88	SER	2.1
2	D	2	ILE	2.1
2	F	76	LYS	2.1
1	A	88	SER	2.1
1	C	268	GLU	2.1
1	C	226	GLN	2.1
1	G	196	ASP	2.1
2	H	45	GLU	2.1
1	A	192	HIS	2.1
1	G	16	GLY	2.1
1	C	110	LEU	2.1
1	A	267	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	272	LEU	2.0
1	E	160	LEU	2.0
1	E	138	THR	2.0
1	E	255	GLN	2.0
2	H	46	ARG	2.0
1	E	106	ASP	2.0
1	E	162	ASP	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
4	GOL	C	306	6/6	0.57	0.17	53,59,62,65	0
4	GOL	D	203	6/6	0.74	0.16	37,42,45,55	0
5	SO4	A	303	5/5	0.75	0.10	67,69,77,82	0
5	SO4	H	202	5/5	0.75	0.11	58,68,75,77	0
5	SO4	F	201	5/5	0.77	0.11	52,70,91,96	0
5	SO4	D	205	5/5	0.78	0.11	50,64,94,112	0
4	GOL	D	202	6/6	0.78	0.19	48,58,60,64	0
5	SO4	C	305	5/5	0.78	0.12	51,55,77,81	0
5	SO4	A	302	5/5	0.79	0.13	55,56,64,66	0
5	SO4	H	205	5/5	0.79	0.11	56,64,86,86	0
4	GOL	G	301	6/6	0.81	0.14	28,36,41,47	0
4	GOL	D	204	6/6	0.81	0.14	39,48,50,51	0
5	SO4	H	203	5/5	0.82	0.11	59,62,70,81	0
4	GOL	A	301	6/6	0.84	0.12	40,43,45,45	0
5	SO4	C	303	5/5	0.84	0.10	55,59,70,73	0
5	SO4	H	204	5/5	0.85	0.10	57,59,65,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	C	302	6/6	0.86	0.15	28,43,45,49	0
5	SO4	G	304	5/5	0.86	0.13	49,51,54,57	0
4	GOL	H	201	6/6	0.87	0.14	22,30,39,54	0
5	SO4	G	303	5/5	0.88	0.13	24,57,67,68	0
5	SO4	A	304	5/5	0.88	0.10	52,52,62,66	0
5	SO4	F	202	5/5	0.88	0.10	55,60,64,67	0
7	PO4	F	203	5/5	0.89	0.09	49,62,69,71	0
5	SO4	G	305	5/5	0.90	0.08	46,51,64,66	0
4	GOL	C	301	6/6	0.93	0.08	27,34,39,39	0
6	ZN	E	301	1/1	0.93	0.10	44,44,44,44	1
5	SO4	C	304	5/5	0.93	0.08	46,47,50,61	0
6	ZN	G	302	1/1	0.97	0.04	25,25,25,25	1
4	GOL	D	201	6/6	0.97	0.07	20,26,27,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.