



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:21 PM UTC

PDB ID : 2XN9 / pdb_00002xn9
Title : Crystal structure of the ternary complex between human T cell receptor, staphylococcal enterotoxin H and human major histocompatibility complex class II
Authors : Salane, M.; Rodstrom, K.E.J.; Fischer, G.; Orekhov, V.Y.; Karlsson, B.G.; Lindkvist-Petersson, K.
Deposited on : 2010-07-31
Resolution : 2.30 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

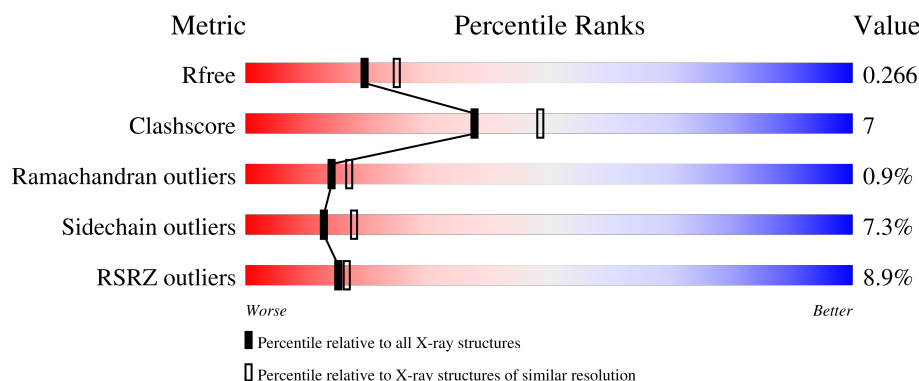
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	204	4% 80% 15% ..
2	B	244	6% 82% 15% ..
3	C	217	2% 81% 17% ..
4	D	182	23% 76% 19% ..

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Mol	Chain	Length	Quality of chain
5	E	190	
6	F	13	

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
7	GOL	B	1246	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8711 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 C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	6	0
			1570	986	265	312	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	CYS	THR	engineered mutation	UNP P01848

- Molecule 2 is a protein called T CELL RECEPTOR BETA-1 CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	3	0
			1960	1234	339	381	6			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	118	LYS	ASN	conflict	UNP P01850
B	119	ASN	LYS	conflict	UNP P01850
B	151	TYR	PHE	conflict	UNP P01850
B	171	CYS	SER	engineered mutation	UNP P01850
B	189	SER	CYS	conflict	UNP P01850

- Molecule 3 is a protein called ENTEROTOXIN H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	215	Total	C	N	O	S	0	1	0
			1757	1108	287	359	3			

- 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	3	0
			1480	956	241	278	5			

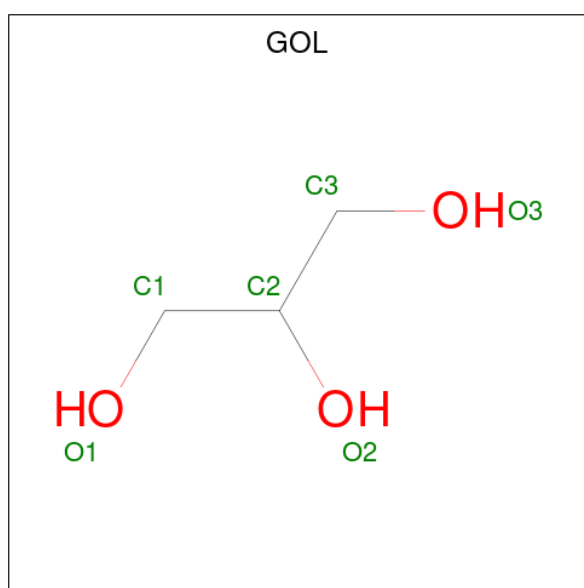
- Molecule 5 is a protein called MAJOR HISTOCOMPATIBILITY COMPLEX CLASS II BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	188	Total	C	N	O	S	0	2	0
			1534	963	274	291	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			

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



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

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Na	0	0
			1	1		

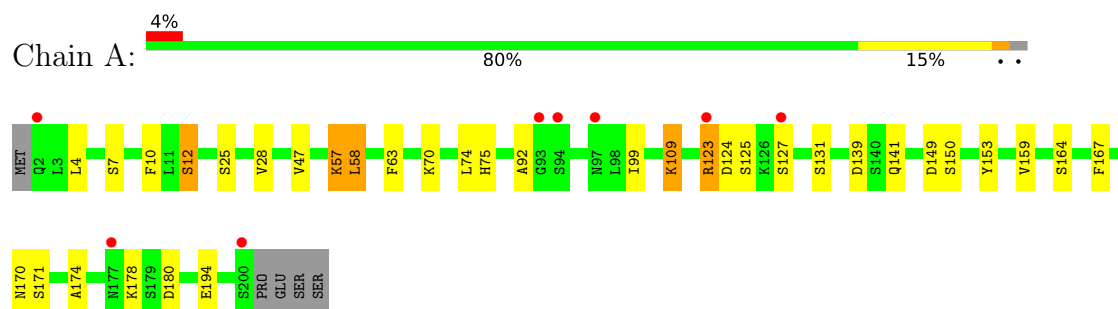
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	92	Total	O	0	0
			92	92		
9	B	74	Total	O	0	0
			74	74		
9	C	67	Total	O	0	0
			67	67		
9	D	25	Total	O	0	0
			25	25		
9	E	17	Total	O	0	0
			17	17		
9	F	5	Total	O	0	0
			5	5		

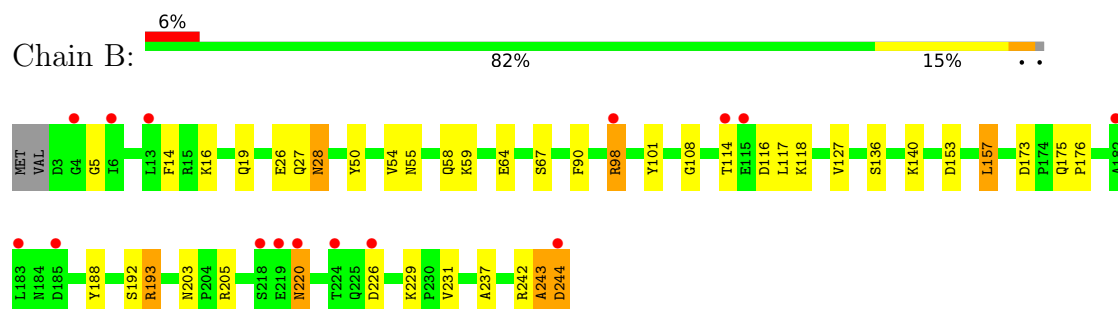
3 Residue-property plots [i](#)

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.

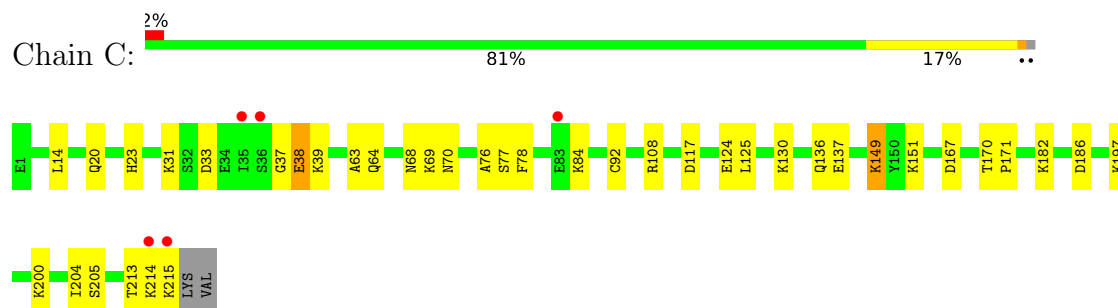
- Molecule 1: T CELL RECEPTOR ALPHA CHAIN C REGION



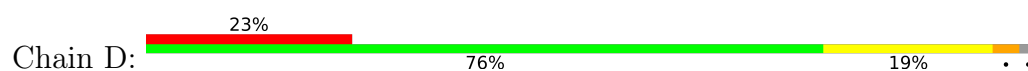
- Molecule 2: T CELL RECEPTOR BETA-1 CHAIN C REGION

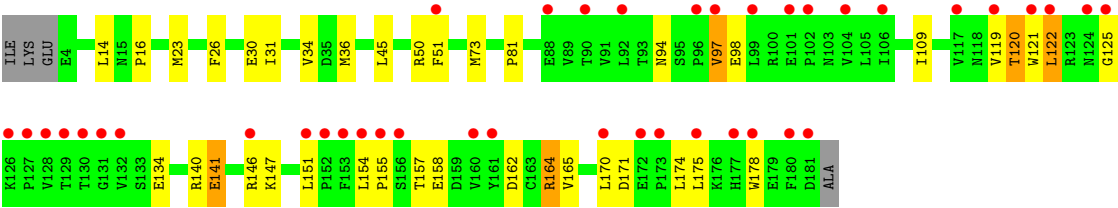


- Molecule 3: ENTEROTOXIN H

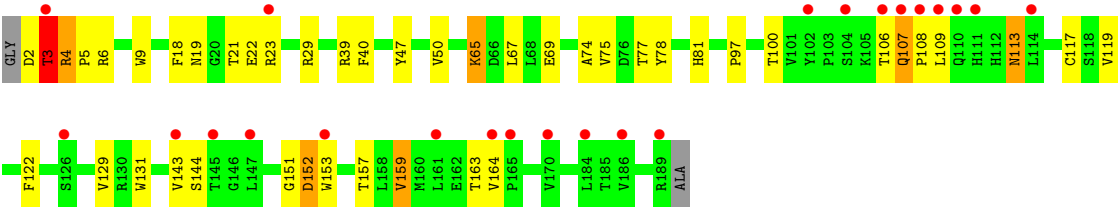


- Molecule 4: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN,

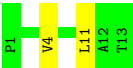
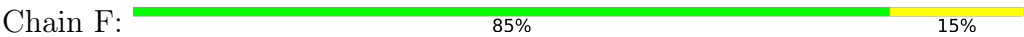




● Molecule 5: MAJOR HISTOCOMPATIBILITY COMPLEX CLASS II BETA CHAIN



● Molecule 6: HEMAGGLUTININ



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	191.18Å 48.89Å 166.72Å 90.00° 113.55° 90.00°	Depositor
Resolution (Å)	152.50 – 2.30 152.50 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.2 (152.50-2.30) 97.2 (152.50-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.222 , 0.272 0.217 , 0.266	Depositor DCC
R_{free} test set	3148 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.8	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	8711	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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: NA, 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	0.91	0/1601	0.97	0/2167
2	B	0.77	0/2013	0.93	1/2739 (0.0%)
3	C	0.75	0/1784	0.93	0/2399
4	D	0.64	0/1525	0.88	0/2081
5	E	0.67	0/1573	0.92	3/2141 (0.1%)
6	F	0.58	0/106	0.80	0/141
All	All	0.75	0/8602	0.93	4/11668 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	152	ASP	N-CA-C	6.03	123.64	110.80
2	B	243	ALA	N-CA-C	5.72	119.43	112.23
5	E	164	VAL	CA-C-N	5.01	124.77	119.76
5	E	164	VAL	C-N-CA	5.01	124.77	119.76

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	1570	0	1508	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1960	0	1834	25	0
3	C	1757	0	1712	22	0
4	D	1480	0	1394	22	0
5	E	1534	0	1428	32	0
6	F	105	0	121	2	0
7	A	6	0	8	1	0
7	B	18	0	24	5	0
8	C	1	0	0	0	0
9	A	92	0	0	1	0
9	B	74	0	0	0	0
9	C	67	0	0	1	0
9	D	25	0	0	0	0
9	E	17	0	0	0	0
9	F	5	0	0	0	0
All	All	8711	0	8029	115	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 7.

All (115) 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:194[B]:GLU:H	1:A:194[B]:GLU:CD	1.56	1.02
5:E:129:VAL:HG11	5:E:159:VAL:HG21	1.57	0.86
5:E:23[B]:ARG:HH11	5:E:23[B]:ARG:HG3	1.43	0.83
3:C:213:THR:HG22	3:C:215:LYS:H	1.45	0.82
1:A:194[B]:GLU:CD	1:A:194[B]:GLU:N	2.38	0.80
2:B:203:ASN:HD21	2:B:205:ARG:HH21	1.31	0.79
5:E:23[B]:ARG:HH11	5:E:23[B]:ARG:CG	1.98	0.75
1:A:171:SER:OG	2:B:193:ARG:HD3	1.89	0.72
5:E:129:VAL:CG1	5:E:159:VAL:HG21	2.19	0.71
5:E:117:CYS:HB3	5:E:159:VAL:HG23	1.75	0.69
5:E:129:VAL:HG11	5:E:159:VAL:CG2	2.23	0.68
5:E:81:HIS:CD2	6:F:4:VAL:HG23	2.28	0.67
4:D:141[A]:GLU:O	4:D:141[A]:GLU:OE2	2.14	0.64
5:E:151:GLY:O	5:E:153:TRP:N	2.29	0.64
1:A:159:VAL:HG22	1:A:170:ASN:OD1	1.98	0.63
3:C:76:ALA:H	3:C:136:GLN:NE2	1.98	0.61
2:B:229:LYS:HG3	2:B:231:VAL:HG13	1.82	0.61
5:E:2:ASP:OD2	5:E:4:ARG:HD3	2.01	0.61
2:B:173:ASP:OD1	2:B:193:ARG:NH2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:GLU:OE2	3:C:149:LYS:HE2	2.01	0.61
3:C:170:THR:HB	3:C:171:PRO:CD	2.32	0.60
5:E:2:ASP:CG	5:E:6:ARG:HH22	2.10	0.59
4:D:120:THR:HB	4:D:164:ARG:HG2	1.85	0.58
2:B:50:TYR:CZ	2:B:58:GLN:HG3	2.39	0.58
2:B:188:TYR:HE1	7:B:1246:GOL:H31	1.68	0.58
4:D:140:ARG:HG2	4:D:146:ARG:HD2	1.86	0.57
4:D:81:PRO:HB3	5:E:5:PRO:HB2	1.86	0.57
1:A:149:ASP:OD1	1:A:149:ASP:C	2.48	0.57
4:D:134:GLU:OE2	4:D:147:LYS:NZ	2.37	0.57
3:C:213:THR:HG23	9:C:2067:HOH:O	2.05	0.56
1:A:194[B]:GLU:N	1:A:194[B]:GLU:OE2	2.38	0.55
2:B:28:ASN:HD22	2:B:28:ASN:H	1.53	0.55
1:A:123[B]:ARG:HD2	1:A:124:ASP:O	2.06	0.55
3:C:130:LYS:HE2	3:C:137:GLU:OE1	2.07	0.54
5:E:23[B]:ARG:CG	5:E:23[B]:ARG:NH1	2.62	0.54
2:B:5:GLY:H	2:B:28:ASN:ND2	2.06	0.54
5:E:119:VAL:CG2	5:E:157:THR:HG22	2.39	0.53
3:C:37:GLY:O	3:C:38:GLU:HG2	2.09	0.53
5:E:97:PRO:HB3	5:E:122:PHE:HB3	1.91	0.52
2:B:98:ARG:H	2:B:98:ARG:HD2	1.74	0.52
1:A:57:LYS:O	1:A:58:LEU:HD13	2.08	0.52
1:A:74[B]:LEU:HD22	1:A:75:HIS:N	2.25	0.51
3:C:167:ASP:O	3:C:205:SER:HB3	2.10	0.51
2:B:188:TYR:CE1	7:B:1246:GOL:H31	2.47	0.49
3:C:170:THR:HB	3:C:171:PRO:HD2	1.95	0.49
2:B:14:PHE:CZ	2:B:114:THR:HB	2.48	0.49
4:D:122:LEU:HB2	4:D:162:ASP:HB2	1.94	0.49
5:E:2:ASP:OD2	5:E:6:ARG:NH2	2.45	0.49
3:C:117:ASP:OD2	3:C:213:THR:HB	2.13	0.49
5:E:2:ASP:O	5:E:3:THR:HG22	2.12	0.49
4:D:109:ILE:HD11	4:D:119:VAL:HG21	1.94	0.49
3:C:108:ARG:NH2	3:C:204:ILE:O	2.42	0.48
5:E:29:ARG:HH12	5:E:39:ARG:NH1	2.11	0.48
3:C:39:LYS:O	3:C:63:ALA:HB2	2.13	0.48
4:D:73:MET:HG2	6:F:11:LEU:CD1	2.44	0.48
1:A:10[B]:PHE:CD1	1:A:10[B]:PHE:C	2.92	0.48
2:B:127:VAL:HG23	2:B:237:ALA:HB3	1.96	0.47
5:E:108:PRO:HA	5:E:109:LEU:HA	1.77	0.47
4:D:26:PHE:HB2	4:D:31:ILE:HD11	1.96	0.47
2:B:5:GLY:H	2:B:28:ASN:HD21	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ALA:N	2:B:244:ASP:HA	2.30	0.47
3:C:213:THR:HG22	3:C:214:LYS:N	2.30	0.46
3:C:77:SER:HA	3:C:92:CYS:O	2.15	0.46
4:D:34:VAL:O	4:D:36:MET:HE2	2.16	0.46
5:E:74:ALA:HA	5:E:77:THR:OG1	2.16	0.46
4:D:51:PHE:N	4:D:51:PHE:CD2	2.83	0.46
5:E:74:ALA:O	5:E:78:TYR:HB3	2.15	0.46
2:B:14:PHE:CE1	2:B:114:THR:HB	2.51	0.46
2:B:176:PRO:HG2	7:B:1246:GOL:H32	1.97	0.46
2:B:101:TYR:HH	3:C:23:HIS:CE1	2.34	0.46
2:B:175:GLN:NE2	7:B:1246:GOL:O2	2.49	0.46
3:C:20:GLN:HE21	3:C:76:ALA:HB1	1.81	0.46
4:D:14:LEU:HD11	5:E:6:ARG:HB3	1.98	0.45
5:E:19:ASN:ND2	5:E:22:GLU:OE1	2.49	0.45
5:E:144:SER:HB2	5:E:159:VAL:HG12	1.97	0.45
2:B:153:ASP:CG	2:B:176:PRO:HG3	2.42	0.45
1:A:167:PHE:CD2	2:B:140:LYS:HE2	2.53	0.44
1:A:74[B]:LEU:HD22	1:A:74[B]:LEU:C	2.42	0.44
7:A:1201:GOL:O3	7:B:1245:GOL:H12	2.17	0.44
1:A:12:SER:OG	1:A:109[B]:LYS:HE2	2.18	0.44
5:E:117:CYS:HB2	5:E:131:TRP:CZ2	2.53	0.44
1:A:153:TYR:O	1:A:174:ALA:HA	2.17	0.44
1:A:109[A]:LYS:HE3	1:A:109[A]:LYS:HB2	1.42	0.43
3:C:213:THR:CG2	3:C:214:LYS:N	2.80	0.43
1:A:139:ASP:OD2	1:A:139:ASP:C	2.59	0.43
5:E:113:ASN:HB3	5:E:163:THR:OG1	2.19	0.43
4:D:16:PRO:HD2	5:E:6:ARG:HD3	2.00	0.43
2:B:28:ASN:HD22	2:B:28:ASN:N	2.15	0.43
5:E:65:LYS:O	5:E:69:GLU:HG3	2.18	0.43
3:C:39:LYS:HE3	3:C:39:LYS:HB2	1.81	0.43
4:D:97:VAL:HG21	4:D:178:TRP:HZ2	1.84	0.43
3:C:182:LYS:HD3	3:C:182:LYS:HA	1.86	0.42
3:C:33:ASP:OD1	3:C:68:ASN:HB2	2.19	0.42
2:B:54:VAL:O	2:B:55:ASN:HB2	2.20	0.42
4:D:119:VAL:HG22	4:D:165:VAL:HG22	2.01	0.42
1:A:4:LEU:HD23	1:A:25:SER:HB2	2.01	0.42
3:C:78:PHE:HB3	3:C:186:ASP:HB3	2.02	0.42
1:A:178:LYS:HE2	1:A:180:ASP:HB3	2.02	0.42
4:D:109:ILE:CD1	4:D:119:VAL:HG21	2.51	0.41
4:D:23:MET:HE2	4:D:30:GLU:HG3	2.02	0.41
4:D:154:LEU:HA	4:D:155:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:51:PHE:N	4:D:51:PHE:HD2	2.18	0.41
4:D:140:ARG:CG	4:D:146:ARG:HD2	2.50	0.41
2:B:16:LYS:HE3	2:B:117:LEU:HG	2.03	0.41
2:B:90:PHE:CZ	2:B:108:GLY:HA3	2.56	0.41
2:B:157:LEU:HD11	2:B:192:SER:CB	2.51	0.41
4:D:121:TRP:CE2	4:D:151:LEU:HB2	2.56	0.41
5:E:18:PHE:HB2	5:E:23[B]:ARG:HB3	2.02	0.41
5:E:40:PHE:HB2	5:E:47:TYR:CE2	2.56	0.41
1:A:92:ALA:O	9:A:2050:HOH:O	2.22	0.40
3:C:31:LYS:HD3	3:C:70:ASN:HD22	1.87	0.40
5:E:18:PHE:HB2	5:E:23[A]:ARG:HB3	2.03	0.40
1:A:47:VAL:HG11	1:A:63:PHE:CG	2.56	0.40
4:D:73:MET:HG3	5:E:9:TRP:CZ3	2.57	0.40
5:E:119:VAL:O	5:E:119:VAL:HG23	2.22	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	203/204 (100%)	193 (95%)	9 (4%)	1 (0%)	24	31
2	B	243/244 (100%)	231 (95%)	9 (4%)	3 (1%)	10	12
3	C	214/217 (99%)	203 (95%)	10 (5%)	1 (0%)	24	31
4	D	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	21	27
5	E	188/190 (99%)	173 (92%)	11 (6%)	4 (2%)	5	4
6	F	11/13 (85%)	11 (100%)	0	0	100	100
All	All	1038/1050 (99%)	979 (94%)	49 (5%)	10 (1%)	14	15

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	152	ASP
3	C	38	GLU
2	B	226[A]	ASP
2	B	226[B]	ASP
4	D	125	GLY
1	A	127	SER
2	B	220	ASN
5	E	3	THR
5	E	106	THR
5	E	107	GLN

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	176/180 (98%)	160 (91%)	16 (9%)	9	11
2	B	212/215 (99%)	195 (92%)	17 (8%)	11	15
3	C	194/197 (98%)	185 (95%)	9 (5%)	24	36
4	D	163/166 (98%)	147 (90%)	16 (10%)	7	10
5	E	165/171 (96%)	153 (93%)	12 (7%)	13	18
6	F	12/12 (100%)	12 (100%)	0	100	100
All	All	922/941 (98%)	852 (92%)	70 (8%)	13	16

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	12	SER
1	A	28	VAL
1	A	57	LYS
1	A	58	LEU
1	A	70	LYS
1	A	99	ILE
1	A	109[A]	LYS
1	A	109[B]	LYS

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Mol	Chain	Res	Type
1	A	123[A]	ARG
1	A	123[B]	ARG
1	A	125	SER
1	A	131	SER
1	A	141	GLN
1	A	150	SER
1	A	164	SER
2	B	19	GLN
2	B	26[A]	GLU
2	B	26[B]	GLU
2	B	27	GLN
2	B	28	ASN
2	B	59	LYS
2	B	64	GLU
2	B	67	SER
2	B	98	ARG
2	B	116	ASP
2	B	118	LYS
2	B	136	SER
2	B	157	LEU
2	B	193	ARG
2	B	220	ASN
2	B	242	ARG
2	B	244	ASP
3	C	14	LEU
3	C	64	GLN
3	C	69	LYS
3	C	84	LYS
3	C	125	LEU
3	C	149	LYS
3	C	151	LYS
3	C	197	LYS
3	C	200	LYS
4	D	45	LEU
4	D	50	ARG
4	D	94	ASN
4	D	97	VAL
4	D	98	GLU
4	D	120	THR
4	D	122	LEU
4	D	141[A]	GLU
4	D	141[B]	GLU

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Mol	Chain	Res	Type
4	D	157	THR
4	D	158	GLU
4	D	164	ARG
4	D	170	LEU
4	D	171	ASP
4	D	174	LEU
4	D	175	LEU
5	E	3	THR
5	E	4	ARG
5	E	21	THR
5	E	50	VAL
5	E	65	LYS
5	E	67	LEU
5	E	75	VAL
5	E	100	THR
5	E	107	GLN
5	E	113	ASN
5	E	143	VAL
5	E	159	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	27	GLN
2	B	28	ASN
2	B	58	GLN
2	B	86	ASN
2	B	175	GLN
2	B	233	GLN
3	C	22	ASN
3	C	29	ASN
3	C	45	ASN
3	C	70	ASN
3	C	136	GLN
4	D	149	HIS
5	E	10	GLN
5	E	113	ASN
5	E	156	GLN
6	F	6	GLN
6	F	7	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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
7	GOL	B	1245	-	5,5,5	0.49	0	5,5,5	0.65	0
7	GOL	B	1247	-	5,5,5	0.39	0	5,5,5	0.20	0
7	GOL	B	1246	-	5,5,5	0.41	0	5,5,5	0.27	0
7	GOL	A	1201	-	5,5,5	0.52	0	5,5,5	0.48	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	B	1245	-	-	1/4/4/4	-
7	GOL	B	1247	-	-	2/4/4/4	-
7	GOL	B	1246	-	-	2/4/4/4	-
7	GOL	A	1201	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1201	GOL	O1-C1-C2-C3
7	A	1201	GOL	C1-C2-C3-O3
7	A	1201	GOL	O2-C2-C3-O3
7	B	1247	GOL	O1-C1-C2-C3
7	A	1201	GOL	O1-C1-C2-O2
7	B	1247	GOL	O1-C1-C2-O2
7	B	1245	GOL	O1-C1-C2-C3
7	B	1246	GOL	O1-C1-C2-C3
7	B	1246	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1245	GOL	1	0
7	B	1246	GOL	4	0
7	A	1201	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	199/204 (97%)	-0.02	8 (4%) 42 44	8, 23, 46, 55	6 (3%)
2	B	242/244 (99%)	0.23	15 (6%) 26 28	10, 32, 53, 67	3 (1%)
3	C	215/217 (99%)	0.26	5 (2%) 61 63	23, 36, 52, 60	1 (0%)
4	D	178/182 (97%)	1.16	41 (23%) 2 2	18, 49, 81, 86	3 (1%)
5	E	188/190 (98%)	0.96	23 (12%) 8 9	20, 50, 71, 86	2 (1%)
6	F	13/13 (100%)	-0.03	0 100 100	30, 34, 41, 43	0
All	All	1035/1050 (98%)	0.48	92 (8%) 15 17	8, 37, 71, 86	15 (1%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	109	LEU	5.4
1	A	93	GLY	4.5
5	E	108	PRO	4.2
4	D	154	LEU	3.6
4	D	97	VAL	3.6
4	D	160	VAL	3.6
4	D	102	PRO	3.6
4	D	99	LEU	3.5
4	D	175	LEU	3.5
5	E	164	VAL	3.4
4	D	88[A]	GLU	3.4
5	E	111	HIS	3.3
2	B	224	THR	3.3
4	D	130	THR	3.2
5	E	102	TYR	3.1
2	B	226[A]	ASP	3.1
4	D	92	LEU	3.1
5	E	110	GLN	3.0
2	B	114	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	123[A]	ARG	3.0
4	D	128	VAL	3.0
2	B	4	GLY	3.0
5	E	165	PRO	3.0
5	E	145	THR	2.9
2	B	182	ALA	2.9
4	D	178	TRP	2.9
5	E	147	LEU	2.8
5	E	186	VAL	2.8
4	D	161	TYR	2.7
5	E	126	SER	2.7
4	D	173	PRO	2.7
1	A	97	ASN	2.7
4	D	106	ILE	2.7
2	B	218	SER	2.7
4	D	181	ASP	2.7
5	E	106	THR	2.7
3	C	36	SER	2.6
5	E	104	SER	2.6
2	B	13	LEU	2.6
4	D	96	PRO	2.6
5	E	114	LEU	2.5
5	E	153	TRP	2.5
4	D	180	PHE	2.5
1	A	127	SER	2.5
4	D	51	PHE	2.5
4	D	119	VAL	2.5
1	A	177	ASN	2.5
4	D	152	PRO	2.5
4	D	127	PRO	2.5
5	E	23[A]	ARG	2.4
4	D	129	THR	2.4
4	D	156	SER	2.4
3	C	35	ILE	2.4
5	E	170	VAL	2.4
5	E	161	LEU	2.4
4	D	153	PHE	2.4
2	B	98	ARG	2.4
5	E	107	GLN	2.4
4	D	172	GLU	2.4
2	B	185	ASP	2.3
2	B	244	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	124	ASN	2.3
3	C	215	LYS	2.3
1	A	2	GLN	2.3
2	B	183	LEU	2.3
4	D	90	THR	2.3
1	A	200	SER	2.3
2	B	220	ASN	2.2
4	D	125	GLY	2.2
5	E	189	ARG	2.2
5	E	3	THR	2.2
4	D	151	LEU	2.2
1	A	94	SER	2.2
4	D	170	LEU	2.2
5	E	143	VAL	2.2
4	D	155	PRO	2.2
4	D	131	GLY	2.2
3	C	83[A]	GLU	2.2
2	B	115	GLU	2.2
4	D	117	VAL	2.1
4	D	122	LEU	2.1
4	D	101	GLU	2.1
4	D	177	HIS	2.1
4	D	146	ARG	2.1
3	C	214	LYS	2.1
2	B	219	GLU	2.1
2	B	6	ILE	2.1
4	D	104	VAL	2.1
4	D	132	VAL	2.0
4	D	121	TRP	2.0
5	E	184	LEU	2.0
4	D	126	LYS	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

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	B	1247	6/6	0.80	0.15	77,78,79,79	0
7	GOL	B	1246	6/6	0.81	0.17	69,69,70,70	0
7	GOL	A	1201	6/6	0.84	0.17	42,49,51,51	0
7	GOL	B	1245	6/6	0.86	0.14	34,38,40,40	0
8	NA	C	1216	1/1	0.99	0.02	22,22,22,22	0

6.5 Other polymers

There are no such residues in this entry.