



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2021 – 02:03 PM EST

PDB ID : 6UJ9
Title : Crystal structure of HLA-B*07:02 with R140Q mutant IDH2 peptide in complex with Fab
Authors : Miller, M.S.; Thirawatananond, P.; Aytenfisu, T.Y.; Wright, K.; Gabelli, S.B.
Deposited on : 2019-10-02
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

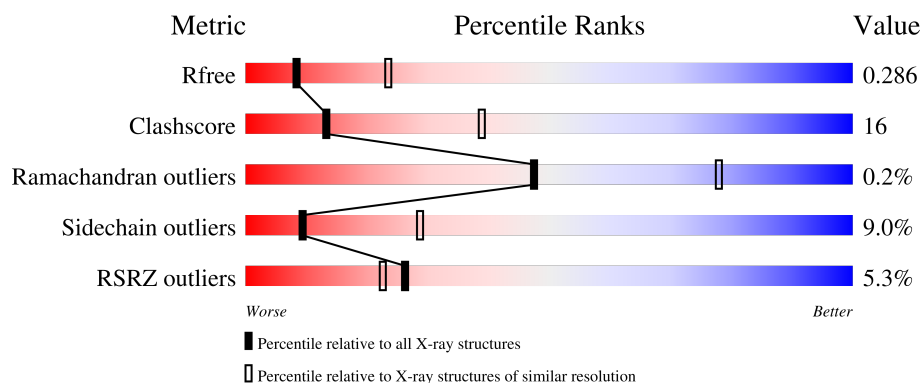
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	298	<div> <div>12%</div> <div>60%</div> <div>30%</div> <div>7%</div> </div>
2	B	119	<div> <div>2%</div> <div>58%</div> <div>22%</div> <div>16%</div> </div>
3	C	10	<div> <div>70%</div> <div>30%</div> </div>
4	L	214	<div> <div>%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
5	H	218	<div> <div>%</div> <div>71%</div> <div>24%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PEG	B	501	-	-	X	-
8	SO4	A	308	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6557 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, B-7 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2270	1409	415	439	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01889
A	281	GLY	-	expression tag	UNP P01889
A	282	SER	-	expression tag	UNP P01889
A	283	LEU	-	expression tag	UNP P01889
A	284	HIS	-	expression tag	UNP P01889
A	285	HIS	-	expression tag	UNP P01889
A	286	ILE	-	expression tag	UNP P01889
A	287	LEU	-	expression tag	UNP P01889
A	288	ASP	-	expression tag	UNP P01889
A	289	ALA	-	expression tag	UNP P01889
A	290	GLN	-	expression tag	UNP P01889
A	291	LYS	-	expression tag	UNP P01889
A	292	MET	-	expression tag	UNP P01889
A	293	VAL	-	expression tag	UNP P01889
A	294	TRP	-	expression tag	UNP P01889
A	295	ASN	-	expression tag	UNP P01889
A	296	HIS	-	expression tag	UNP P01889
A	297	ARG	-	expression tag	UNP P01889

- 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
			834	531	141	159	3			

- Molecule 3 is a protein called Isocitrate dehydrogenase [NADP], mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			74	45	13	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	7	GLN	ARG	engineered mutation	UNP P48735

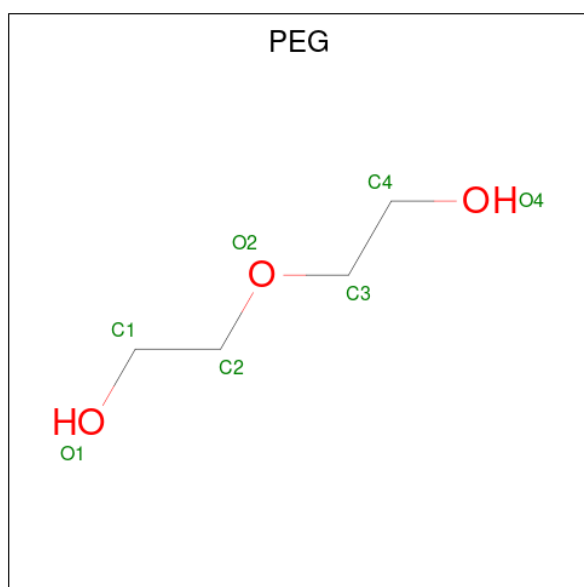
- Molecule 4 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	213	Total	C	N	O	S	0	0	0
			1642	1030	274	333	5			

- Molecule 5 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	218	Total	C	N	O	S	0	0	0
			1640	1040	272	321	7			

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



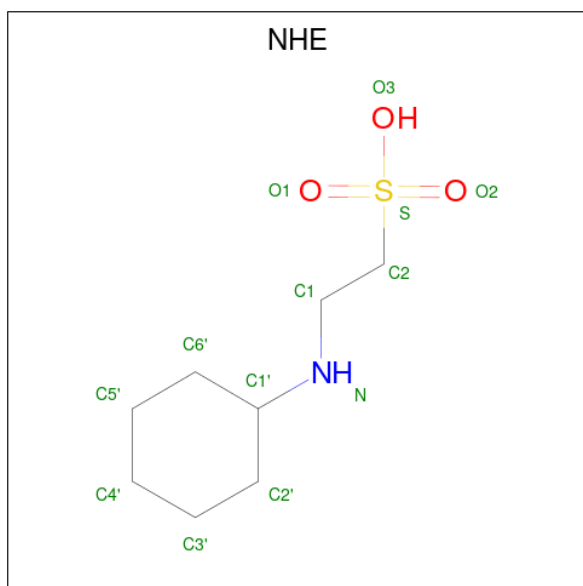
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	L	1	Total	C	O	0	0
			7	4	3		
6	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C₈H₁₇NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

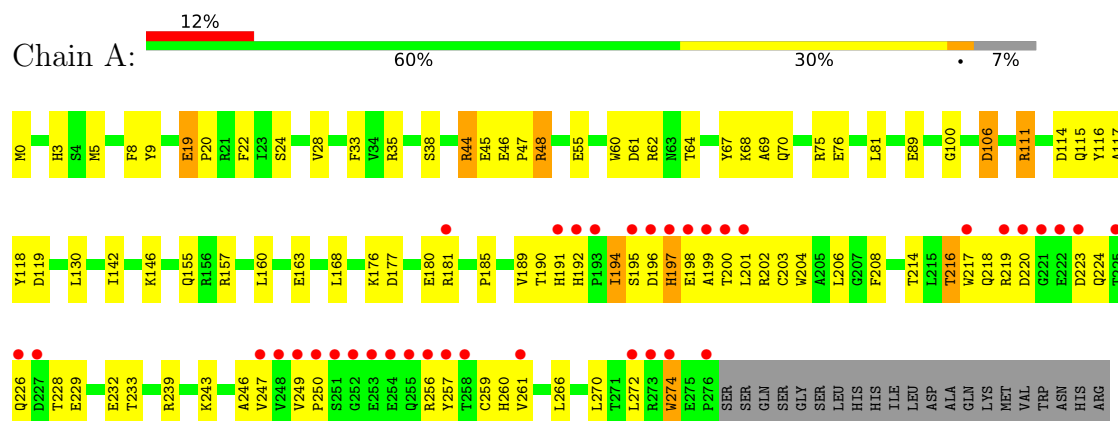
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	O	0	0
			1	1		
9	H	1	Total	O	0	0
			1	1		

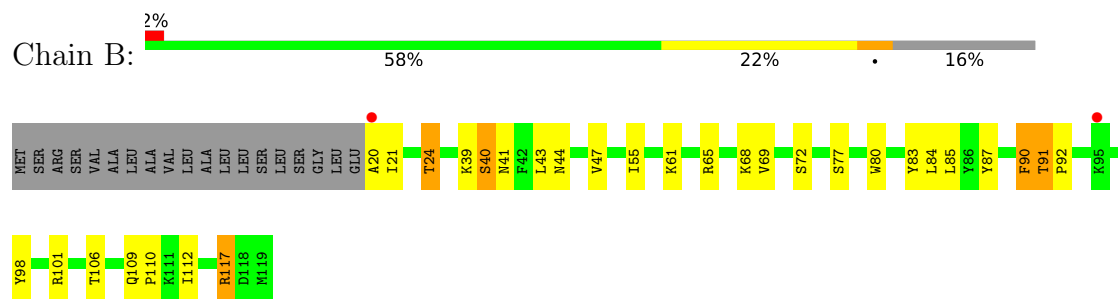
3 Residue-property plots

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.

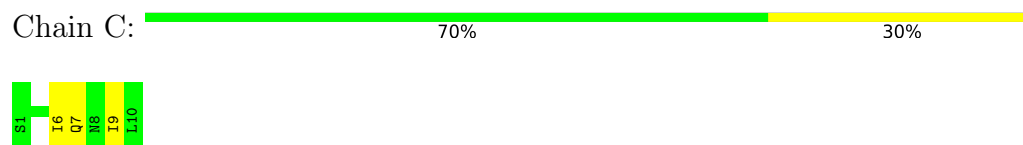
- Molecule 1: HLA class I histocompatibility antigen, B-7 alpha chain



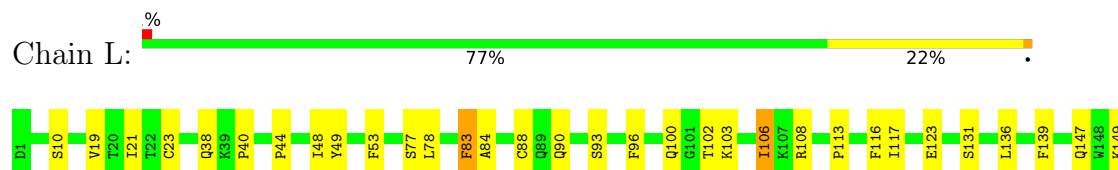
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Isocitrate dehydrogenase [NADP], mitochondrial



- Molecule 4: Fab light chain





● Molecule 5: Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.61Å 42.01Å 125.18Å 90.00° 92.75° 90.00°	Depositor
Resolution (Å)	48.93 – 2.90 48.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.93-2.90) 98.2 (48.93-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.214 , 0.287 0.222 , 0.286	Depositor DCC
R_{free} test set	973 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6557	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.08% 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, 0.333 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: PEG, SO4, NHE

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	0.68	0/2333	0.91	0/3169
2	B	0.63	0/857	0.82	0/1159
3	C	0.63	0/74	0.75	0/99
4	L	0.67	0/1678	0.84	0/2279
5	H	0.67	0/1683	0.85	0/2297
All	All	0.67	0/6625	0.86	0/9003

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	2270	0	2114	107	0
2	B	834	0	796	31	0
3	C	74	0	77	4	0
4	L	1642	0	1595	34	0
5	H	1640	0	1598	49	0
6	A	21	0	30	1	0
6	B	7	0	10	4	0
6	L	14	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	13	0	17	3	0
8	A	25	0	0	0	0
8	B	5	0	0	0	0
8	H	10	0	0	0	0
9	C	1	0	0	0	0
9	H	1	0	0	0	0
All	All	6557	0	6257	207	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 16.

All (207) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:HG21	1:A:257:TYR:CE1	1.67	1.28
1:A:249:VAL:HG22	1:A:250:PRO:HD2	1.26	1.12
1:A:249:VAL:CG2	1:A:250:PRO:HD2	1.82	1.10
1:A:76:GLU:HG3	5:H:103:TYR:OH	1.60	1.01
1:A:119:ASP:HB3	2:B:20:ALA:CB	1.93	0.97
1:A:192:HIS:ND1	1:A:200:THR:HG22	1.83	0.92
1:A:249:VAL:HG21	1:A:257:TYR:CZ	2.05	0.91
1:A:119:ASP:HB3	2:B:20:ALA:HB2	1.51	0.90
1:A:249:VAL:HG22	1:A:250:PRO:CD	2.02	0.89
1:A:261:VAL:HG21	1:A:272:LEU:HD11	1.54	0.89
1:A:233:THR:OG1	1:A:243:LYS:HD2	1.75	0.87
1:A:192:HIS:CE1	1:A:200:THR:HG22	2.09	0.86
1:A:249:VAL:HG21	1:A:257:TYR:HE1	1.41	0.85
1:A:203:CYS:SG	1:A:272:LEU:HD12	2.18	0.84
1:A:218:GLN:HA	1:A:224:GLN:HG2	1.58	0.84
1:A:219:ARG:HH21	1:A:256:ARG:HH21	1.25	0.83
1:A:224:GLN:O	1:A:228:THR:HG23	1.78	0.83
1:A:249:VAL:CG2	1:A:250:PRO:CD	2.56	0.82
1:A:185:PRO:HD2	1:A:266:LEU:HD21	1.61	0.81
1:A:259:CYS:HB3	1:A:272:LEU:HB2	1.62	0.81
2:B:61:LYS:HE3	2:B:98:TYR:OH	1.83	0.77
1:A:249:VAL:CG2	1:A:257:TYR:CZ	2.69	0.76
5:H:83:MET:HE2	5:H:86:LEU:HD21	1.68	0.75
1:A:69:ALA:HB1	3:C:6:ILE:HD12	1.68	0.75
1:A:106:ASP:OD1	1:A:106:ASP:N	2.21	0.74
1:A:249:VAL:HG23	1:A:257:TYR:OH	1.89	0.73
1:A:119:ASP:HB3	2:B:20:ALA:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ILE:HD11	1:A:199:ALA:HA	1.72	0.72
1:A:201:LEU:HB2	1:A:247:VAL:HG12	1.72	0.72
1:A:20:PRO:HD2	1:A:75:ARG:HD2	1.70	0.71
1:A:189:VAL:CG1	1:A:274:TRP:HB2	2.20	0.71
5:H:132:SER:O	5:H:136:THR:HG23	1.90	0.71
1:A:249:VAL:HG23	1:A:250:PRO:HD2	1.72	0.71
1:A:9:TYR:CD1	1:A:24:SER:OG	2.44	0.70
2:B:47:VAL:HG11	2:B:55:ILE:CD1	2.21	0.70
4:L:210:ASN:HB2	4:L:213:GLU:HG3	1.75	0.69
7:A:304:NHE:H6'2	7:A:304:NHE:HC22	1.74	0.69
1:A:233:THR:OG1	1:A:243:LYS:CD	2.41	0.69
1:A:270:LEU:HD23	1:A:272:LEU:HD21	1.75	0.69
1:A:189:VAL:HG12	1:A:274:TRP:HB2	1.74	0.68
2:B:47:VAL:HG11	2:B:55:ILE:HD11	1.76	0.68
1:A:203:CYS:SG	1:A:272:LEU:CD1	2.82	0.68
1:A:64:THR:O	1:A:68:LYS:HG3	1.94	0.67
5:H:136:THR:O	5:H:136:THR:OG1	2.08	0.67
1:A:219:ARG:HE	1:A:256:ARG:NH2	1.94	0.66
1:A:176:LYS:HG3	1:A:180:GLU:OE1	1.95	0.66
2:B:83:TYR:OH	6:B:501:PEG:H21	1.95	0.66
5:H:6:GLU:OE2	5:H:6:GLU:N	2.26	0.66
5:H:131:PRO:HG3	5:H:143:LEU:HB3	1.76	0.66
1:A:44:ARG:NH2	1:A:61:ASP:OD1	2.29	0.66
1:A:261:VAL:CG2	1:A:272:LEU:HD11	2.26	0.65
2:B:101:ARG:HG3	2:B:112:ILE:HG12	1.79	0.65
5:H:197:GLN:OE1	5:H:197:GLN:HA	1.95	0.65
1:A:239:ARG:HG2	7:A:304:NHE:HC11	1.79	0.65
1:A:249:VAL:CG2	1:A:257:TYR:OH	2.44	0.65
2:B:44:ASN:HB3	2:B:85:LEU:HD11	1.78	0.65
1:A:100:GLY:O	1:A:160:LEU:HD22	1.96	0.65
3:C:9:ILE:HD12	5:H:102:ARG:HA	1.77	0.65
1:A:194:ILE:HD11	1:A:198:GLU:O	1.96	0.65
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.31	0.65
4:L:117:ILE:HG22	5:H:135:SER:HB3	1.77	0.65
1:A:130:LEU:HB3	1:A:157:ARG:HG3	1.78	0.65
1:A:249:VAL:CG2	1:A:257:TYR:CE1	2.62	0.65
1:A:35:ARG:NH1	1:A:46:GLU:OE1	2.32	0.63
4:L:40:PRO:HB3	4:L:165:GLU:HG3	1.81	0.63
4:L:19:VAL:HG21	4:L:78:LEU:HD13	1.81	0.63
5:H:149:ASP:OD1	5:H:176:GLN:NE2	2.31	0.63
2:B:61:LYS:HG3	2:B:98:TYR:CE1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ASP:O	2:B:20:ALA:HB3	2.00	0.62
1:A:9:TYR:CE1	1:A:24:SER:OG	2.51	0.61
5:H:132:SER:H	5:H:136:THR:CG2	2.12	0.61
1:A:130:LEU:CB	1:A:157:ARG:HG3	2.32	0.60
1:A:197:HIS:N	1:A:197:HIS:ND1	2.50	0.60
5:H:202:ASN:HB3	5:H:213:ASP:OD1	2.01	0.60
5:H:183:LEU:C	5:H:183:LEU:HD12	2.23	0.59
1:A:192:HIS:HE2	1:A:202:ARG:CZ	2.16	0.59
1:A:100:GLY:O	1:A:160:LEU:CD2	2.50	0.58
1:A:261:VAL:HG21	1:A:272:LEU:CD1	2.30	0.58
1:A:19:GLU:OE1	1:A:19:GLU:HA	2.03	0.58
2:B:39:LYS:C	2:B:91:THR:HG23	2.24	0.58
1:A:217:TRP:O	1:A:224:GLN:HB2	2.05	0.57
4:L:83:PHE:HB2	4:L:106:ILE:HD13	1.87	0.57
1:A:9:TYR:HD1	1:A:24:SER:HG	1.40	0.57
5:H:132:SER:H	5:H:136:THR:HG23	1.70	0.57
4:L:90:GLN:HE21	4:L:93:SER:H	1.52	0.57
1:A:69:ALA:HB1	3:C:6:ILE:CD1	2.34	0.56
1:A:194:ILE:CD1	1:A:198:GLU:O	2.54	0.56
1:A:261:VAL:CG2	1:A:272:LEU:CD1	2.83	0.56
1:A:185:PRO:HB3	1:A:208:PHE:HB3	1.86	0.56
1:A:0:MET:HB2	1:A:180:GLU:HG2	1.87	0.56
2:B:24:THR:HG22	2:B:106:THR:OG1	2.06	0.56
5:H:168:VAL:HG22	5:H:187:VAL:HG23	1.87	0.56
1:A:204:TRP:HE3	1:A:206:LEU:HD21	1.71	0.56
2:B:83:TYR:OH	6:B:501:PEG:C1	2.54	0.55
4:L:136:LEU:N	4:L:136:LEU:HD12	2.20	0.55
2:B:83:TYR:OH	6:B:501:PEG:C2	2.54	0.55
1:A:192:HIS:ND1	1:A:200:THR:CG2	2.64	0.55
1:A:116:TYR:OH	3:C:7:GLN:OE1	2.24	0.55
1:A:47:PRO:HG3	1:A:60:TRP:CH2	2.42	0.54
2:B:43:LEU:O	2:B:87:TYR:HA	2.07	0.54
1:A:192:HIS:ND1	1:A:200:THR:C	2.61	0.54
1:A:119:ASP:CB	2:B:20:ALA:HB2	2.29	0.53
5:H:168:VAL:HG22	5:H:187:VAL:CG2	2.39	0.53
1:A:192:HIS:HB2	1:A:200:THR:H	1.73	0.53
4:L:48:ILE:HA	4:L:53:PHE:O	2.09	0.53
4:L:49:TYR:O	4:L:53:PHE:HB2	2.08	0.53
5:H:157:VAL:HG11	5:H:185:SER:CB	2.38	0.53
1:A:0:MET:HA	1:A:3:HIS:CE1	2.43	0.53
2:B:24:THR:CG2	2:B:106:THR:OG1	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:58:THR:OG1	5:H:70:ILE:HG22	2.09	0.53
1:A:163:GLU:OE2	6:A:302:PEG:H31	2.08	0.53
1:A:219:ARG:NH2	1:A:256:ARG:HH21	2.00	0.53
2:B:109:GLN:HG3	2:B:110:PRO:HD2	1.91	0.53
4:L:179:LEU:HG	4:L:181:LEU:HD13	1.91	0.53
1:A:9:TYR:CE2	1:A:70:GLN:HG2	2.44	0.52
4:L:113:PRO:HB3	4:L:139:PHE:HB3	1.89	0.52
4:L:100:GLN:OE1	4:L:100:GLN:N	2.40	0.52
1:A:47:PRO:HG3	1:A:60:TRP:CZ2	2.45	0.52
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.92	0.51
2:B:40:SER:N	2:B:91:THR:HG23	2.25	0.50
4:L:147:GLN:OE1	4:L:154:LEU:HD11	2.11	0.50
1:A:216:THR:O	1:A:260:HIS:N	2.38	0.50
2:B:47:VAL:HG11	2:B:55:ILE:HD13	1.93	0.50
4:L:96:PHE:CZ	5:H:103:TYR:CD2	3.00	0.49
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.47	0.49
4:L:40:PRO:CB	4:L:165:GLU:HG3	2.43	0.49
5:H:4:LEU:HD22	5:H:22:CYS:SG	2.52	0.49
5:H:29:VAL:HG12	5:H:29:VAL:O	2.12	0.49
1:A:185:PRO:HD2	1:A:266:LEU:CD2	2.39	0.49
2:B:72:SER:O	2:B:84:LEU:CD2	2.61	0.49
5:H:132:SER:N	5:H:136:THR:HG23	2.28	0.48
4:L:150:VAL:HG23	4:L:155:GLN:HG3	1.95	0.48
5:H:97:SER:HB2	5:H:105:VAL:HB	1.95	0.48
5:H:206:LYS:N	5:H:207:PRO:CD	2.76	0.48
7:A:304:NHE:HC22	7:A:304:NHE:C6'	2.43	0.48
4:L:96:PHE:CE1	5:H:103:TYR:CG	3.01	0.48
1:A:117:ALA:HB2	2:B:80:TRP:CE2	2.48	0.48
5:H:22:CYS:SG	5:H:22:CYS:O	2.72	0.48
4:L:44:PRO:HD2	5:H:108:TRP:CE3	2.49	0.48
1:A:28:VAL:HG23	1:A:33:PHE:CE1	2.49	0.47
1:A:146:LYS:HE2	5:H:32:TYR:CE1	2.50	0.47
1:A:48:ARG:HD2	1:A:48:ARG:HA	1.50	0.47
1:A:190:THR:HB	1:A:202:ARG:HB3	1.97	0.47
4:L:193:ALA:HB2	4:L:208:SER:HB3	1.96	0.47
1:A:44:ARG:NH2	1:A:61:ASP:HA	2.30	0.46
4:L:83:PHE:CE2	4:L:166:GLN:O	2.68	0.46
1:A:45:GLU:HG3	1:A:67:TYR:HE2	1.80	0.46
1:A:55:GLU:HA	1:A:55:GLU:OE1	2.15	0.46
4:L:90:GLN:NE2	4:L:93:SER:O	2.48	0.46
2:B:72:SER:O	2:B:84:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:TYR:HD1	1:A:24:SER:OG	1.88	0.46
1:A:229:GLU:HB3	1:A:246:ALA:HB3	1.98	0.46
4:L:193:ALA:CB	4:L:208:SER:HB3	2.46	0.46
1:A:44:ARG:HG2	1:A:44:ARG:HH11	1.80	0.45
2:B:90:PHE:CZ	2:B:92:PRO:HG3	2.51	0.45
1:A:119:ASP:O	2:B:20:ALA:CB	2.65	0.45
4:L:108:ARG:HD2	4:L:171:SER:HB2	1.98	0.45
4:L:136:LEU:HD13	4:L:175:LEU:HD23	1.98	0.45
5:H:11:LEU:HD21	5:H:119:ALA:O	2.17	0.45
5:H:132:SER:H	5:H:136:THR:HG21	1.80	0.45
4:L:162:SER:OG	5:H:172:PRO:O	2.33	0.45
1:A:201:LEU:HB2	1:A:247:VAL:CG1	2.46	0.45
2:B:90:PHE:CD1	2:B:90:PHE:O	2.70	0.45
5:H:38:ARG:HG2	5:H:48:VAL:CG2	2.47	0.45
5:H:132:SER:O	5:H:136:THR:N	2.48	0.45
5:H:202:ASN:N	5:H:202:ASN:ND2	2.64	0.44
2:B:41:ASN:HB3	2:B:90:PHE:CE1	2.52	0.44
5:H:144:GLY:HA2	5:H:159:TRP:CH2	2.53	0.44
1:A:76:GLU:HG3	5:H:103:TYR:HH	1.77	0.43
4:L:149:LYS:HE3	4:L:154:LEU:HD13	2.01	0.43
5:H:143:LEU:C	5:H:143:LEU:HD12	2.39	0.43
1:A:202:ARG:HG2	1:A:204:TRP:NE1	2.34	0.43
4:L:116:PHE:HD1	5:H:136:THR:HA	1.82	0.43
5:H:11:LEU:HB2	5:H:152:PRO:HG3	2.01	0.43
5:H:51:ILE:HD11	5:H:55:TYR:HB3	2.01	0.43
5:H:58:THR:OG1	5:H:70:ILE:CG2	2.67	0.43
2:B:90:PHE:CD1	2:B:90:PHE:C	2.90	0.43
4:L:90:GLN:NE2	4:L:93:SER:H	2.15	0.43
4:L:83:PHE:CB	4:L:106:ILE:HD13	2.49	0.43
1:A:111:ARG:HD2	1:A:111:ARG:HA	1.78	0.42
5:H:157:VAL:HG11	5:H:185:SER:HB2	2.00	0.42
4:L:40:PRO:CG	4:L:165:GLU:HG3	2.49	0.42
1:A:8:PHE:HZ	6:B:501:PEG:H31	1.83	0.42
5:H:30:LYS:HE3	5:H:31:TYR:CE1	2.54	0.42
5:H:51:ILE:HG12	5:H:55:TYR:HA	2.01	0.42
2:B:117:ARG:HH11	2:B:117:ARG:CG	2.33	0.42
1:A:0:MET:O	1:A:0:MET:SD	2.78	0.41
1:A:190:THR:N	1:A:202:ARG:O	2.52	0.41
1:A:247:VAL:O	1:A:247:VAL:HG13	2.20	0.41
1:A:191:HIS:ND1	1:A:274:TRP:CH2	2.89	0.41
4:L:38:GLN:O	4:L:84:ALA:HB1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:O	1:A:146:LYS:HG3	2.20	0.41
1:A:192:HIS:HB2	1:A:200:THR:N	2.34	0.41
5:H:197:GLN:OE1	5:H:197:GLN:CA	2.66	0.41
1:A:130:LEU:HB2	1:A:157:ARG:CG	2.50	0.41
2:B:117:ARG:NH1	2:B:117:ARG:HG3	2.36	0.41
5:H:128:PRO:HD3	5:H:214:LYS:HD3	2.02	0.41
1:A:194:ILE:HD12	1:A:195:SER:H	1.86	0.41
1:A:22:PHE:H	1:A:38:SER:HG	1.64	0.40
5:H:151:PHE:CE1	5:H:181:TYR:HE1	2.38	0.40
4:L:10:SER:HA	4:L:103:LYS:O	2.22	0.40
4:L:21:ILE:HD13	4:L:102:THR:HG21	2.03	0.40
4:L:163:VAL:HB	4:L:175:LEU:HD12	2.02	0.40
5:H:144:GLY:HA2	5:H:159:TRP:CZ2	2.57	0.40
1:A:176:LYS:HG3	1:A:180:GLU:CD	2.41	0.40
5:H:27:PHE:CE2	5:H:29:VAL:HG22	2.56	0.40
1:A:177:ASP:O	1:A:181:ARG:CD	2.69	0.40

There are no symmetry-related clashes.

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	275/298 (92%)	264 (96%)	10 (4%)	1 (0%)	34	66
2	B	98/119 (82%)	96 (98%)	2 (2%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
4	L	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
5	H	216/218 (99%)	206 (95%)	9 (4%)	1 (0%)	29	61
All	All	808/859 (94%)	780 (96%)	26 (3%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	ILE
5	H	29	VAL

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	235/254 (92%)	216 (92%)	19 (8%)	11	33
2	B	94/109 (86%)	84 (89%)	10 (11%)	6	20
3	C	9/9 (100%)	9 (100%)	0	100	100
4	L	188/189 (100%)	179 (95%)	9 (5%)	25	58
5	H	182/182 (100%)	156 (86%)	26 (14%)	3	10
All	All	708/743 (95%)	644 (91%)	64 (9%)	9	29

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	44	ARG
1	A	48	ARG
1	A	62	ARG
1	A	89	GLU
1	A	106	ASP
1	A	111	ARG
1	A	114	ASP
1	A	115	GLN
1	A	155	GLN
1	A	196	ASP
1	A	197	HIS
1	A	214	THR
1	A	216	THR
1	A	220	ASP
1	A	223	ASP
1	A	226	GLN
1	A	232	GLU

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Mol	Chain	Res	Type
1	A	274	TRP
2	B	21	ILE
2	B	24	THR
2	B	40	SER
2	B	65	ARG
2	B	68	LYS
2	B	69	VAL
2	B	77	SER
2	B	90	PHE
2	B	91	THR
2	B	117	ARG
4	L	23	CYS
4	L	77	SER
4	L	83	PHE
4	L	88	CYS
4	L	106	ILE
4	L	123	GLU
4	L	131	SER
4	L	151	ASP
4	L	160	GLN
5	H	21	SER
5	H	28	ASN
5	H	30	LYS
5	H	55	TYR
5	H	62	ASP
5	H	70	ILE
5	H	71	SER
5	H	75	SER
5	H	89	GLU
5	H	97	SER
5	H	118	SER
5	H	125	SER
5	H	132	SER
5	H	136	THR
5	H	154	PRO
5	H	156	THR
5	H	183	LEU
5	H	184	SER
5	H	186	VAL
5	H	188	THR
5	H	192	SER
5	H	196	THR

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Mol	Chain	Res	Type
5	H	197	GLN
5	H	198	THR
5	H	202	ASN
5	H	214	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
8	SO4	A	305	-	4,4,4	0.35	0	6,6,6	0.06	0
8	SO4	H	302	-	4,4,4	0.36	0	6,6,6	0.05	0
6	PEG	A	303	-	6,6,6	0.18	0	5,5,5	0.09	0
8	SO4	A	308	-	4,4,4	0.37	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	B	502	-	4,4,4	0.36	0	6,6,6	0.06	0
6	PEG	B	501	-	6,6,6	0.17	0	5,5,5	0.09	0
6	PEG	A	301	-	6,6,6	0.18	0	5,5,5	0.20	0
8	SO4	A	306	-	4,4,4	0.36	0	6,6,6	0.08	0
6	PEG	L	301	-	6,6,6	0.14	0	5,5,5	0.17	0
8	SO4	A	307	-	4,4,4	0.37	0	6,6,6	0.12	0
7	NHE	A	304	-	13,13,13	2.70	2 (15%)	16,17,17	2.62	7 (43%)
8	SO4	A	309	-	4,4,4	0.39	0	6,6,6	0.05	0
6	PEG	L	302	-	6,6,6	0.14	0	5,5,5	0.10	0
6	PEG	A	302	-	6,6,6	0.15	0	5,5,5	0.10	0
8	SO4	H	301	-	4,4,4	0.71	0	6,6,6	0.20	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
6	PEG	A	303	-	-	0/4/4/4	-
6	PEG	B	501	-	-	2/4/4/4	-
6	PEG	A	301	-	-	1/4/4/4	-
6	PEG	L	301	-	-	3/4/4/4	-
7	NHE	A	304	-	-	2/7/15/15	0/1/1/1
6	PEG	L	302	-	-	0/4/4/4	-
6	PEG	A	302	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	304	NHE	C2-S	-8.01	1.66	1.77
7	A	304	NHE	O3-S	5.18	1.65	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	304	NHE	C1-N-C1'	4.68	123.32	114.14
7	A	304	NHE	O3-S-C2	4.59	113.20	105.77
7	A	304	NHE	O1-S-C2	4.48	112.31	106.92
7	A	304	NHE	O2-S-C2	-3.78	102.36	106.92
7	A	304	NHE	C5'-C6'-C1'	3.58	117.84	111.11
7	A	304	NHE	O2-S-O1	-2.33	105.89	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	A	304	NHE	C6'-C1'-C2'	2.17	114.57	110.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	304	NHE	N-C1-C2-S
6	L	301	PEG	O2-C3-C4-O4
6	L	301	PEG	O1-C1-C2-O2
7	A	304	NHE	C2-C1-N-C1'
6	B	501	PEG	C4-C3-O2-C2
6	B	501	PEG	O1-C1-C2-O2
6	A	301	PEG	O1-C1-C2-O2
6	L	301	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	PEG	4	0
7	A	304	NHE	3	0
6	A	302	PEG	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	277/298 (92%)	0.51	37 (13%) 3 2	20, 42, 114, 155	0
2	B	100/119 (84%)	0.11	2 (2%) 65 63	25, 45, 66, 84	0
3	C	10/10 (100%)	-0.19	0 100 100	24, 26, 35, 41	0
4	L	213/214 (99%)	-0.09	2 (0%) 84 84	22, 35, 55, 68	0
5	H	218/218 (100%)	-0.04	2 (0%) 84 84	22, 38, 63, 95	0
All	All	818/859 (95%)	0.15	43 (5%) 26 22	20, 38, 79, 155	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ASP	7.4
1	A	250	PRO	6.5
1	A	257	TYR	6.4
5	H	133	SER	6.4
1	A	221	GLY	6.3
1	A	254	GLU	6.0
2	B	95	LYS	5.7
1	A	248	VAL	5.4
1	A	198	GLU	4.9
1	A	249	VAL	4.9
1	A	251	SER	4.2
1	A	225	THR	4.0
1	A	222	GLU	4.0
1	A	196	ASP	3.8
1	A	197	HIS	3.7
1	A	256	ARG	3.7
1	A	193	PRO	3.6
1	A	255	GLN	3.5
1	A	195	SER	3.5
1	A	181	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
5	H	110	GLN	3.1
1	A	191	HIS	3.1
1	A	253	GLU	3.1
1	A	258	THR	3.0
1	A	226	GLN	3.0
1	A	252	GLY	2.9
1	A	199	ALA	2.8
1	A	201	LEU	2.7
1	A	200	THR	2.5
1	A	273	ARG	2.4
1	A	276	PRO	2.4
2	B	20	ALA	2.4
1	A	247	VAL	2.4
1	A	274	TRP	2.3
4	L	203	SER	2.3
1	A	227	ASP	2.2
1	A	217	TRP	2.2
1	A	223	ASP	2.2
1	A	192	HIS	2.2
1	A	261	VAL	2.2
1	A	272	LEU	2.0
4	L	151	ASP	2.0
1	A	219	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	SO4	A	307	5/5	0.65	0.37	108,110,117,123	0
8	SO4	H	302	5/5	0.67	0.34	99,100,108,109	0
8	SO4	A	308	5/5	0.73	0.43	113,115,121,123	0
7	NHE	A	304	13/13	0.76	0.32	92,96,118,127	0
6	PEG	A	301	7/7	0.80	0.26	47,53,55,58	0
8	SO4	A	306	5/5	0.81	0.37	79,80,85,85	0
6	PEG	B	501	7/7	0.83	0.23	76,78,80,80	0
8	SO4	B	502	5/5	0.84	0.31	79,84,87,89	0
8	SO4	A	309	5/5	0.84	0.29	124,127,128,129	0
6	PEG	L	301	7/7	0.85	0.23	57,57,59,65	0
8	SO4	A	305	5/5	0.85	0.29	84,89,95,96	0
8	SO4	H	301	5/5	0.86	0.40	89,91,94,97	0
6	PEG	L	302	7/7	0.86	0.20	70,73,77,78	0
6	PEG	A	302	7/7	0.88	0.28	60,61,62,62	0
6	PEG	A	303	7/7	0.88	0.20	48,54,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.