



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 12:06 PM EDT

PDB ID : 3UTP
Title : 1E6 TCR specific for HLA-A*0201-ALWGPDPAAA
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Deposited on : 2011-11-26
Resolution : 2.57 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

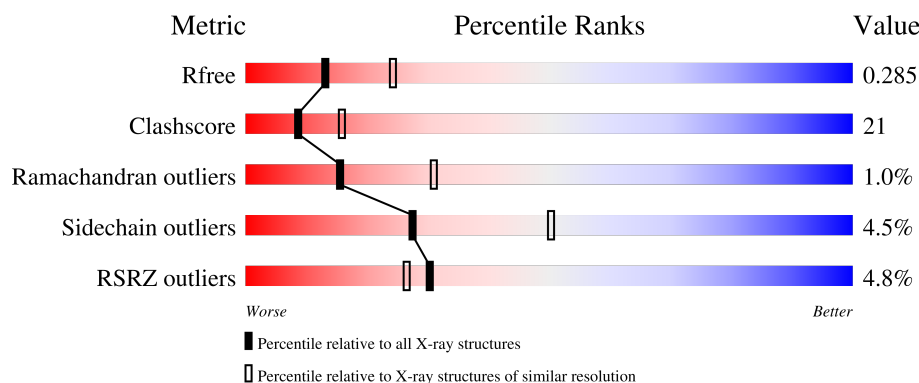
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	D	201	<div> <div>11%</div> <div>62%</div> <div>32%</div> <div>5%</div> </div>
1	K	201	<div> <div>2%</div> <div>62%</div> <div>35%</div> </div>
2	E	246	<div> <div>3%</div> <div>71%</div> <div>26%</div> </div>
2	L	246	<div> <div>4%</div> <div>67%</div> <div>29%</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
4	SO4	D	204	-	-	-	X
4	SO4	E	248	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7261 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.

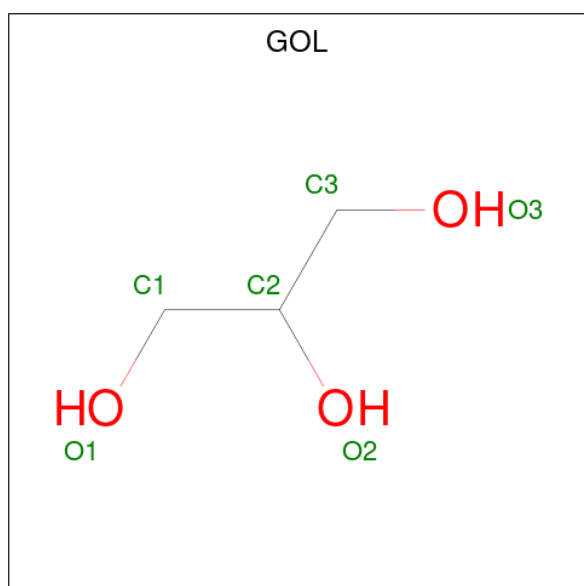
- Molecule 1 is a protein called 1E6 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	199	Total	C	N	O	S	0	0	0
			1573	986	259	318	10			
1	K	201	Total	C	N	O	S	0	0	0
			1586	994	261	321	10			

- Molecule 2 is a protein called 1E6 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	246	Total	C	N	O	S	0	0	0
			1974	1249	341	374	10			
2	L	246	Total	C	N	O	S	0	0	0
			1974	1249	341	374	10			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		

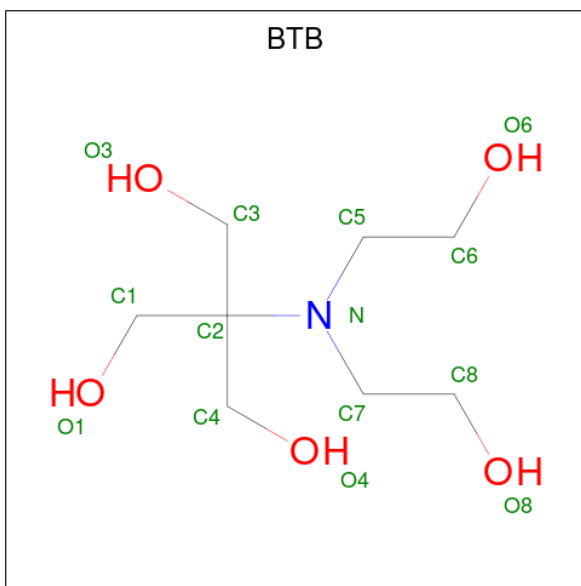
- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN

E-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



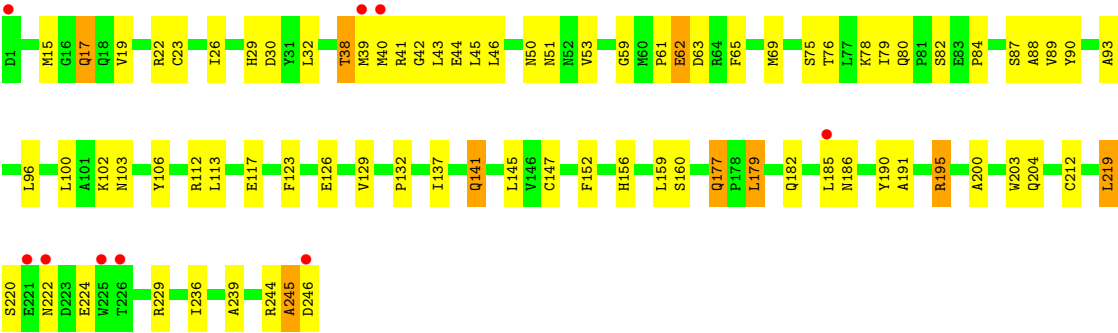
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	20	Total	O	0	0
			20	20		
6	E	22	Total	O	0	0
			22	22		
6	K	21	Total	O	0	0
			21	21		
6	L	20	Total	O	0	0
			20	20		



● Molecule 2: 1E6 TCR beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	192.03Å 43.26Å 124.71Å 90.00° 101.25° 90.00°	Depositor
Resolution (Å)	30.58 – 2.57 30.58 – 2.57	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.58-2.57) 99.5 (30.58-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.57Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.230 , 0.291 0.225 , 0.285	Depositor DCC
R_{free} test set	1644 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7261	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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

5.1 Standard geometry

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

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	D	0.77	0/1609	0.48	0/2177
1	K	0.78	0/1623	0.50	0/2197
2	E	0.70	1/2029 (0.0%)	0.47	0/2759
2	L	0.76	2/2029 (0.1%)	0.48	0/2759
All	All	0.75	3/7290 (0.0%)	0.48	0/9892

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	92	CYS	CB-SG	-6.74	1.70	1.82
2	L	147	CYS	CB-SG	-6.60	1.71	1.82
2	L	212	CYS	CB-SG	-6.03	1.72	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1573	0	1489	89	0
1	K	1586	0	1501	82	0
2	E	1974	0	1887	64	0
2	L	1974	0	1887	77	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	6	0	8	0	0
3	K	6	0	8	0	0
4	D	10	0	0	1	0
4	E	15	0	0	2	0
4	K	10	0	0	0	0
4	L	10	0	0	1	0
5	E	14	0	19	0	0
6	D	20	0	0	0	0
6	E	22	0	0	3	0
6	K	21	0	0	1	0
6	L	20	0	0	0	0
All	All	7261	0	6799	288	1

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 21.

All (288) 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:D:33:PHE:CD1	1:D:72:ILE:HD11	1.94	1.03
1:K:98:LYS:HG3	2:L:45:LEU:HD23	1.39	1.00
1:K:129:SER:HA	1:K:131:LYS:HE3	1.48	0.93
1:D:64:GLN:HE22	1:K:18:ILE:H	1.20	0.88
2:E:118:ASP:HB3	6:E:257:HOH:O	1.74	0.87
1:K:160:VAL:HG22	1:K:171:ASN:ND2	1.90	0.85
2:L:177:GLN:HA	2:L:177:GLN:HE21	1.39	0.84
2:L:179:LEU:HD23	2:L:191:ALA:O	1.78	0.84
1:K:131:LYS:HD2	1:K:132:SER:N	1.93	0.84
1:D:122:GLN:HG2	1:D:184:CYS:SG	2.16	0.83
1:D:11:LEU:CD1	1:D:107:LEU:HD12	2.08	0.83
2:E:21:LEU:HD22	2:E:111:THR:HG21	1.60	0.83
2:E:14:GLU:HB2	2:E:119:LEU:HD21	1.61	0.82
4:D:1:SO4:O2	1:K:18:ILE:HD13	1.79	0.82
1:K:34:MET:HE3	1:K:49:TYR:HB2	1.60	0.81
1:D:11:LEU:CD1	1:D:107:LEU:CD1	2.59	0.81
1:K:160:VAL:HG22	1:K:171:ASN:HD22	1.45	0.80
2:L:22:ARG:HD2	2:L:23:CYS:N	1.95	0.80
2:L:219:LEU:HD23	2:L:219:LEU:H	1.45	0.80
2:E:226:THR:HG22	6:E:260:HOH:O	1.82	0.79
1:K:11:LEU:CD1	1:K:107:LEU:HD12	2.12	0.79
1:D:178:ASN:HD22	1:D:178:ASN:H	1.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:ASN:C	1:D:186:ASN:HD22	1.84	0.78
2:E:50:ASN:O	2:E:53:VAL:HG22	1.84	0.77
1:D:18:ILE:H	1:K:64:GLN:HE22	1.29	0.77
1:D:34:MET:HE2	2:E:103:ASN:HB2	1.66	0.77
1:D:33:PHE:CD1	1:D:72:ILE:CD1	2.68	0.76
1:D:113:ILE:CD1	1:D:113:ILE:H	1.99	0.75
2:L:15:MET:HE1	2:L:117:GLU:HG2	1.67	0.75
2:L:159:LEU:HD23	2:L:160:SER:N	2.03	0.74
1:D:184:CYS:O	1:D:185:ALA:CB	2.37	0.72
2:L:220:SER:OG	2:L:222:ASN:OD1	2.07	0.72
2:E:134:GLU:N	2:E:134:GLU:OE2	2.22	0.72
1:K:60:ARG:NH2	1:K:83:ASP:OD2	2.23	0.72
2:E:129:VAL:HG23	2:E:239:ALA:HB3	1.71	0.71
2:E:159:LEU:C	2:E:159:LEU:HD23	2.10	0.71
1:K:11:LEU:CD1	1:K:107:LEU:CD1	2.68	0.71
1:D:195:GLU:OE2	1:D:195:GLU:N	2.23	0.71
1:D:186:ASN:C	1:D:186:ASN:ND2	2.44	0.70
2:E:182:GLN:NE2	2:E:184:ALA:HB3	2.07	0.70
1:D:19:VAL:HG13	1:D:76:ILE:HB	1.73	0.69
1:D:52:SER:HA	1:D:67:LYS:HE3	1.73	0.69
2:L:179:LEU:HD23	2:L:179:LEU:H	1.57	0.69
2:L:26:ILE:HB	2:L:29:HIS:CD2	2.27	0.69
2:E:7:SER:HB3	4:E:248:SO4:O4	1.92	0.69
1:D:11:LEU:HD11	1:D:107:LEU:HD13	1.75	0.68
2:L:219:LEU:HD23	2:L:219:LEU:N	2.07	0.68
1:K:80:GLN:O	1:K:109:VAL:HG11	1.94	0.68
2:L:32:LEU:C	2:L:32:LEU:HD23	2.14	0.68
1:D:11:LEU:O	1:D:11:LEU:HD12	1.94	0.68
2:L:46:LEU:HA	2:L:59:GLY:O	1.93	0.68
1:K:33:PHE:CD1	1:K:72:ILE:CD1	2.76	0.67
1:D:97:TYR:O	1:D:99:LEU:HD12	1.95	0.67
1:K:124:ARG:HA	1:K:131:LYS:HZ3	1.57	0.67
1:D:113:ILE:H	1:D:113:ILE:HD13	1.59	0.67
1:D:122:GLN:CG	1:D:184:CYS:SG	2.83	0.66
2:E:179:LEU:HD23	2:E:179:LEU:H	1.59	0.66
1:D:47:LEU:HD22	1:D:48:MET:HG2	1.78	0.66
1:D:60:ARG:NH2	1:D:83:ASP:OD2	2.28	0.66
1:K:33:PHE:CD1	1:K:72:ILE:HD11	2.30	0.66
1:K:62:THR:OG1	1:K:77:ARG:NH2	2.28	0.66
1:D:34:MET:HE1	2:E:103:ASN:HD22	1.59	0.65
2:L:46:LEU:O	2:L:59:GLY:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:15:MET:CE	2:E:117:GLU:HA	2.27	0.65
1:D:34:MET:CE	2:E:103:ASN:HD22	2.10	0.64
1:D:11:LEU:HD11	1:D:107:LEU:CD1	2.27	0.64
1:K:192:ILE:N	1:K:192:ILE:HD12	2.12	0.64
2:L:50:ASN:O	2:L:53:VAL:HG22	1.98	0.64
1:D:125:ASP:HB3	1:D:129:SER:HB3	1.81	0.63
1:D:178:ASN:HD22	1:D:178:ASN:N	1.96	0.63
2:E:19:VAL:HG22	2:E:79:ILE:HB	1.80	0.63
1:D:184:CYS:O	1:D:185:ALA:HB3	1.97	0.63
1:K:81:PRO:HA	1:K:109:VAL:HG13	1.81	0.63
1:D:11:LEU:HD13	1:D:107:LEU:HD12	1.79	0.62
1:K:161:LEU:C	1:K:161:LEU:HD12	2.20	0.62
2:E:175:ASP:HB2	2:E:192:LEU:HD12	1.82	0.62
1:K:11:LEU:HD12	1:K:107:LEU:HA	1.82	0.62
1:D:11:LEU:HD13	1:D:107:LEU:CD1	2.30	0.61
1:D:80:GLN:O	1:D:109:VAL:HG11	1.99	0.61
1:D:11:LEU:CD1	1:D:107:LEU:HD13	2.29	0.61
1:D:88:LEU:HD23	1:D:104:GLY:HA3	1.80	0.61
1:K:101:PHE:CE2	2:L:43:LEU:HD22	2.35	0.61
1:K:124:ARG:H	1:K:124:ARG:HD2	1.66	0.60
1:D:126:SER:O	1:D:128:SER:N	2.34	0.60
1:D:148:SER:HB2	1:D:155:ILE:HD11	1.82	0.60
1:K:11:LEU:HD11	1:K:107:LEU:CD1	2.33	0.59
2:L:159:LEU:HD23	2:L:159:LEU:C	2.23	0.59
2:E:122:VAL:HG12	2:E:232:PRO:HB2	1.85	0.59
1:D:18:ILE:H	1:K:64:GLN:NE2	2.00	0.58
1:D:34:MET:HB3	1:D:49:TYR:HB2	1.86	0.58
2:L:145:LEU:HD12	2:L:145:LEU:N	2.19	0.58
2:E:89:VAL:HG22	2:E:112:ARG:HG2	1.85	0.57
2:L:38:THR:CG2	2:L:41:ARG:HB3	2.34	0.57
1:D:11:LEU:HD12	1:D:107:LEU:HA	1.86	0.57
1:D:113:ILE:HD13	1:D:113:ILE:N	2.18	0.57
1:D:55:ASN:HB3	1:D:64:GLN:HG2	1.86	0.57
2:E:211:ARG:NH2	2:E:213:GLN:OE1	2.37	0.57
2:L:129:VAL:HG23	2:L:239:ALA:HB3	1.86	0.57
1:K:34:MET:HE1	2:L:103:ASN:CG	2.24	0.57
2:L:126:GLU:OE1	2:L:126:GLU:HA	2.06	0.56
1:D:52:SER:O	1:D:65:VAL:HG11	2.05	0.56
2:L:19:VAL:HG13	2:L:79:ILE:HB	1.86	0.56
1:D:33:PHE:CE1	1:D:72:ILE:HD11	2.39	0.56
2:E:60:MET:HE2	2:E:60:MET:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:14:GLU:HB2	2:E:119:LEU:CD2	2.34	0.55
2:E:53:VAL:HG23	2:E:53:VAL:O	2.05	0.55
1:D:161:LEU:C	1:D:161:LEU:HD12	2.27	0.55
2:E:15:MET:HE3	2:E:117:GLU:HA	1.89	0.55
1:K:11:LEU:HD11	1:K:107:LEU:HD13	1.88	0.55
1:D:88:LEU:HD23	1:D:104:GLY:CA	2.37	0.55
2:E:182:GLN:HE22	2:E:184:ALA:HB3	1.72	0.55
2:L:43:LEU:HD23	2:L:44:GLU:N	2.21	0.55
2:E:7:SER:CB	4:E:248:SO4:O4	2.55	0.54
1:K:11:LEU:HD12	1:K:11:LEU:O	2.07	0.54
1:K:97:TYR:CE1	2:L:100:LEU:HB3	2.42	0.54
1:D:52:SER:O	1:D:65:VAL:CG1	2.56	0.54
2:L:245:ALA:O	2:L:246:ASP:CB	2.55	0.54
1:D:161:LEU:HD12	1:D:161:LEU:O	2.08	0.54
2:L:179:LEU:CD2	2:L:191:ALA:O	2.55	0.53
2:E:186:ASN:C	2:E:186:ASN:HD22	2.11	0.53
2:L:87:SER:O	2:L:88:ALA:HB2	2.08	0.53
1:D:178:ASN:H	1:D:178:ASN:ND2	2.03	0.52
2:E:175:ASP:HB2	2:E:192:LEU:CD1	2.39	0.52
2:E:47:ILE:HA	2:E:56:ASP:O	2.10	0.52
1:D:192:ILE:N	1:D:192:ILE:HD12	2.24	0.52
1:K:161:LEU:HD12	1:K:161:LEU:O	2.10	0.52
2:L:38:THR:HG21	2:L:41:ARG:HB3	1.91	0.52
1:D:46:LEU:HD22	2:E:104:ILE:HG12	1.92	0.52
1:K:33:PHE:CE1	1:K:72:ILE:HD11	2.44	0.52
1:D:90:ALA:HB2	1:D:101:PHE:CE1	2.44	0.52
2:E:195:ARG:HD2	2:E:195:ARG:N	2.25	0.52
2:L:15:MET:HE2	2:L:84:PRO:CD	2.40	0.52
1:D:34:MET:HB3	1:D:49:TYR:CB	2.40	0.52
2:L:29:HIS:HA	2:L:96:LEU:HD23	1.92	0.52
1:D:2:LYS:HZ1	1:D:98:LYS:HD3	1.75	0.51
2:L:61:PRO:HB2	2:L:65:PHE:CD1	2.46	0.51
2:L:179:LEU:HD23	2:L:179:LEU:N	2.23	0.51
1:D:108:LEU:C	1:D:108:LEU:HD13	2.31	0.51
1:K:48:MET:CE	1:K:74:LEU:CD1	2.88	0.51
2:L:46:LEU:CA	2:L:59:GLY:O	2.59	0.51
2:L:100:LEU:C	2:L:102:LYS:H	2.13	0.51
1:D:99:LEU:HD13	2:E:105:GLN:NE2	2.26	0.51
2:E:182:GLN:HE22	2:E:184:ALA:CB	2.24	0.51
2:L:204:GLN:HA	2:L:244:ARG:O	2.10	0.51
1:K:131:LYS:HD2	1:K:131:LYS:C	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:62:GLU:CA	2:E:62:GLU:OE1	2.59	0.50
2:L:76:THR:CG2	2:L:78:LYS:HG3	2.42	0.50
2:L:177:GLN:HE21	2:L:177:GLN:CA	2.17	0.50
2:L:30:ASP:HB2	2:L:51:ASN:ND2	2.27	0.50
1:D:113:ILE:CD1	1:D:113:ILE:N	2.69	0.49
1:D:133:VAL:HG11	2:E:130:PHE:CD2	2.47	0.49
2:L:89:VAL:HG22	2:L:112:ARG:HG2	1.95	0.49
2:L:123:PHE:CE1	2:L:229:ARG:NH1	2.81	0.49
1:D:34:MET:CE	2:E:103:ASN:ND2	2.76	0.49
1:K:187:ALA:O	1:K:188:PHE:HB2	2.12	0.49
2:L:43:LEU:HD23	2:L:43:LEU:C	2.33	0.49
2:E:222:ASN:HD22	2:E:223:ASP:N	2.11	0.48
1:D:34:MET:HE3	1:D:49:TYR:HB2	1.95	0.48
1:D:123:LEU:N	1:D:123:LEU:HD12	2.29	0.48
1:D:150:ASP:OD1	1:D:179:LYS:NZ	2.45	0.48
2:E:199:SER:O	2:E:200:ALA:C	2.50	0.48
1:D:97:TYR:O	1:D:99:LEU:CD1	2.62	0.48
1:D:127:LYS:HD3	1:D:127:LYS:C	2.34	0.48
2:L:19:VAL:HG12	2:L:82:SER:HB3	1.94	0.48
2:L:182:GLN:NE2	2:L:185:LEU:HD22	2.28	0.48
1:K:172:SER:C	2:L:195:ARG:HH22	2.18	0.48
1:D:92:ARG:NH1	1:D:93:GLY:O	2.47	0.47
1:K:11:LEU:CD1	1:K:107:LEU:HD13	2.43	0.47
1:D:136:PHE:HB2	1:D:188:PHE:CZ	2.49	0.47
1:K:148:SER:N	1:K:155:ILE:HD12	2.29	0.47
2:E:145:LEU:HD12	2:E:145:LEU:N	2.29	0.47
1:D:123:LEU:O	1:D:133:VAL:CG1	2.62	0.47
2:E:159:LEU:HD23	2:E:160:SER:N	2.29	0.47
1:K:39:TYR:O	1:K:40:SER:C	2.52	0.47
1:K:88:LEU:HD23	1:K:104:GLY:HA3	1.95	0.47
1:K:131:LYS:NZ	1:K:132:SER:OG	2.31	0.47
1:K:192:ILE:N	1:K:192:ILE:CD1	2.77	0.47
1:K:166:MET:O	1:K:167:ASP:C	2.53	0.47
2:L:195:ARG:HD2	2:L:195:ARG:N	2.30	0.47
2:L:245:ALA:O	2:L:246:ASP:HB2	2.15	0.47
2:E:15:MET:HE2	2:E:117:GLU:HA	1.96	0.47
1:K:11:LEU:HD13	1:K:107:LEU:HD12	1.92	0.47
1:D:136:PHE:O	1:D:172:SER:HA	2.15	0.46
1:D:81:PRO:HA	1:D:109:VAL:HG13	1.98	0.46
1:D:98:LYS:HE2	1:D:100:ILE:HD11	1.96	0.46
1:D:52:SER:HA	1:D:67:LYS:CE	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:17:GLN:HE21	2:L:17:GLN:HA	1.79	0.46
2:E:204:GLN:HA	2:E:244:ARG:O	2.14	0.46
2:L:40:MET:HG3	2:L:41:ARG:N	2.31	0.46
2:L:62:GLU:HG3	2:L:63:ASP:H	1.80	0.46
1:K:34:MET:CE	2:L:103:ASN:CG	2.84	0.46
1:D:153:VAL:HG13	1:D:182:PHE:CE1	2.51	0.46
2:L:132:PRO:HD2	2:L:203:TRP:CZ2	2.50	0.46
2:L:38:THR:HG23	2:L:42:GLY:H	1.81	0.46
2:L:137:ILE:O	2:L:141:GLN:N	2.49	0.46
2:E:222:ASN:HD22	2:E:223:ASP:H	1.64	0.45
1:K:27:ASN:HB3	1:K:30:PHE:CE2	2.51	0.45
2:L:61:PRO:O	2:L:62:GLU:C	2.55	0.45
1:K:11:LEU:HD13	1:K:107:LEU:CD1	2.46	0.45
1:K:148:SER:H	1:K:155:ILE:HD12	1.80	0.45
2:E:221:GLU:HG3	2:E:222:ASN:N	2.31	0.45
1:K:19:VAL:HG23	1:K:79:SER:OG	2.16	0.45
2:L:93:ALA:HA	2:L:106:TYR:O	2.17	0.45
1:D:34:MET:SD	1:D:34:MET:N	2.89	0.45
2:E:168:VAL:HG23	2:E:168:VAL:O	2.16	0.45
1:K:11:LEU:CD1	1:K:107:LEU:HA	2.45	0.45
2:E:87:SER:O	2:E:88:ALA:HB2	2.17	0.45
2:L:22:ARG:HD2	2:L:23:CYS:H	1.80	0.45
1:K:101:PHE:CD2	2:L:43:LEU:HD22	2.52	0.44
2:L:100:LEU:C	2:L:102:LYS:N	2.70	0.44
2:E:119:LEU:HD13	2:E:219:LEU:HD22	1.99	0.44
2:L:112:ARG:HB3	2:L:156:HIS:CE1	2.52	0.44
1:D:181:ASP:OD2	1:D:182:PHE:N	2.51	0.44
1:K:64:GLN:O	1:K:72:ILE:HG23	2.18	0.44
1:K:48:MET:CE	1:K:74:LEU:HD11	2.48	0.44
2:E:225:TRP:CZ2	2:E:232:PRO:HD3	2.52	0.44
1:K:2:LYS:HE3	1:K:100:ILE:HD11	1.99	0.44
1:K:72:ILE:HG22	1:K:73:SER:N	2.32	0.44
1:K:69:SER:O	1:K:70:LYS:C	2.55	0.43
1:K:136:PHE:HB2	1:K:188:PHE:CE1	2.53	0.43
1:D:18:ILE:N	1:K:64:GLN:HE22	2.06	0.43
2:E:179:LEU:HD23	2:E:191:ALA:O	2.18	0.43
1:D:43:GLY:HA2	2:E:91:PHE:CE2	2.54	0.43
2:E:147:CYS:HB2	2:E:161:TRP:CZ2	2.54	0.43
1:K:181:ASP:OD1	1:K:181:ASP:O	2.37	0.43
2:L:236:ILE:HG13	4:L:248:SO4:O1	2.19	0.43
1:K:88:LEU:HD23	1:K:104:GLY:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:172:SER:OG	2:L:195:ARG:NH2	2.52	0.43
1:K:48:MET:HE1	1:K:74:LEU:CD1	2.49	0.43
1:K:77:ARG:O	1:K:78:ASP:C	2.57	0.43
1:K:34:MET:HE2	2:L:103:ASN:CB	2.49	0.42
1:D:21:LEU:HD13	1:D:87:TYR:HB2	2.00	0.42
2:L:15:MET:CE	2:L:84:PRO:CG	2.97	0.42
1:D:24:THR:HG22	1:D:71:TYR:CD2	2.54	0.42
1:D:97:TYR:CB	2:E:100:LEU:HD13	2.49	0.42
1:D:184:CYS:HA	1:D:187:ALA:HB2	2.01	0.42
2:E:121:ASN:N	2:E:121:ASN:HD22	2.16	0.42
1:K:12:SER:HB3	1:K:110:ARG:HH11	1.84	0.42
1:K:201:SER:N	1:K:202:PRO:HD3	2.35	0.42
1:D:120:VAL:HA	1:D:135:LEU:O	2.19	0.42
1:K:108:LEU:C	1:K:108:LEU:CD2	2.88	0.42
1:K:111:PRO:CG	1:K:160:VAL:HG21	2.49	0.42
1:K:129:SER:CA	1:K:131:LYS:HE3	2.36	0.42
2:L:32:LEU:C	2:L:32:LEU:CD2	2.86	0.42
1:D:108:LEU:HD11	1:D:110:ARG:HG2	2.02	0.42
2:E:69:MET:HG2	2:E:75:SER:HB2	2.01	0.42
1:D:108:LEU:CD1	1:D:110:ARG:HG2	2.50	0.42
2:L:22:ARG:CD	2:L:23:CYS:N	2.76	0.42
1:K:120:VAL:HA	1:K:135:LEU:O	2.19	0.42
2:L:39:MET:HG3	2:L:40:MET:N	2.35	0.42
1:D:99:LEU:HD12	1:D:99:LEU:N	2.35	0.42
1:D:18:ILE:CB	1:K:64:GLN:HE22	2.32	0.41
1:D:19:VAL:HG12	1:D:79:SER:OG	2.20	0.41
1:K:33:PHE:O	1:K:49:TYR:HA	2.20	0.41
2:E:222:ASN:ND2	2:E:223:ASP:N	2.68	0.41
1:K:19:VAL:HG12	1:K:20:SER:N	2.33	0.41
2:L:76:THR:HG22	2:L:78:LYS:HG3	2.02	0.41
1:D:131:LYS:O	1:D:131:LYS:CG	2.69	0.41
1:K:37:ARG:HB2	1:K:47:LEU:HD11	2.01	0.41
1:K:148:SER:HA	1:K:190:ASN:OD1	2.20	0.41
1:K:31:GLN:HG3	1:K:51:TYR:CE1	2.55	0.41
2:L:152:PHE:CE2	2:L:190:TYR:HB2	2.55	0.41
1:K:26:SER:HA	1:K:70:LYS:HD3	2.03	0.41
2:L:69:MET:HG2	2:L:75:SER:HB2	2.03	0.41
2:L:145:LEU:HD12	2:L:145:LEU:H	1.84	0.41
1:D:98:LYS:HG3	2:E:45:LEU:CD2	2.50	0.41
2:L:224:GLU:OE2	2:L:224:GLU:HA	2.21	0.41
2:E:14:GLU:CB	2:E:119:LEU:HD21	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:62:GLU:OE1	2:E:62:GLU:N	2.54	0.41
1:K:25:TYR:CZ	1:K:70:LYS:HA	2.55	0.41
2:E:53:VAL:O	2:E:53:VAL:CG2	2.67	0.41
1:K:19:VAL:CG1	1:K:20:SER:N	2.84	0.41
1:K:131:LYS:C	1:K:131:LYS:CD	2.90	0.41
2:L:219:LEU:N	2:L:219:LEU:CD2	2.78	0.41
1:D:62:THR:OG1	1:D:77:ARG:NH2	2.35	0.41
2:E:66:SER:HB3	6:E:267:HOH:O	2.19	0.41
2:E:80:GLN:HA	2:E:81:PRO:HA	1.87	0.40
1:K:125:ASP:HB3	1:K:131:LYS:HE2	2.02	0.40
2:E:222:ASN:HD22	2:E:222:ASN:N	2.19	0.40
1:K:9:GLY:HA3	1:K:10:PRO:HA	1.91	0.40
2:L:61:PRO:HG2	2:L:65:PHE:CE1	2.56	0.40
2:L:141:GLN:C	2:L:200:ALA:HB2	2.42	0.40
1:D:90:ALA:HB2	1:D:101:PHE:CD1	2.57	0.40
1:K:179:LYS:NZ	6:K:218:HOH:O	2.53	0.40
2:E:46:LEU:HB3	2:E:60:MET:HE2	2.04	0.40
2:L:177:GLN:HA	2:L:177:GLN:NE2	2.22	0.40
2:E:29:HIS:CD2	2:E:95:SER:HA	2.56	0.40
2:L:90:TYR:CE2	2:L:113:LEU:HD23	2.56	0.40

All (1) 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)
2:L:62:GLU:OE1	2:L:102:LYS:NZ[1_565]	2.04	0.16

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	D	197/201 (98%)	179 (91%)	14 (7%)	4 (2%)	7 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	199/201 (99%)	184 (92%)	13 (6%)	2 (1%)	15	31
2	E	244/246 (99%)	220 (90%)	23 (9%)	1 (0%)	34	55
2	L	244/246 (99%)	229 (94%)	13 (5%)	2 (1%)	19	37
All	All	884/894 (99%)	812 (92%)	63 (7%)	9 (1%)	15	31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	185	ALA
2	L	62	GLU
1	D	127	LYS
1	D	189	ASN
1	K	200	PRO
1	D	131	LYS
1	K	40	SER
2	L	245	ALA
2	E	61	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	180/182 (99%)	172 (96%)	8 (4%)	28	51
1	K	182/182 (100%)	173 (95%)	9 (5%)	25	46
2	E	216/216 (100%)	206 (95%)	10 (5%)	27	49
2	L	216/216 (100%)	207 (96%)	9 (4%)	30	53
All	All	794/796 (100%)	758 (96%)	36 (4%)	27	50

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	11	LEU
1	D	19	VAL

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Mol	Chain	Res	Type
1	D	31	GLN
1	D	34	MET
1	D	113	ILE
1	D	125	ASP
1	D	178	ASN
1	D	186	ASN
2	E	22	ARG
2	E	43	LEU
2	E	60	MET
2	E	62	GLU
2	E	64	ARG
2	E	80	GLN
2	E	182	GLN
2	E	186	ASN
2	E	195	ARG
2	E	222	ASN
1	K	34	MET
1	K	56	LYS
1	K	65	VAL
1	K	108	LEU
1	K	109	VAL
1	K	114	GLN
1	K	124	ARG
1	K	131	LYS
1	K	174	VAL
2	L	17	GLN
2	L	38	THR
2	L	80	GLN
2	L	141	GLN
2	L	177	GLN
2	L	179	LEU
2	L	186	ASN
2	L	195	ARG
2	L	219	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	22	ASN
1	D	64	GLN
1	D	114	GLN
1	D	142	GLN

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Mol	Chain	Res	Type
1	D	144	ASN
1	D	178	ASN
1	D	186	ASN
2	E	51	ASN
2	E	80	GLN
2	E	121	ASN
2	E	182	GLN
2	E	186	ASN
2	E	222	ASN
2	E	235	GLN
1	K	64	GLN
1	K	147	GLN
1	K	171	ASN
1	K	178	ASN
1	K	189	ASN
2	L	17	GLN
2	L	18	GLN
2	L	51	ASN
2	L	80	GLN
2	L	121	ASN
2	L	177	GLN
2	L	182	GLN
2	L	204	GLN
2	L	215	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	K	203	-	4,4,4	0.35	0	6,6,6	0.19	0
4	SO4	L	247	-	4,4,4	0.36	0	6,6,6	0.08	0
3	GOL	K	1	-	5,5,5	0.49	0	5,5,5	0.26	0
4	SO4	E	249	-	4,4,4	0.33	0	6,6,6	0.14	0
4	SO4	D	1	-	4,4,4	0.60	0	6,6,6	0.11	0
4	SO4	L	248	-	4,4,4	0.23	0	6,6,6	0.07	0
5	BTB	E	247	-	13,13,13	1.30	2 (15%)	7,16,16	0.59	0
3	GOL	D	203	-	5,5,5	0.60	0	5,5,5	0.17	0
4	SO4	E	248	-	4,4,4	0.51	0	6,6,6	0.11	0
4	SO4	E	250	-	4,4,4	0.45	0	6,6,6	0.12	0
4	SO4	D	204	-	4,4,4	0.29	0	6,6,6	0.09	0
4	SO4	K	204	-	4,4,4	0.24	0	6,6,6	0.11	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
3	GOL	D	203	-	-	4/4/4/4	-
3	GOL	K	1	-	-	4/4/4/4	-
5	BTB	E	247	-	-	13/21/21/21	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	247	BTB	C4-C2	3.07	1.56	1.53
5	E	247	BTB	C1-C2	2.03	1.55	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	203	GOL	O1-C1-C2-C3
5	E	247	BTB	N-C2-C3-O3
5	E	247	BTB	C1-C2-C4-O4
5	E	247	BTB	C3-C2-C4-O4
5	E	247	BTB	N-C2-C4-O4
5	E	247	BTB	C8-C7-N-C5
5	E	247	BTB	N-C5-C6-O6
3	D	203	GOL	C1-C2-C3-O3
3	K	1	GOL	O1-C1-C2-C3
3	K	1	GOL	C1-C2-C3-O3
3	K	1	GOL	O2-C2-C3-O3
3	D	203	GOL	O1-C1-C2-O2
3	D	203	GOL	O2-C2-C3-O3
3	K	1	GOL	O1-C1-C2-O2
5	E	247	BTB	C1-C2-N-C5
5	E	247	BTB	C3-C2-N-C5
5	E	247	BTB	C3-C2-N-C7
5	E	247	BTB	C4-C2-N-C7
5	E	247	BTB	C1-C2-C3-O3
5	E	247	BTB	C1-C2-N-C7
5	E	247	BTB	C4-C2-N-C5

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	SO4	1	0
4	L	248	SO4	1	0
4	E	248	SO4	2	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	D	199/201 (99%)	0.55	22 (11%) 5 4	23, 53, 121, 156	0
1	K	201/201 (100%)	0.05	5 (2%) 57 53	24, 46, 87, 119	0
2	E	246/246 (100%)	0.18	7 (2%) 53 49	25, 55, 100, 137	0
2	L	246/246 (100%)	0.15	9 (3%) 41 37	26, 54, 92, 114	0
All	All	892/894 (99%)	0.23	43 (4%) 30 26	23, 52, 104, 156	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	51	TYR	9.2
2	L	246	ASP	5.9
1	D	49	TYR	5.8
1	D	52	SER	5.0
1	K	114	GLN	4.8
2	E	246	ASP	4.5
2	E	1	ASP	4.1
1	D	130	ASP	4.1
1	D	199	PHE	3.8
1	D	124	ARG	3.7
1	K	202	PRO	3.7
2	L	226	THR	3.6
1	D	53	SER	3.5
1	D	164	ARG	3.2
1	D	167	ASP	3.1
1	K	201	SER	3.1
2	L	1	ASP	3.0
1	K	130	ASP	3.0
2	E	245	ALA	3.0
1	D	127	LYS	2.9
2	L	221	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	L	185	LEU	2.8
2	E	186	ASN	2.7
1	D	197	THR	2.6
1	D	5	GLU	2.6
2	L	225	TRP	2.6
1	D	196	ASP	2.5
2	E	220	SER	2.4
1	D	200	PRO	2.4
1	D	50	THR	2.4
1	D	132	SER	2.2
2	L	40	MET	2.2
1	D	149	LYS	2.2
1	D	55	ASN	2.2
1	D	114	GLN	2.2
2	L	39	MET	2.2
2	E	221	GLU	2.2
2	L	222	ASN	2.1
1	D	192	ILE	2.1
1	D	181	ASP	2.1
1	K	2	LYS	2.1
2	E	185	LEU	2.1
1	D	150	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 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BTB	E	247	14/14	0.55	0.33	72,80,85,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	K	1	6/6	0.71	0.25	58,69,75,77	0
4	SO4	D	204	5/5	0.75	0.54	100,100,100,100	0
3	GOL	D	203	6/6	0.75	0.35	54,62,66,68	0
4	SO4	E	249	5/5	0.92	0.29	56,60,74,80	0
4	SO4	L	247	5/5	0.94	0.18	70,72,76,80	0
4	SO4	E	250	5/5	0.94	0.24	53,56,61,62	0
4	SO4	K	203	5/5	0.95	0.20	51,59,67,68	0
4	SO4	L	248	5/5	0.97	0.32	84,84,89,89	0
4	SO4	K	204	5/5	0.97	0.26	64,70,73,78	0
4	SO4	E	248	5/5	0.98	0.16	31,36,52,57	0
4	SO4	D	1	5/5	0.99	0.15	19,21,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.