



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 09:56 PM UTC

PDB ID : 8T59 / pdb_00008t59
Title : Crystal structure of Para.09 bound to TREM2
Authors : Wallweber, H.; Hsu, P.L.
Deposited on : 2023-06-12
Resolution : 2.00 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

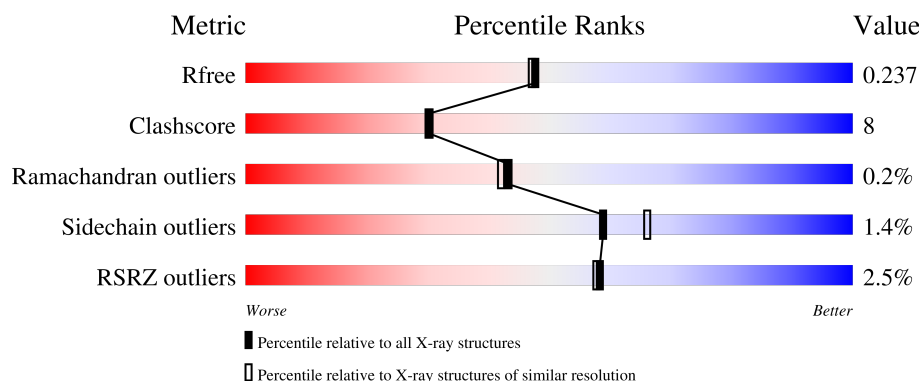
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	225	4% 79% 13% 7%
1	C	225	% 82% 13% •
2	B	219	% 83% 16%
2	D	219	2% 86% 13% •
3	E	19	5% 68% 11% 21%

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Mol	Chain	Length	Quality of chain
3	F	19	

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	GOL	B	305	-	X	-	-
4	GOL	C	302	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7624 atoms, of which 90 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 Para.09 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	1	0
			1587	1008	261	313	5			
1	C	216	Total	C	N	O	S	0	5	0
			1658	1051	273	329	5			

- Molecule 2 is a protein called Para.09 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	2	0
			1691	1068	280	337	6			
2	D	219	Total	C	N	O	S	0	1	0
			1691	1067	280	337	7			

- Molecule 3 is a protein called Triggering receptor expressed on myeloid cells 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	15	Total	C	N	O	0	0	0
			116	70	22	24			
3	F	17	Total	C	N	O	0	0	0
			131	78	24	29			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

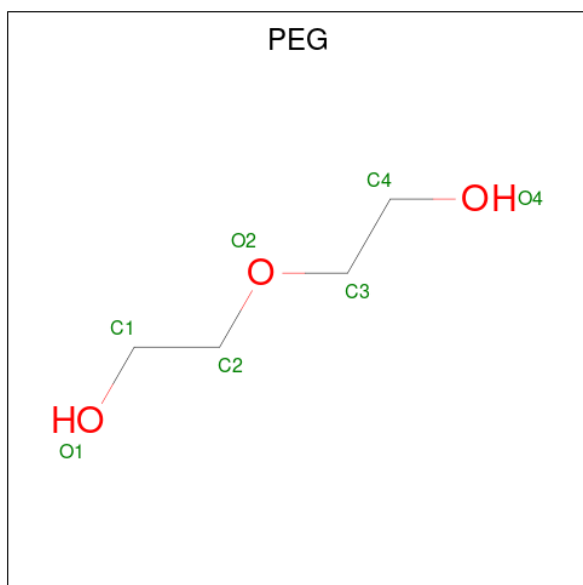
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Zn	0	0
			3	3		
5	D	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total	Zn	0	0
			1	1		
5	F	1	Total	Zn	0	0
			1	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	116	Total	O	0	1
			117	117		
7	B	114	Total	O	0	2
			116	116		
7	C	154	Total	O	0	6
			160	160		
7	D	159	Total	O	0	3
			162	162		
7	E	14	Total	O	0	2
			16	16		
7	F	15	Total	O	0	0
			15	15		

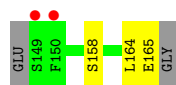
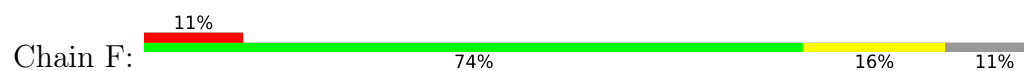
- Molecule 1: Para.09 heavy chain



- Molecule 3: Triggering receptor expressed on myeloid cells 2



- Molecule 3: Triggering receptor expressed on myeloid cells 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.17Å 68.16Å 254.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.78 – 2.00 33.78 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.78-2.00) 93.8 (33.78-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.78 (at 1.92Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.200 , 0.237 0.200 , 0.237	Depositor DCC
R_{free} test set	3629 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.3	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	0.96	EDS
Total number of atoms	7624	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: PEG, ZN, 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	0.30	0/1626	0.55	1/2218 (0.0%)
1	C	0.29	0/1699	0.52	0/2318
2	B	0.27	0/1729	0.54	0/2350
2	D	0.29	0/1729	0.56	0/2350
3	E	0.25	0/117	0.39	0/157
3	F	0.31	0/132	0.52	0/177
All	All	0.29	0/7032	0.54	1/9570 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	100	ASP	N-CA-C	-6.46	105.27	113.02

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	98	VAL	Peptide

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Mol	Chain	Res	Type	Group
2	D	98	VAL	Peptide

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	1587	0	1552	29	0
1	C	1658	0	1627	31	0
2	B	1691	0	1667	28	0
2	D	1691	0	1666	32	0
3	E	116	0	106	2	0
3	F	131	0	117	2	0
4	A	12	16	16	2	0
4	B	24	32	32	5	0
4	C	18	24	22	4	0
4	D	6	8	8	0	0
5	B	3	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	C	7	10	10	0	0
7	A	117	0	0	3	0
7	B	116	0	0	3	0
7	C	160	0	0	4	1
7	D	162	0	0	5	1
7	E	16	0	0	1	0
7	F	15	0	0	0	0
All	All	7534	90	6823	115	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 8.

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)
2:D:14:THR:HG23	2:D:17:GLU:HG3	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:HIS:HB3	2:B:206:LEU:HD23	1.46	0.95
2:D:218:GLU:OE1	7:D:401:HOH:O	1.84	0.94
1:A:128:PRO:HG3	1:A:140:LEU:HB3	1.54	0.89
1:C:41:SER:HB3	4:C:301:GOL:O2	1.76	0.86
1:C:216:LYS:NZ	2:D:219:CYS:SG	2.52	0.81
2:D:14:THR:HG23	2:D:17:GLU:CG	2.14	0.77
1:A:194:GLN:HB3	7:A:464:HOH:O	1.84	0.76
2:B:128:GLU:OE1	2:B:128:GLU:N	2.16	0.75
2:B:110:GLU:OE1	2:B:178:TYR:OH	2.07	0.73
2:D:14:THR:CG2	2:D:17:GLU:HG3	2.19	0.73
2:B:118:PRO:HD2	2:B:206:LEU:HD21	1.69	0.73
1:C:150:GLU:HG3	7:C:403:HOH:O	1.88	0.73
1:C:210:ASP:OD1	7:C:401:HOH:O	2.07	0.71
1:A:41:SER:HB3	4:A:302:GOL:H31	1.73	0.71
2:D:14:THR:HG22	7:D:514:HOH:O	1.92	0.69
2:B:53:ILE:HD12	2:B:78:LEU:CD1	2.23	0.68
1:A:169:PRO:HD2	2:B:167:SER:OG	1.94	0.68
1:A:100:ASP:O	1:A:101:ILE:HG22	1.94	0.67
2:B:203:HIS:HB3	2:B:206:LEU:CD2	2.21	0.67
2:D:218:GLU:HG2	2:D:219:CYS:H	1.60	0.66
1:C:103:GLU:OE2	7:C:402:HOH:O	2.13	0.66
2:D:3:VAL:HG12	2:D:26:SER:HB3	1.79	0.64
1:C:132:SER:HA	2:D:121:PHE:HD2	1.64	0.63
2:D:3:VAL:CG1	2:D:26:SER:HB3	2.30	0.62
3:E:161:ARG:HD2	7:E:311[B]:HOH:O	1.98	0.61
2:D:130:LEU:O	2:D:188:LYS:HD2	2.01	0.60
2:D:218:GLU:HG2	2:D:219:CYS:N	2.16	0.60
1:A:145:LYS:HE2	7:B:408:HOH:O	1.99	0.60
2:D:38:LEU:HD13	2:D:76:PHE:CD2	2.36	0.60
1:A:134:SER:N	7:A:403:HOH:O	2.34	0.59
2:B:42:LEU:HB2	2:B:52:LEU:HD11	1.84	0.59
1:A:1:GLU:N	7:A:401:HOH:O	2.23	0.59
2:D:78:LEU:C	2:D:78:LEU:HD23	2.28	0.58
1:A:194:GLN:NE2	1:C:7[A]:SER:HB2	2.19	0.58
2:B:59:LEU:HD21	2:B:65:ASP:HA	1.86	0.57
1:C:41:SER:HB3	4:C:301:GOL:HO2	1.66	0.57
1:C:150:GLU:OE2	7:C:403:HOH:O	2.17	0.57
2:B:126:SER:HB2	2:B:128:GLU:OE1	2.05	0.56
1:C:70:PHE:CE2	1:C:85:MET:HE3	2.41	0.56
1:A:75:ASP:OD2	1:A:78:LYS:NZ	2.36	0.56
1:A:50:HIS:ND1	2:B:99:TYR:OH	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:VAL:HG11	2:D:165:GLN:HB3	1.89	0.53
2:D:110:GLU:OE2	2:D:178:TYR:OH	2.20	0.53
1:A:41:SER:H	4:A:302:GOL:H31	1.74	0.53
2:B:88:VAL:HG11	2:B:111:ILE:HG12	1.91	0.52
1:A:12:VAL:HG11	1:A:88:LEU:HD13	1.91	0.52
2:B:186:LEU:HD11	4:B:306:GOL:C1	2.40	0.52
1:A:180:LEU:C	1:A:180:LEU:HD12	2.35	0.51
2:B:130:LEU:O	2:B:188:LYS:HD2	2.10	0.51
1:A:194:GLN:NE2	1:C:7[B]:SER:HB3	2.24	0.51
1:C:121:PRO:HB3	1:C:147:TYR:HB3	1.93	0.51
2:D:218:GLU:O	2:D:219:CYS:CB	2.58	0.51
1:A:85:MET:HB3	1:A:88:LEU:HD21	1.92	0.50
2:B:100:PRO:O	2:B:102:THR:HG23	2.11	0.50
2:B:3:VAL:HG12	2:B:26:SER:HB3	1.94	0.50
1:C:133[B]:THR:HG22	1:C:133[B]:THR:O	2.11	0.50
1:C:64:GLU:OE2	1:C:67:LYS:NZ	2.43	0.49
1:A:169:PRO:HD2	2:B:167:SER:HG	1.76	0.49
1:C:12:VAL:HG11	1:C:88:LEU:HD13	1.93	0.49
4:B:305:GOL:H32	7:B:433:HOH:O	2.12	0.49
1:C:50:HIS:ND1	2:D:99:TYR:OH	2.40	0.49
2:D:42:LEU:HB2	2:D:52:LEU:HD11	1.95	0.49
2:D:100:PRO:O	2:D:102:THR:HG23	2.12	0.49
1:A:70:PHE:CE2	1:A:85:MET:HE3	2.48	0.49
1:C:132:SER:CA	2:D:121:PHE:HD2	2.26	0.48
3:F:164:LEU:O	3:F:165:GLU:HB2	2.13	0.48
2:B:180:LEU:C	2:B:180:LEU:HD23	2.39	0.48
2:D:218:GLU:O	2:D:219:CYS:HB2	2.13	0.48
1:C:101:ILE:HG23	1:C:101:ILE:O	2.14	0.47
2:D:180:LEU:C	2:D:180:LEU:HD23	2.39	0.47
1:A:128:PRO:O	1:A:129:SER:HB2	2.15	0.47
2:B:38:LEU:HG	2:B:39:TYR:N	2.29	0.47
2:B:128:GLU:HA	2:B:131:LYS:HE2	1.97	0.47
2:B:94:ALA:HB2	2:B:103:PHE:CD2	2.50	0.46
1:C:85:MET:HE1	1:C:96:TYR:CZ	2.51	0.46
2:D:31:THR:O	2:D:33:LYS:O	2.34	0.46
2:B:88:VAL:CG1	2:B:111:ILE:HG12	2.46	0.46
2:D:3:VAL:HG12	2:D:26:SER:CB	2.43	0.45
1:A:58:TYR:CD1	1:A:74:ARG:HD3	2.52	0.45
1:C:100:ASP:O	1:C:101:ILE:HG22	2.16	0.45
4:B:305:GOL:H11	7:B:433:HOH:O	2.16	0.45
2:D:180:LEU:HD23	2:D:181:SER:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:LEU:HD21	4:B:306:GOL:H11	1.99	0.45
1:C:128:PRO:HG2	1:C:215:PRO:HA	1.99	0.45
1:C:180:LEU:HD12	1:C:180:LEU:C	2.42	0.45
1:A:208:LYS:HB3	1:A:208:LYS:HE3	1.71	0.44
2:D:185:THR:C	2:D:186:LEU:HD12	2.42	0.44
1:C:172:LEU:HD23	1:C:173:GLN:O	2.18	0.44
2:D:170:GLU:OE2	7:D:402:HOH:O	2.21	0.44
1:C:93:THR:O	1:C:94:ALA:HB2	2.17	0.44
2:B:17:GLU:HB3	2:B:18:PRO:HD2	2.00	0.44
2:D:170:GLU:HG3	7:D:402:HOH:O	2.17	0.44
1:C:102:LEU:HD12	3:F:158:SER:HB3	2.00	0.44
2:B:129:GLN:HG2	2:B:134:THR:O	2.17	0.43
2:D:128:GLU:OE1	2:D:128:GLU:N	2.47	0.43
1:A:2:VAL:HG11	1:A:104:TYR:CD1	2.53	0.43
1:A:101:ILE:HD12	1:A:101:ILE:HA	1.80	0.43
2:B:53:ILE:HD12	2:B:78:LEU:HD13	1.98	0.43
1:A:30:SER:O	1:A:53:ALA:HB1	2.19	0.43
2:B:186:LEU:HD12	2:B:186:LEU:HA	1.83	0.43
1:C:12:VAL:O	1:C:113:VAL:HA	2.19	0.42
1:A:128:PRO:HA	1:A:139:ALA:O	2.19	0.42
2:B:194:HIS:NE2	4:B:306:GOL:H2	2.34	0.42
2:D:78:LEU:HD23	2:D:79:LYS:N	2.35	0.42
1:A:121:PRO:HB3	1:A:147:TYR:HB3	2.02	0.42
1:A:58:TYR:HD1	1:A:74:ARG:HD3	1.85	0.42
1:A:193:THR:HG22	1:A:193:THR:O	2.20	0.42
1:C:70:PHE:HA	1:C:84:GLN:O	2.20	0.42
1:C:67:LYS:HE2	4:C:302:GOL:H31	2.01	0.41
2:D:99:TYR:HB2	7:D:475:HOH:O	2.20	0.41
1:C:67:LYS:CE	4:C:302:GOL:H31	2.50	0.41
1:A:22:CYS:HB3	1:A:81:VAL:HG13	2.02	0.40
1:C:172:LEU:HD23	1:C:172:LEU:C	2.46	0.40
3:E:152:ASP:OD1	3:E:152:ASP:C	2.65	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)
7:C:524:HOH:O	7:D:540:HOH:O[3_644]	1.79	0.41

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	207/225 (92%)	199 (96%)	7 (3%)	1 (0%)	24	21
1	C	219/225 (97%)	212 (97%)	6 (3%)	1 (0%)	24	21
2	B	218/219 (100%)	212 (97%)	6 (3%)	0	100	100
2	D	218/219 (100%)	212 (97%)	6 (3%)	0	100	100
3	E	13/19 (68%)	13 (100%)	0	0	100	100
3	F	15/19 (79%)	14 (93%)	1 (7%)	0	100	100
All	All	890/926 (96%)	862 (97%)	26 (3%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ILE
1	C	101	ILE

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	179/193 (93%)	175 (98%)	4 (2%)	45	50
1	C	189/193 (98%)	186 (98%)	3 (2%)	55	62
2	B	195/194 (100%)	193 (99%)	2 (1%)	68	75
2	D	195/194 (100%)	192 (98%)	3 (2%)	57	64
3	E	13/17 (76%)	13 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	15/17 (88%)	15 (100%)	0	100	100
All	All	786/808 (97%)	774 (98%)	12 (2%)	59	64

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	ILE
1	A	152[A]	VAL
1	A	152[B]	VAL
1	A	180	LEU
2	B	9	LEU
2	B	99	TYR
1	C	180	LEU
1	C	188	SER
1	C	216	LYS
2	D	14	THR
2	D	97	LEU
2	D	99	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
2	B	165	GLN
1	C	79	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 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 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
4	GOL	A	302	-	5,5,5	0.92	0	5,5,5	1.09	0
6	PEG	C	304	-	6,6,6	0.50	0	5,5,5	0.28	0
4	GOL	C	303	-	5,5,5	1.37	1 (20%)	5,5,5	1.56	1 (20%)
4	GOL	B	302	-	5,5,5	0.92	0	5,5,5	1.23	1 (20%)
4	GOL	A	301	-	5,5,5	0.78	0	5,5,5	1.30	1 (20%)
4	GOL	B	305	-	5,5,5	1.42	1 (20%)	5,5,5	1.53	1 (20%)
4	GOL	C	301	-	5,5,5	0.94	0	5,5,5	1.42	1 (20%)
4	GOL	D	301	-	5,5,5	0.94	0	5,5,5	1.55	1 (20%)
4	GOL	C	302	-	5,5,5	1.23	1 (20%)	5,5,5	1.58	1 (20%)
4	GOL	B	301	-	5,5,5	1.28	0	5,5,5	1.52	1 (20%)
4	GOL	B	306	-	5,5,5	1.20	1 (20%)	5,5,5	1.53	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	302	-	-	2/4/4/4	-
6	PEG	C	304	-	-	2/4/4/4	-
4	GOL	C	303	-	-	2/4/4/4	-
4	GOL	B	302	-	-	2/4/4/4	-
4	GOL	A	301	-	-	2/4/4/4	-
4	GOL	B	305	-	-	4/4/4/4	-
4	GOL	C	301	-	-	0/4/4/4	-
4	GOL	D	301	-	-	2/4/4/4	-
4	GOL	C	302	-	-	4/4/4/4	-
4	GOL	B	301	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	306	-	-	1/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	302	GOL	O2-C2	-2.70	1.35	1.43
4	C	303	GOL	O2-C2	-2.49	1.36	1.43
4	B	305	GOL	O2-C2	-2.19	1.37	1.43
4	B	306	GOL	O2-C2	-2.06	1.37	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	303	GOL	C3-C2-C1	-3.21	100.03	111.80
4	B	305	GOL	C3-C2-C1	-3.03	100.68	111.80
4	B	301	GOL	C3-C2-C1	-2.92	101.07	111.80
4	B	306	GOL	C3-C2-C1	-2.87	101.26	111.80
4	C	301	GOL	C3-C2-C1	-2.65	102.09	111.80
4	C	302	GOL	C3-C2-C1	-2.56	102.40	111.80
4	D	301	GOL	C3-C2-C1	-2.55	102.45	111.80
4	B	302	GOL	C3-C2-C1	-2.46	102.78	111.80
4	A	301	GOL	C3-C2-C1	-2.11	104.08	111.80

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GOL	C1-C2-C3-O3
4	A	302	GOL	O1-C1-C2-O2
4	B	305	GOL	O1-C1-C2-O2
4	B	305	GOL	O1-C1-C2-C3
4	B	305	GOL	C1-C2-C3-O3
4	C	302	GOL	C1-C2-C3-O3
4	C	303	GOL	O1-C1-C2-O2
4	C	303	GOL	O1-C1-C2-C3
4	D	301	GOL	O1-C1-C2-C3
4	D	301	GOL	O1-C1-C2-O2
4	A	302	GOL	O1-C1-C2-C3
4	B	302	GOL	C1-C2-C3-O3
4	C	302	GOL	O1-C1-C2-C3
4	C	302	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	C	304	PEG	O2-C3-C4-O4
4	B	305	GOL	O2-C2-C3-O3
4	C	302	GOL	O1-C1-C2-O2
4	A	301	GOL	O2-C2-C3-O3
4	B	306	GOL	O2-C2-C3-O3
6	C	304	PEG	C4-C3-O2-C2
4	B	302	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	GOL	2	0
4	B	305	GOL	2	0
4	C	301	GOL	2	0
4	C	302	GOL	2	0
4	B	306	GOL	3	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	210/225 (93%)	0.02	8 (3%)	44 43	16, 36, 55, 84	1 (0%)
1	C	216/225 (96%)	-0.12	3 (1%)	73 73	14, 30, 46, 82	5 (2%)
2	B	218/219 (99%)	-0.03	3 (1%)	73 73	16, 35, 54, 81	2 (0%)
2	D	219/219 (100%)	-0.16	5 (2%)	61 60	17, 32, 44, 98	1 (0%)
3	E	15/19 (78%)	0.13	1 (6%)	24 22	33, 37, 64, 65	0
3	F	17/19 (89%)	0.26	2 (11%)	9 8	28, 33, 81, 88	0
All	All	895/926 (96%)	-0.06	22 (2%)	58 58	14, 33, 53, 98	9 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	133[A]	THR	12.4
2	D	202[A]	THR	7.7
1	C	152[A]	VAL	5.0
2	D	34	GLY	3.8
3	F	149	SER	3.8
2	B	99	TYR	3.7
1	A	135	GLY	3.6
2	D	219	CYS	3.2
1	A	193	THR	3.1
2	D	99	TYR	3.0
3	E	150	PHE	3.0
1	A	192	GLY	2.9
3	F	150	PHE	2.9
1	A	127	ALA	2.9
1	A	134	SER	2.8
2	B	100	PRO	2.4
2	D	100	PRO	2.4
2	B	186	LEU	2.3
1	A	194	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	128	PRO	2.2
1	A	129	SER	2.1
1	C	216	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	305	6/6	0.67	0.14	49,70,85,90	0
4	GOL	C	301	6/6	0.78	0.15	59,72,85,90	0
4	GOL	B	306	6/6	0.80	0.12	40,62,78,82	0
4	GOL	A	302	6/6	0.80	0.11	54,68,80,85	0
4	GOL	C	303	6/6	0.81	0.13	53,70,84,87	0
4	GOL	A	301	6/6	0.83	0.11	43,55,77,84	0
6	PEG	C	304	7/7	0.84	0.11	50,61,74,82	0
4	GOL	C	302	6/6	0.85	0.12	39,63,75,86	0
4	GOL	D	301	6/6	0.90	0.10	31,47,57,57	0
4	GOL	B	301	6/6	0.92	0.14	30,39,43,47	0
4	GOL	B	302	6/6	0.93	0.08	43,52,54,54	0
5	ZN	D	302	1/1	0.99	0.02	37,37,37,37	0
5	ZN	D	303	1/1	0.99	0.02	33,33,33,33	0
5	ZN	E	201	1/1	0.99	0.03	50,50,50,50	0
5	ZN	F	201	1/1	0.99	0.02	42,42,42,42	0
5	ZN	B	304	1/1	0.99	0.02	42,42,42,42	0
5	ZN	B	307	1/1	1.00	0.01	36,36,36,36	0
5	ZN	B	303	1/1	1.00	0.01	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.