



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 02:05 PM UTC

PDB ID : 4C56 / pdb_00004c56
Title : X-ray structure of the complex between staphylococcal enterotoxin B, T cell receptor and major histocompatibility complex class II
Authors : Rodstrom, K.E.J.; Elbing, K.; Lindkvist-Petersson, K.
Deposited on : 2013-09-10
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 types of validation reports are described at

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

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

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

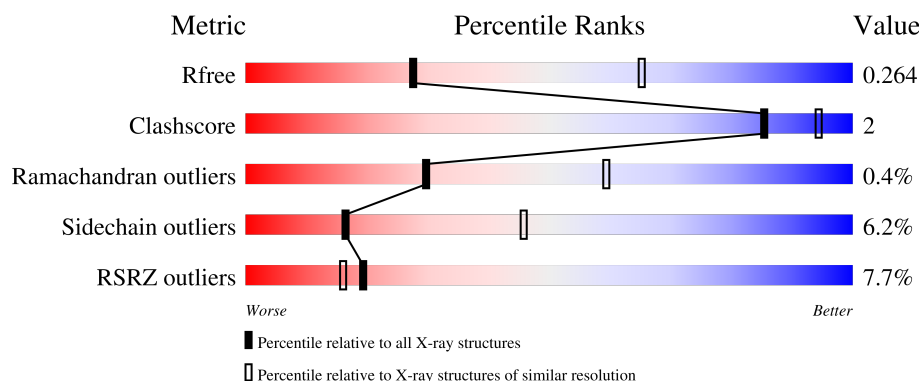
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



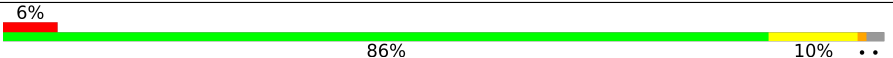
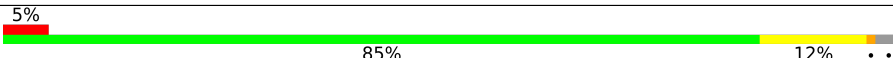
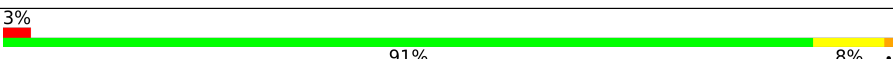
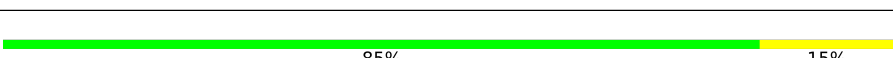
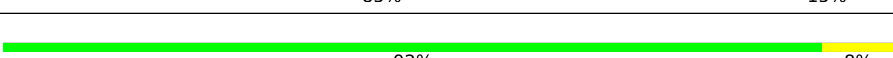
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	206	23% 79% 14% 7%
1	G	206	8% 85% 11% .
2	B	244	17% 85% 12% ..
2	H	244	3% 86% 11% ..
3	C	238	3% 90% 5% 5%

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Mol	Chain	Length	Quality of chain
3	I	238	
4	D	182	
4	J	182	
5	E	190	
5	K	190	
6	F	13	
6	L	13	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16311 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 T CELL RECEPTOR ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1393	879	236	274	4			
1	G	198	Total	C	N	O	S	0	0	0
			1512	947	253	307	5			

- Molecule 2 is a protein called T CELL RECEPTOR BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	240	Total	C	N	O	S	0	0	0
			1872	1184	319	363	6			
2	H	239	Total	C	N	O	S	0	0	0
			1858	1178	319	355	6			

- Molecule 3 is a protein called ENTEROTOXIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	227	Total	C	N	O	S	0	0	0
			1806	1158	287	351	10			
3	I	227	Total	C	N	O	S	0	0	0
			1777	1138	280	349	10			

- Molecule 4 is a protein called HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1429	929	235	260	5			
4	J	178	Total	C	N	O	S	0	0	0
			1427	927	235	260	5			

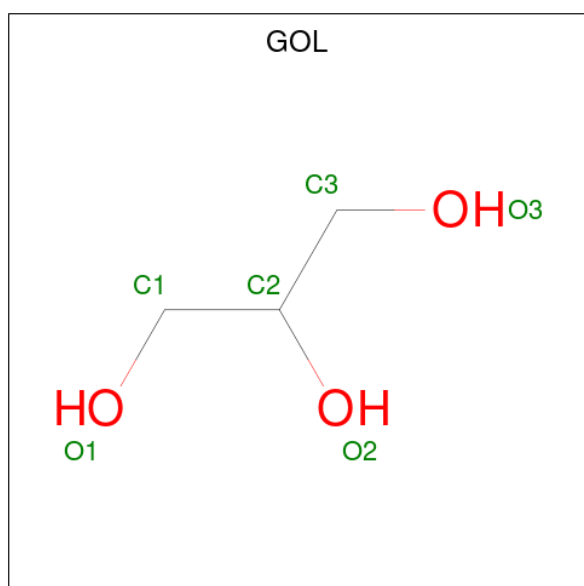
- Molecule 5 is a protein called MHC CLASS II ANTIGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	184	Total	C	N	O	S	0	0	0
			1494	941	266	281	6			
5	K	189	Total	C	N	O	S	0	0	0
			1505	951	264	284	6			

- Molecule 6 is a protein called HEMAGGLUTININ.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	13	Total	C	N	O	0	0	0
			105	69	18	18			
6	L	13	Total	C	N	O	0	0	0
			101	66	17	18			

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	O	0	0
			3	3		
8	B	1	Total	O	0	0
			1	1		

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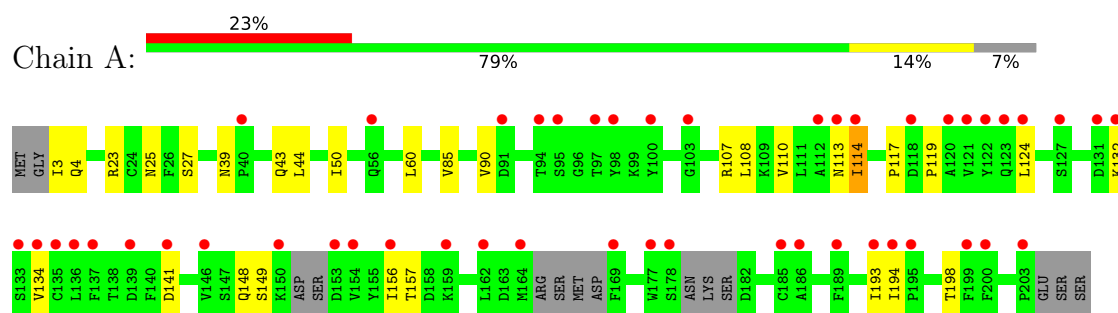
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total 1	O 1	0	0
8	D	6	Total 6	O 6	0	0
8	E	3	Total 3	O 3	0	0
8	G	4	Total 4	O 4	0	0
8	H	2	Total 2	O 2	0	0
8	I	2	Total 2	O 2	0	0
8	J	3	Total 3	O 3	0	0
8	K	1	Total 1	O 1	0	0

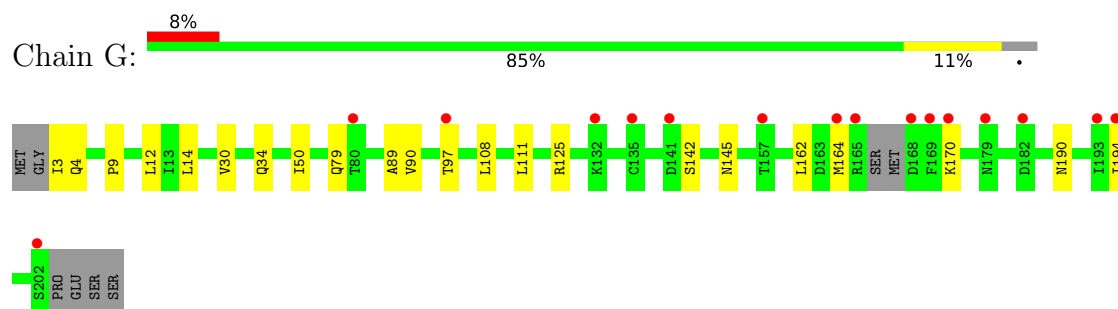
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

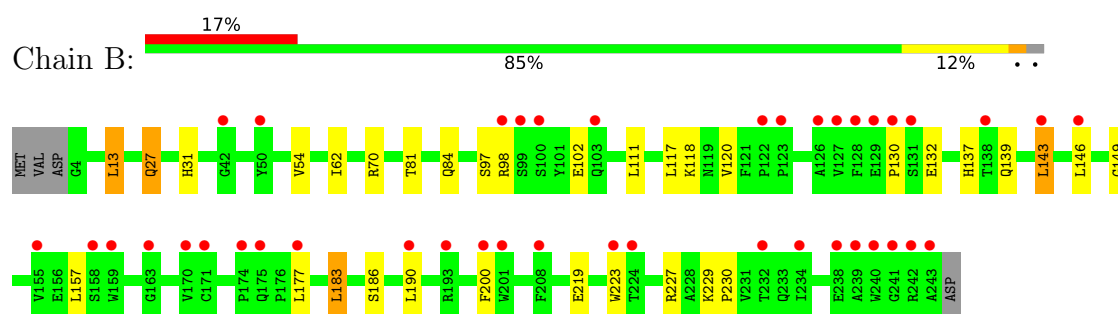
• Molecule 1: T CELL RECEPTOR ALPHA CHAIN



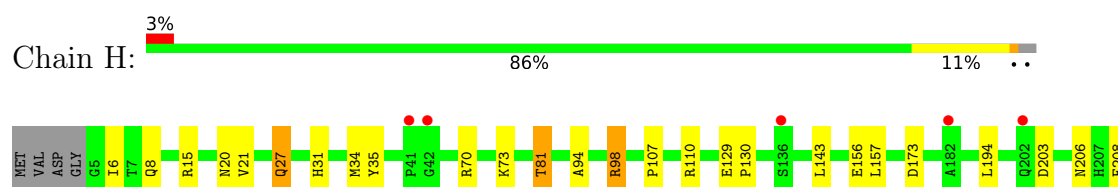
• Molecule 1: T CELL RECEPTOR ALPHA CHAIN

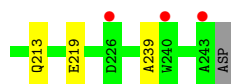


• Molecule 2: T CELL RECEPTOR BETA CHAIN

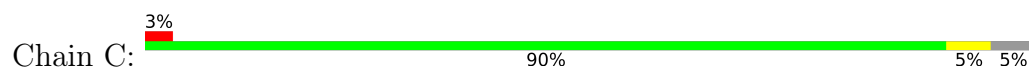


• Molecule 2: T CELL RECEPTOR BETA CHAIN

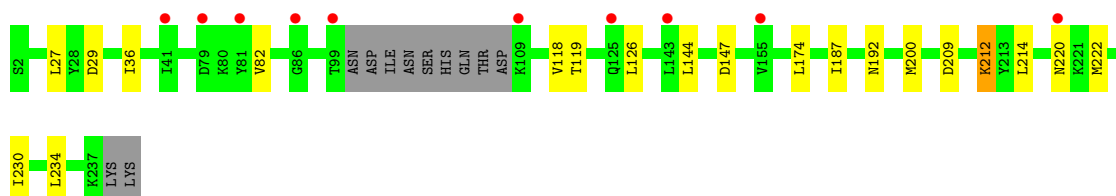
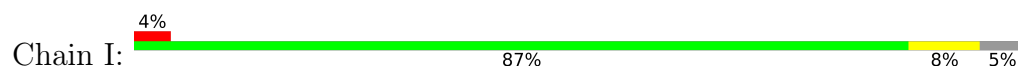




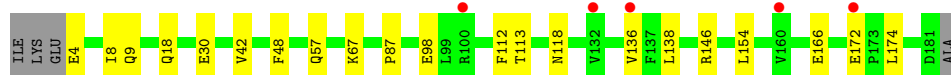
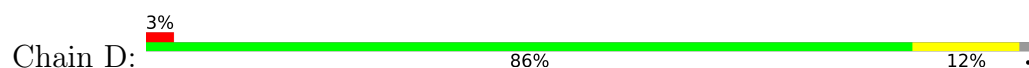
• Molecule 3: ENTEROTOXIN B



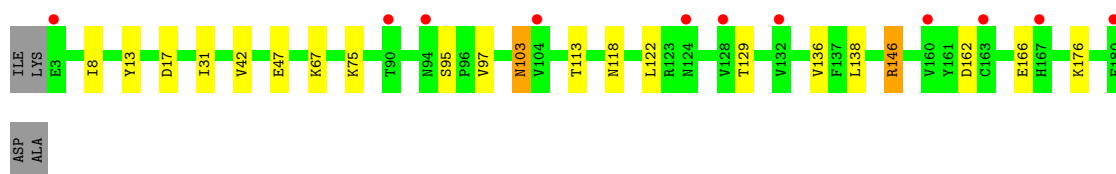
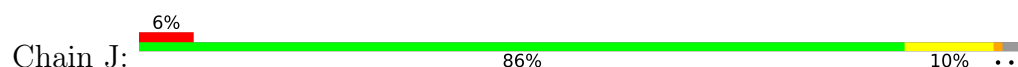
• Molecule 3: ENTEROTOXIN B



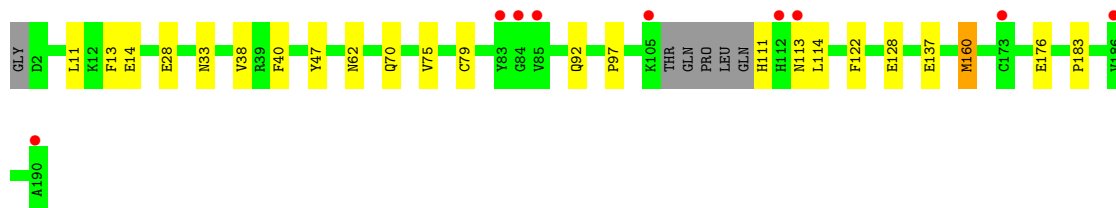
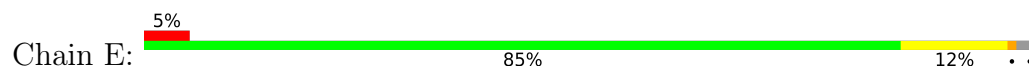
• Molecule 4: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN



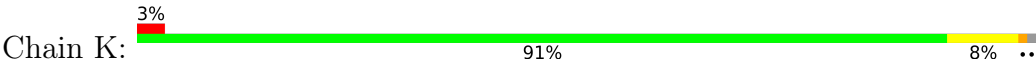
• Molecule 4: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN



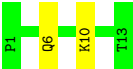
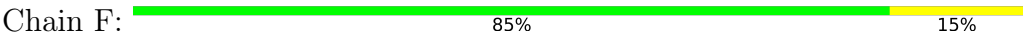
• Molecule 5: MHC CLASS II ANTIGEN



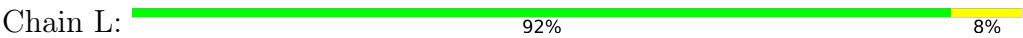
• Molecule 5: MHC CLASS II ANTIGEN



● Molecule 6: HEMAGGLUTININ



● Molecule 6: HEMAGGLUTININ



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.35Å 217.65Å 101.41Å 90.00° 99.82° 90.00°	Depositor
Resolution (Å)	29.23 – 2.90 29.23 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.23-2.90) 98.9 (29.23-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.233 , 0.251 0.245 , 0.264	Depositor DCC
R_{free} test set	3135 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16311	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: 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	A	0.72	0/1420	1.13	1/1946 (0.1%)
1	G	0.69	0/1543	1.08	0/2103
2	B	0.68	0/1925	1.06	0/2631
2	H	0.65	0/1911	1.03	0/2612
3	C	0.67	0/1849	1.11	1/2509 (0.0%)
3	I	0.70	0/1820	1.15	0/2476
4	D	0.70	0/1473	1.16	1/2013 (0.0%)
4	J	0.72	0/1471	1.17	1/2010 (0.0%)
5	E	0.64	0/1532	1.05	0/2083
5	K	0.67	0/1545	1.06	0/2107
6	F	0.57	0/106	0.95	0/141
6	L	0.55	0/102	0.85	0/137
All	All	0.68	0/16697	1.10	4/22768 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	31	ILE	N-CA-C	-5.59	106.25	111.45
4	D	48	PHE	CA-CB-CG	5.49	119.29	113.80
1	A	27	SER	N-CA-C	5.49	117.06	111.14
3	C	111	LYS	N-CA-C	5.21	116.98	109.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1393	0	1254	11	0
1	G	1512	0	1407	6	0
2	B	1872	0	1709	9	0
2	H	1858	0	1696	13	0
3	C	1806	0	1637	2	0
3	I	1777	0	1575	5	0
4	D	1429	0	1361	7	0
4	J	1427	0	1354	6	0
5	E	1494	0	1403	11	0
5	K	1505	0	1400	6	0
6	F	105	0	121	1	0
6	L	101	0	110	0	0
7	E	6	0	8	0	0
8	A	3	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	6	0	0	0	0
8	E	3	0	0	0	0
8	G	4	0	0	0	0
8	H	2	0	0	0	0
8	I	2	0	0	0	0
8	J	3	0	0	0	0
8	K	1	0	0	0	0
All	All	16311	0	15035	69	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 2.

All (69) 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)
5:E:47:TYR:H	5:E:62:ASN:HD21	1.44	0.66
1:G:125:ARG:HB2	2:H:129:GLU:HB2	1.81	0.62
1:A:148:GLN:HA	1:A:156:ILE:HG21	1.85	0.59
1:G:30:VAL:HG11	1:G:90:VAL:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:95:SER:H	4:J:103:ASN:HD21	1.53	0.56
4:D:118:ASN:HB3	4:D:166:GLU:HB2	1.87	0.56
3:I:187:ILE:HB	3:I:200:MET:HE3	1.86	0.56
4:J:118:ASN:HB3	4:J:166:GLU:HB2	1.88	0.55
1:A:148:GLN:HG2	1:A:149:SER:H	1.72	0.54
4:D:8:ILE:HG12	5:E:14:GLU:HG2	1.88	0.54
1:A:114:ILE:HD13	1:A:117:PRO:HG3	1.89	0.54
5:E:128:GLU:HB2	5:E:176:GLU:HB2	1.89	0.53
2:H:156:GLU:HB2	2:H:213:GLN:HB3	1.91	0.53
4:J:8:ILE:HG12	5:K:14:GLU:HG2	1.89	0.53
2:H:208:PHE:HB2	2:H:239:ALA:HB3	1.91	0.53
3:C:96:SER:HB3	4:D:67:LYS:HD3	1.91	0.53
2:H:27:GLN:HE22	2:H:31:HIS:H	1.58	0.52
2:H:203:ASP:HB3	2:H:206:ASN:HD22	1.74	0.52
2:B:183:LEU:HB3	2:B:186:SER:HB3	1.91	0.52
3:I:27:LEU:HD22	3:I:214:LEU:HD11	1.92	0.50
2:H:8:GLN:HB2	2:H:107:PRO:HD2	1.93	0.50
5:E:97:PRO:HB3	5:E:122:PHE:HB3	1.93	0.50
2:B:120:VAL:HG13	2:B:230:PRO:HG2	1.94	0.50
2:B:117:LEU:O	2:B:120:VAL:HG12	2.12	0.49
4:D:9:GLN:HB3	5:E:13:PHE:HB2	1.93	0.49
3:C:27:LEU:HD22	3:C:214:LEU:HD11	1.94	0.48
1:G:14:LEU:HD12	1:G:108:LEU:HD11	1.94	0.48
2:H:15:ARG:HG3	2:H:21:VAL:HB	1.96	0.48
3:I:209:ASP:HB3	3:I:212:LYS:HB2	1.95	0.48
4:J:138:LEU:HB2	4:J:146:ARG:HB3	1.96	0.47
5:K:47:TYR:H	5:K:62:ASN:HD21	1.62	0.47
5:K:128:GLU:HB2	5:K:176:GLU:HB2	1.96	0.46
1:A:124:LEU:HB3	1:A:134:VAL:HG13	1.96	0.46
3:I:118:VAL:H	3:I:220:ASN:HD21	1.61	0.46
1:G:34:GLN:HB2	1:G:89:ALA:HB3	1.98	0.46
4:J:122:LEU:HB2	4:J:162:ASP:HB2	1.98	0.46
2:H:20:ASN:HD21	2:H:81:THR:HG23	1.81	0.45
2:B:54:VAL:HA	2:B:70:ARG:HG2	1.98	0.45
2:H:98:ARG:HE	2:H:98:ARG:H	1.63	0.45
1:A:85:VAL:HG22	1:A:107:ARG:HG2	1.99	0.45
5:E:28:GLU:HB3	5:E:40:PHE:HB3	1.98	0.45
1:G:111:LEU:HB3	1:G:142:SER:HB3	1.99	0.45
2:H:35:TYR:HB2	2:H:94:ALA:HB3	1.99	0.45
1:A:23:ARG:HE	1:A:25:ASN:HD21	1.64	0.45
2:H:143:LEU:HD13	2:H:194:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:THR:HG22	2:B:177:LEU:HD13	1.98	0.45
5:E:92:GLN:HG2	5:K:92:GLN:HG2	1.99	0.44
4:D:30:GLU:HB2	4:D:138:LEU:HD21	2.00	0.44
1:A:39:ASN:HD21	1:A:43:GLN:HB3	1.83	0.44
5:E:114:LEU:HD22	5:E:160:MET:HB3	2.00	0.44
4:D:138:LEU:HB2	4:D:146:ARG:HG3	2.00	0.43
1:G:9:PRO:HG2	1:G:12:LEU:HD13	1.99	0.43
4:D:87:PRO:HB3	4:D:112:PHE:HB3	2.01	0.43
5:E:70:GLN:HE22	6:F:6:GLN:HE22	1.67	0.42
2:B:27:GLN:HE22	2:B:31:HIS:H	1.66	0.42
5:E:75:VAL:HA	5:E:79:CYS:HB2	2.00	0.42
2:H:70:ARG:HH21	2:H:73:LYS:HA	1.84	0.42
2:B:223:TRP:HB3	2:B:229:LYS:HE2	2.01	0.42
2:H:130:PRO:HD3	2:H:143:LEU:HG	2.00	0.42
2:B:130:PRO:HD3	2:B:143:LEU:HG	2.02	0.42
1:A:119:PRO:HB2	1:A:198:THR:HG22	2.02	0.41
4:J:13:TYR:CZ	4:J:67:LYS:HG3	2.55	0.41
5:E:176:GLU:HG2	5:E:183:PRO:HB3	2.03	0.41
1:A:114:ILE:HG21	1:A:141:ASP:HA	2.03	0.41
5:K:76:ASP:HA	5:K:80:ARG:HB2	2.02	0.41
3:I:119:THR:HG22	3:I:222:MET:HE3	2.02	0.41
5:K:64:GLN:H	5:K:64:GLN:HG2	1.73	0.41
2:B:13:LEU:HB3	2:B:111:LEU:HD12	2.04	0.40
1:A:114:ILE:H	1:A:114:ILE:HG13	1.71	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	184/206 (89%)	167 (91%)	17 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	194/206 (94%)	189 (97%)	4 (2%)	1 (0%)	24	54
2	B	238/244 (98%)	220 (92%)	15 (6%)	3 (1%)	9	32
2	H	237/244 (97%)	226 (95%)	11 (5%)	0	100	100
3	C	223/238 (94%)	213 (96%)	9 (4%)	1 (0%)	30	59
3	I	223/238 (94%)	210 (94%)	12 (5%)	1 (0%)	30	59
4	D	176/182 (97%)	171 (97%)	5 (3%)	0	100	100
4	J	176/182 (97%)	173 (98%)	3 (2%)	0	100	100
5	E	180/190 (95%)	169 (94%)	10 (6%)	1 (1%)	21	51
5	K	187/190 (98%)	173 (92%)	13 (7%)	1 (0%)	24	54
6	F	11/13 (85%)	11 (100%)	0	0	100	100
6	L	11/13 (85%)	11 (100%)	0	0	100	100
All	All	2040/2146 (95%)	1933 (95%)	99 (5%)	8 (0%)	30	59

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	192	ASN
2	B	118	LYS
3	C	192	ASN
5	E	33	ASN
5	K	33	ASN
2	B	98	ARG
1	G	164	MET
2	B	149	GLY

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	141/185 (76%)	128 (91%)	13 (9%)	8	27
1	G	168/185 (91%)	158 (94%)	10 (6%)	17	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	195/214 (91%)	177 (91%)	18 (9%)	8	27
2	H	191/214 (89%)	182 (95%)	9 (5%)	23	56
3	C	188/224 (84%)	179 (95%)	9 (5%)	23	55
3	I	182/224 (81%)	172 (94%)	10 (6%)	19	50
4	D	155/166 (93%)	145 (94%)	10 (6%)	15	44
4	J	154/166 (93%)	143 (93%)	11 (7%)	13	40
5	E	162/171 (95%)	156 (96%)	6 (4%)	30	64
5	K	161/171 (94%)	153 (95%)	8 (5%)	22	53
6	F	12/12 (100%)	11 (92%)	1 (8%)	10	32
6	L	11/12 (92%)	10 (91%)	1 (9%)	9	28
All	All	1720/1944 (88%)	1614 (94%)	106 (6%)	16	46

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	4	GLN
1	A	44	LEU
1	A	50	ILE
1	A	60	LEU
1	A	90	VAL
1	A	108	LEU
1	A	110	VAL
1	A	113	ASN
1	A	114	ILE
1	A	132	LYS
1	A	193	ILE
1	A	194	ILE
2	B	13	LEU
2	B	27	GLN
2	B	62	ILE
2	B	81	THR
2	B	84	GLN
2	B	97	SER
2	B	102	GLU
2	B	132	GLU
2	B	137	HIS
2	B	139	GLN

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Mol	Chain	Res	Type
2	B	143	LEU
2	B	146	LEU
2	B	157	LEU
2	B	183	LEU
2	B	190	LEU
2	B	200	PHE
2	B	219	GLU
2	B	227	ARG
3	C	56	THR
3	C	69	LYS
3	C	97	LYS
3	C	111	LYS
3	C	125	GLN
3	C	143	LEU
3	C	144	LEU
3	C	174	LEU
3	C	212	LYS
4	D	4	GLU
4	D	18	GLN
4	D	42	VAL
4	D	57	GLN
4	D	98	GLU
4	D	113	THR
4	D	136	VAL
4	D	154	LEU
4	D	172	GLU
4	D	174	LEU
5	E	11	LEU
5	E	38	VAL
5	E	111	HIS
5	E	113	ASN
5	E	137	GLU
5	E	160	MET
6	F	10	LYS
1	G	3	ILE
1	G	4	GLN
1	G	50	ILE
1	G	79	GLN
1	G	97	THR
1	G	145	ASN
1	G	162	LEU
1	G	170	LYS

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Mol	Chain	Res	Type
1	G	190	ASN
1	G	194	ILE
2	H	6	ILE
2	H	27	GLN
2	H	34	MET
2	H	81	THR
2	H	98	ARG
2	H	110	ARG
2	H	157	LEU
2	H	173	ASP
2	H	219	GLU
3	I	29	ASP
3	I	36	ILE
3	I	82	VAL
3	I	126	LEU
3	I	144	LEU
3	I	147	ASP
3	I	174	LEU
3	I	212	LYS
3	I	230	ILE
3	I	234	LEU
4	J	17	ASP
4	J	42	VAL
4	J	47	GLU
4	J	75	LYS
4	J	97	VAL
4	J	103	ASN
4	J	113	THR
4	J	129	THR
4	J	136	VAL
4	J	146	ARG
4	J	176	LYS
5	K	11	LEU
5	K	21	THR
5	K	38	VAL
5	K	64	GLN
5	K	67	LEU
5	K	107	GLN
5	K	138	GLU
5	K	164	VAL
6	L	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	7	GLN
1	A	25	ASN
1	A	38	GLN
1	A	39	ASN
1	A	143	GLN
1	A	145	ASN
2	B	27	GLN
2	B	39	GLN
2	B	58	GLN
2	B	202	GLN
2	B	233	GLN
3	C	37	ASN
3	C	121	HIS
3	C	124	ASN
3	C	125	GLN
3	C	142	ASN
3	C	151	ASN
3	C	218	ASN
4	D	18	GLN
4	D	84	ASN
4	D	177	HIS
5	E	34	GLN
5	E	62	ASN
5	E	70	GLN
5	E	92	GLN
5	E	113	ASN
5	E	156	GLN
5	E	174	GLN
1	G	15	GLN
1	G	32	ASN
1	G	113	ASN
1	G	115	GLN
1	G	179	ASN
1	G	187	ASN
2	H	20	ASN
2	H	27	GLN
2	H	84	GLN
3	I	37	ASN
3	I	122	ASN
3	I	158	GLN
3	I	220	ASN

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Mol	Chain	Res	Type
4	J	5	HIS
4	J	18	GLN
4	J	57	GLN
4	J	84	ASN
4	J	94	ASN
4	J	103	ASN
4	J	143	HIS
5	K	62	ASN
5	K	70	GLN
5	K	92	GLN
5	K	113	ASN
5	K	156	GLN
5	K	174	GLN
6	L	6	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
7	GOL	E	1191	-	5,5,5	0.05	0	5,5,5	0.15	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
7	GOL	E	1191	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	192/206 (93%)	1.31	48 (25%) 2 1	47, 76, 126, 138	0
1	G	198/206 (96%)	0.71	16 (8%) 18 15	35, 56, 75, 96	0
2	B	240/244 (98%)	1.23	41 (17%) 4 3	51, 91, 110, 126	0
2	H	239/244 (97%)	0.53	8 (3%) 49 40	37, 54, 73, 94	0
3	C	227/238 (95%)	0.60	7 (3%) 51 42	46, 60, 76, 92	0
3	I	227/238 (95%)	0.84	10 (4%) 39 30	46, 66, 80, 102	0
4	D	178/182 (97%)	0.46	5 (2%) 55 46	35, 51, 66, 88	0
4	J	178/182 (97%)	0.88	11 (6%) 26 21	48, 67, 82, 99	0
5	E	184/190 (96%)	0.63	9 (4%) 35 27	38, 59, 79, 96	0
5	K	189/190 (99%)	0.77	6 (3%) 50 41	41, 66, 84, 100	0
6	F	13/13 (100%)	0.25	0 100 100	39, 42, 55, 68	0
6	L	13/13 (100%)	0.44	0 100 100	45, 49, 59, 83	0
All	All	2078/2146 (96%)	0.79	161 (7%) 19 16	35, 62, 104, 138	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	99	SER	6.1
1	A	189	PHE	4.8
1	A	153	ASP	4.6
1	A	150	LYS	4.5
2	B	100	SER	4.3
3	I	155	VAL	4.1
2	H	42	GLY	4.0
1	A	114	ILE	4.0
1	A	194	ILE	3.7
2	B	98	ARG	3.7
3	C	236	THR	3.6

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Mol	Chain	Res	Type	RSRZ
2	H	243	ALA	3.6
2	B	243	ALA	3.5
2	B	131	SER	3.4
2	B	143	LEU	3.3
1	A	97	THR	3.3
1	A	136	LEU	3.3
1	A	177	TRP	3.3
1	A	178	SER	3.3
1	A	135	CYS	3.3
1	A	98	TYR	3.3
1	A	164	MET	3.3
3	I	220	ASN	3.2
1	A	195	PRO	3.2
1	A	127	SER	3.2
1	A	200	PHE	3.2
2	B	208	PHE	3.1
3	C	100	ASN	3.1
4	J	180	PHE	3.1
1	A	193	ILE	3.1
1	A	154	VAL	3.1
2	B	129	GLU	3.1
1	A	118	ASP	3.1
1	A	146	VAL	3.0
2	B	190	LEU	2.9
2	B	175	GLN	2.9
1	G	168	ASP	2.9
1	A	137	PHE	2.9
1	A	120	ALA	2.9
2	B	241	GLY	2.9
1	A	133	SER	2.9
1	A	123	GLN	2.9
5	E	190	ALA	2.9
2	B	224	THR	2.9
2	B	146	LEU	2.8
2	B	138	THR	2.8
2	H	136	SER	2.8
2	B	171	CYS	2.8
2	B	177	LEU	2.7
2	H	41	PRO	2.7
1	A	162	LEU	2.7
5	K	190	ALA	2.6
1	G	179	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	238	GLU	2.6
1	A	169	PHE	2.6
1	A	91	ASP	2.6
1	A	141	ASP	2.6
3	C	127	ASP	2.6
5	K	179	SER	2.6
1	A	124	LEU	2.6
3	I	41	ILE	2.6
5	K	21	THR	2.6
2	B	103	GLN	2.6
2	B	239	ALA	2.6
5	E	113	ASN	2.6
1	G	164	MET	2.5
1	A	186	ALA	2.5
5	K	113	ASN	2.5
5	E	84	GLY	2.5
1	A	132	LYS	2.5
1	G	182	ASP	2.5
4	J	104	VAL	2.5
2	B	50	TYR	2.5
1	A	94	THR	2.5
1	G	169	PHE	2.5
1	A	103	GLY	2.5
3	C	148	VAL	2.5
2	B	159	TRP	2.5
1	A	100	TYR	2.5
5	K	140	ALA	2.5
1	A	199	PHE	2.4
1	A	131	ASP	2.4
1	A	112	ALA	2.4
2	B	234	ILE	2.4
2	B	155	VAL	2.4
1	A	122	TYR	2.4
1	A	121	VAL	2.4
4	J	132	VAL	2.4
1	G	165	ARG	2.4
2	B	240	TRP	2.4
1	G	157	THR	2.4
4	J	128	VAL	2.3
2	B	223	TRP	2.3
3	I	99	THR	2.3
1	G	193	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	194	ILE	2.3
4	D	160	VAL	2.3
4	J	94	ASN	2.3
4	J	124	ASN	2.3
1	A	139	ASP	2.3
1	A	95	SER	2.3
1	G	202	SER	2.3
1	G	80	THR	2.3
2	B	130	PRO	2.3
1	A	134	VAL	2.3
2	B	127	VAL	2.3
3	C	9	ASP	2.3
1	G	97	THR	2.3
4	D	100	ARG	2.3
2	B	174	PRO	2.3
4	J	160	VAL	2.3
2	B	163	GLY	2.3
4	J	3	GLU	2.3
5	E	112	HIS	2.3
5	E	105	LYS	2.2
3	I	79	ASP	2.2
2	H	240	TRP	2.2
2	B	200	PHE	2.2
1	A	40	PRO	2.2
3	I	81	TYR	2.2
2	B	42	GLY	2.2
3	I	109	LYS	2.2
4	D	172	GLU	2.2
3	I	125	GLN	2.2
2	B	123	PRO	2.2
2	B	126	ALA	2.2
5	E	186	VAL	2.2
3	C	164	THR	2.2
2	B	201	TRP	2.2
1	A	185	CYS	2.2
2	B	128	PHE	2.2
2	B	158	SER	2.2
5	E	85	VAL	2.1
1	G	141	ASP	2.1
3	I	86	GLY	2.1
5	K	168	GLY	2.1
3	C	198	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	242	ARG	2.1
1	A	56	GLN	2.1
2	H	202	GLN	2.1
2	B	122	PRO	2.1
2	B	232	THR	2.1
1	G	135	CYS	2.1
1	G	170	LYS	2.1
4	J	90	THR	2.1
1	G	132	LYS	2.1
4	D	132	VAL	2.1
2	H	226	ASP	2.1
1	A	156	ILE	2.1
5	E	83	TYR	2.1
5	E	173	CYS	2.0
2	B	170	VAL	2.0
1	A	113	ASN	2.0
2	B	193	ARG	2.0
1	A	159	LYS	2.0
4	D	136	VAL	2.0
4	J	167	HIS	2.0
1	A	203	PRO	2.0
4	J	163	CYS	2.0
3	I	143	LEU	2.0
2	H	182	ALA	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($\text{\AA}^2$)	Q<0.9
7	GOL	E	1191	6/6	0.56	0.20	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.