



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:48 AM UTC

PDB ID : 9CGS / pdb_00009cgs
Title : Structure of human MAIT A-F7 TCR in complex with human MR1-Pyridoxal-5'-phosphate
Authors : Awad, W.; Rossjohn, R.
Deposited on : 2024-06-30
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

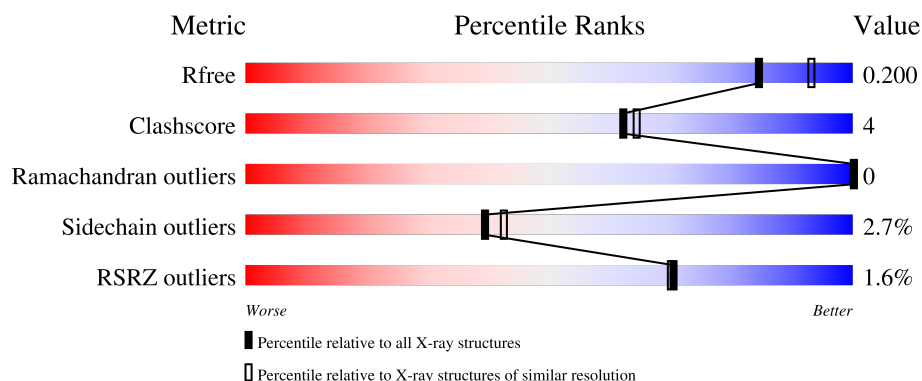
1 Overall quality at a glance

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	271	0% 85% 12% 3%
1	C	271	3% 85% 11% 4%
2	B	100	90% 8% 2%
2	F	100	95% 5%
3	D	204	3% 90% 5% 2%

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Mol	Chain	Length	Quality of chain
3	G	204	87% 10%
4	E	246	3% 85% 13%
4	H	246	% 88% 10%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13983 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 Major histocompatibility complex class I-related gene protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	P	S	6	9	0
			2234	1432	383	406	1	12			
1	C	267	Total	C	N	O	P	S	2	5	0
			2236	1438	383	403	1	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q95460
A	261	SER	CYS	conflict	UNP Q95460
C	0	MET	-	initiating methionine	UNP Q95460
C	261	SER	CYS	conflict	UNP Q95460

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			784	503	134	144	3			
2	F	100	Total	C	N	O	S	0	0	0
			812	518	138	152	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
F	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called TCR TRAV1-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	194	Total	C	N	O	S	0	4	0
			1498	957	237	294	10			

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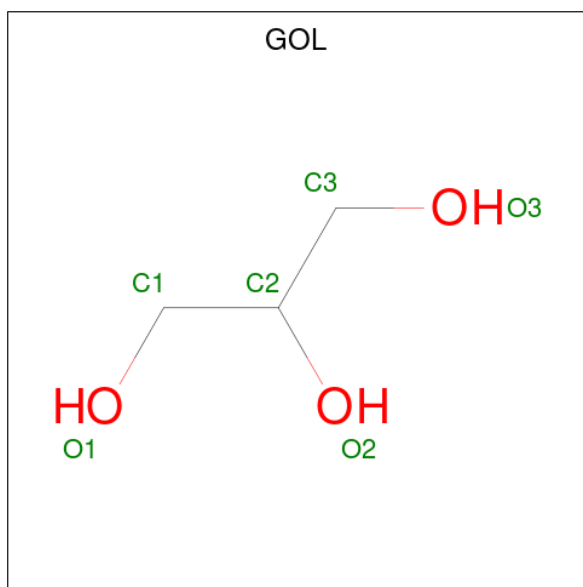
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	200	Total	C	N	O	S	1	9	0
			1600	1016	254	319	11			

- Molecule 4 is a protein called TCR TRBV6-1.

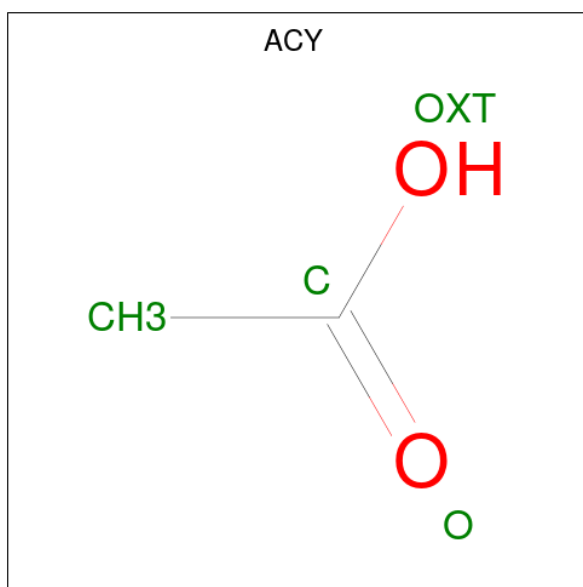
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	242	Total	C	N	O	S	0	4	0
			1887	1191	325	362	9			
4	H	245	Total	C	N	O	S	0	10	0
			1948	1231	336	368	13			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Na	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	164	Total	O	0	0
			164	164		
8	B	53	Total	O	0	0
			53	53		
8	C	156	Total	O	0	0
			156	156		
8	D	77	Total	O	0	0
			77	77		
8	E	68	Total	O	0	0
			68	68		
8	F	82	Total	O	0	0
			82	82		

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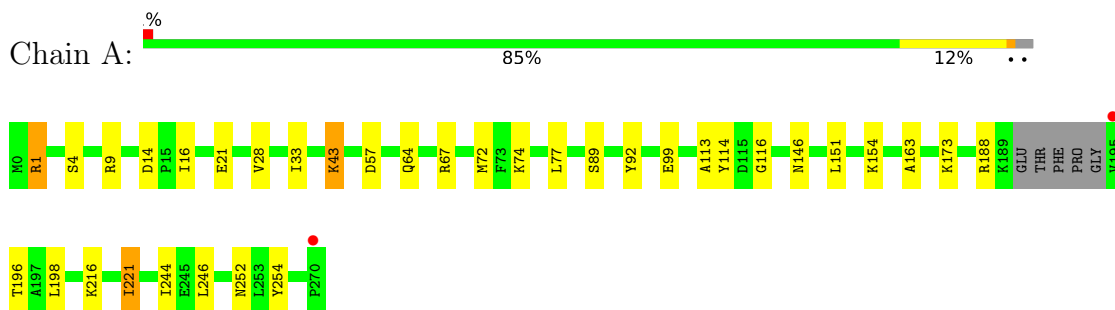
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	155	Total 155	O 155	0	0
8	H	202	Total 202	O 202	0	0

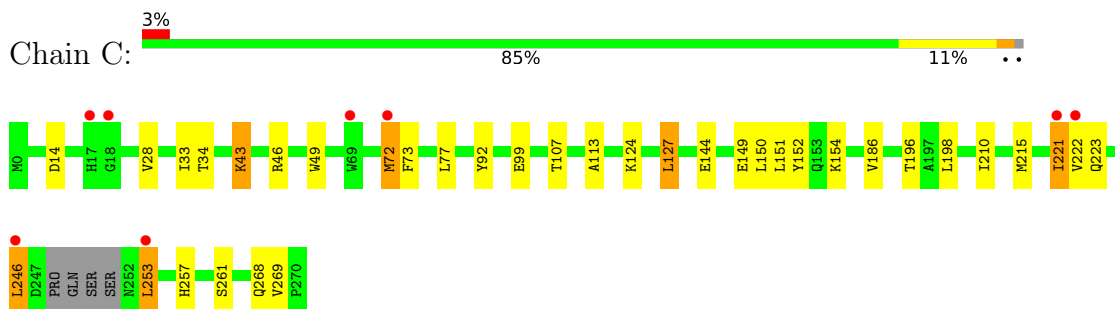
3 Residue-property plots

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

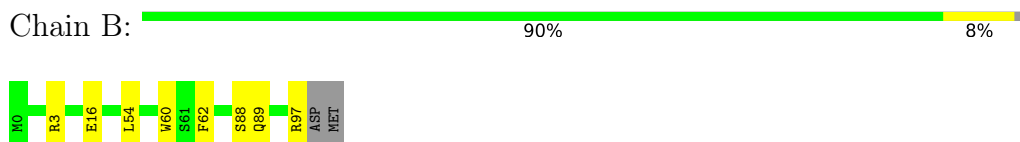
- Molecule 1: Major histocompatibility complex class I-related gene protein



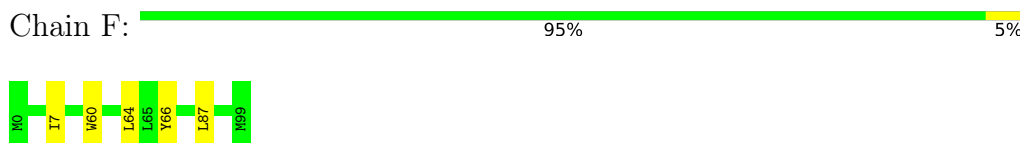
- Molecule 1: Major histocompatibility complex class I-related gene protein



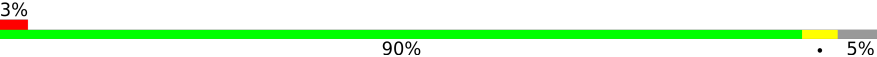
- Molecule 2: Beta-2-microglobulin

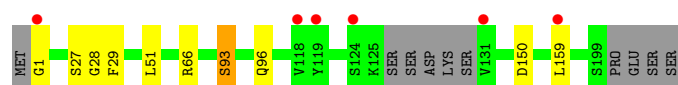


- Molecule 2: Beta-2-microglobulin



- Molecule 3: TCR TRAV1-2

Chain D:  3% 90% 5%



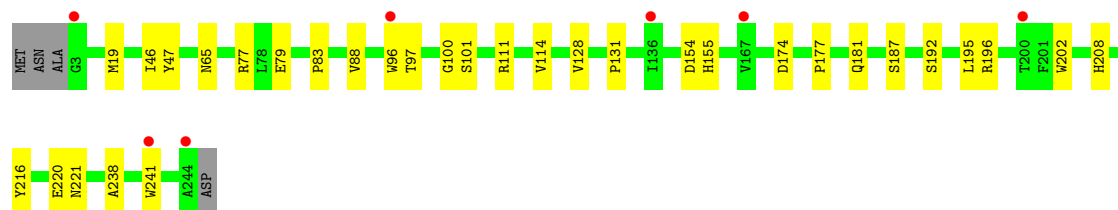
• Molecule 3: TCR TRAV1-2

Chain G:  87% 10% 3%



• Molecule 4: TCR TRBV6-1

Chain E:  3% 85% 13%



• Molecule 4: TCR TRBV6-1

Chain H:  88% 10% 2%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	216.80Å 70.08Å 142.88Å 90.00° 104.55° 90.00°	Depositor
Resolution (Å)	44.18 – 2.00 44.18 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (44.18-2.00) 92.0 (44.18-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.173 , 0.200 0.173 , 0.200	Depositor DCC
R_{free} test set	2000 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.9	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	0.97	EDS
Total number of atoms	13983	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: LLP, GOL, NA, ACY

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	0.14	0/2299	0.34	0/3124
1	C	0.16	0/2295	0.35	0/3121
2	B	0.12	0/807	0.35	0/1100
2	F	0.12	0/835	0.35	0/1135
3	D	0.13	0/1543	0.36	0/2096
3	G	0.13	0/1662	0.39	0/2252
4	E	0.12	0/1944	0.35	0/2652
4	H	0.14	0/2026	0.37	0/2757
All	All	0.14	0/13411	0.36	0/18237

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
4	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	99	GLU	Peptide

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	2234	0	2127	25	0
1	C	2236	0	2127	25	0
2	B	784	0	723	3	0
2	F	812	0	758	4	0
3	D	1498	0	1399	8	0
3	G	1600	0	1545	17	0
4	E	1887	0	1747	17	0
4	H	1948	0	1848	19	0
5	A	6	0	8	2	0
5	F	6	0	8	0	0
5	H	6	0	8	3	0
6	A	4	0	3	1	0
6	F	4	0	3	1	0
7	H	1	0	0	0	0
8	A	164	0	0	2	0
8	B	53	0	0	0	0
8	C	156	0	0	2	0
8	D	77	0	0	0	0
8	E	68	0	0	1	0
8	F	82	0	0	1	0
8	G	155	0	0	3	0
8	H	202	0	0	4	0
All	All	13983	0	12304	104	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 4.

All (104) 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:F:7:ILE:H	6:F:202:ACY:H3	1.41	0.84
1:A:43:LLP:O3	1:A:43:LLP:NZ	2.12	0.83
1:A:67:ARG:HH12	5:H:301:GOL:H31	1.50	0.74
3:G:19:GLN:NE2	8:G:303:HOH:O	2.21	0.73
1:C:221:ILE:HG12	1:C:223:GLN:H	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLN:HE22	5:H:301:GOL:H32	1.56	0.70
4:E:155:HIS:HB3	4:E:216:TYR:HB2	1.73	0.69
1:A:163:ALA:HB3	5:A:501:GOL:H12	1.76	0.68
4:H:155:HIS:ND1	8:H:401:HOH:O	2.27	0.67
4:H:19[A]:MET:HE2	4:H:112:LEU:HD11	1.79	0.64
1:C:43:LLP:NZ	1:C:43:LLP:O3	2.30	0.64
3:G:95:TYR:OH	8:G:301:HOH:O	2.14	0.64
1:C:99:GLU:HB2	1:C:107:THR:HG22	1.81	0.63
1:A:146:ASN:OD1	8:A:601:HOH:O	2.15	0.63
4:H:13:LEU:HD21	4:H:19[A]:MET:HG3	1.79	0.62
3:D:159:LEU:HD21	4:E:196:ARG:HB2	1.80	0.62
1:A:114:TYR:HB3	6:A:502:ACY:H3	1.86	0.58
4:E:111:ARG:NH1	8:E:303:HOH:O	2.35	0.58
2:F:87:LEU:O	8:F:301:HOH:O	2.17	0.57
4:H:65[A]:ASN:ND2	8:H:404:HOH:O	2.38	0.56
1:C:124:LYS:NZ	8:C:1201:HOH:O	2.38	0.56
1:A:77:LEU:HD13	1:A:92:TYR:HB2	1.86	0.55
4:E:65[A]:ASN:OD1	4:E:77:ARG:NH1	2.37	0.55
1:A:9:ARG:NE	1:A:43:LLP:OP3	2.26	0.55
3:G:91:LYS:HG2	3:G:95:TYR:HA	1.89	0.54
4:H:174:ASP:HB2	4:H:191:LEU:HD12	1.89	0.54
3:D:28:GLY:HA3	3:D:93[B]:SER:HB3	1.90	0.53
1:C:196:THR:HB	1:C:246:LEU:HB2	1.92	0.52
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.45	0.52
3:G:28:GLY:HA3	3:G:93[A]:SER:OG	2.10	0.52
1:A:151:LEU:HD22	3:G:51:LEU:HD12	1.91	0.51
1:C:222:VAL:HA	4:H:200:THR:HG21	1.91	0.51
4:E:128:VAL:HG23	4:E:238:ALA:HB3	1.92	0.51
3:G:4[A]:ILE:HD11	3:G:90:VAL:HB	1.93	0.51
3:G:159[A]:LEU:HB3	4:H:172[A]:CYS:HB2	1.93	0.51
3:G:28:GLY:HA3	3:G:93[B]:SER:HB3	1.93	0.50
1:A:196:THR:HG22	1:A:246:LEU:HD12	1.93	0.50
1:C:215:MET:HG3	1:C:257:HIS:CD2	2.46	0.50
1:C:28:VAL:HG23	1:C:33:ILE:HD13	1.93	0.49
1:C:221:ILE:HG12	1:C:223:GLN:N	2.26	0.49
1:C:77:LEU:HD13	1:C:92:TYR:HB2	1.93	0.49
1:C:186:VAL:HG11	1:C:269:VAL:HG22	1.94	0.49
1:C:198:LEU:HD13	1:C:269:VAL:HG21	1.93	0.49
4:H:65[B]:ASN:ND2	8:H:409:HOH:O	2.45	0.49
1:A:21:GLU:OE2	1:A:74:LYS:NZ	2.40	0.49
3:G:108[B]:LYS:HB3	3:G:139:SER:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LYS:HB2	1:A:221:ILE:HD13	1.95	0.48
1:A:163:ALA:CB	5:A:501:GOL:H12	2.42	0.48
2:F:64:LEU:HD13	2:F:66:TYR:HE1	1.78	0.48
3:G:41:GLU:OE1	8:G:302:HOH:O	2.20	0.47
4:H:120:ASN:HB2	8:H:413:HOH:O	2.13	0.47
1:A:72:MET:HE2	4:H:96:TRP:CG	2.49	0.47
4:E:208:HIS:HB2	4:E:241:TRP:CZ3	2.50	0.47
1:A:252:ASN:HB2	1:A:254:TYR:CE2	2.50	0.47
4:H:69:LEU:HD22	4:H:69:LEU:H	1.80	0.47
1:C:152:TYR:CD1	4:E:100:GLY:HA3	2.50	0.47
1:C:113:ALA:HB2	2:F:60:TRP:CE2	2.49	0.47
4:E:174:ASP:OD2	4:E:192:SER:OG	2.31	0.47
3:G:4[B]:ILE:HD11	3:G:100:GLY:HA3	1.96	0.47
4:H:11:GLN:HG2	4:H:19[B]:MET:HE3	1.97	0.47
1:A:67:ARG:NH1	5:H:301:GOL:H31	2.25	0.46
3:G:121:LEU:HD11	3:G:133:LEU:HB2	1.98	0.46
4:E:88:VAL:HG22	4:E:111:ARG:HD3	1.98	0.46
1:C:151:LEU:HD22	3:D:51:LEU:HD12	1.97	0.45
1:C:34:THR:HB	1:C:43:LLP:HE3	1.99	0.45
1:C:43:LLP:H5'2	8:C:1211:HOH:O	2.17	0.45
1:C:253:LEU:HD23	1:C:253:LEU:HA	1.76	0.44
2:B:54:LEU:HD11	2:B:62:PHE:HB3	1.99	0.44
3:G:138[A]:ASP:OD1	3:G:139:SER:N	2.49	0.44
4:H:128:VAL:HG23	4:H:238:ALA:HB3	2.00	0.44
3:D:1:GLY:N	3:D:27:SER:H	2.16	0.44
4:H:86:THR:HG23	4:H:113:THR:HA	1.99	0.44
1:A:154:LYS:HD3	3:G:51:LEU:HD11	1.99	0.44
4:E:83:PRO:HA	4:E:114:VAL:HB	1.99	0.44
1:C:72:MET:HB3	4:E:96:TRP:CZ2	2.53	0.43
3:D:28:GLY:HA3	3:D:93[A]:SER:OG	2.18	0.43
1:C:46:ARG:HA	1:C:46:ARG:HD3	1.77	0.43
1:C:210:ILE:O	4:H:206:ARG:HG2	2.18	0.43
4:H:13:LEU:HD21	4:H:19[B]:MET:HE3	1.99	0.43
4:H:131:PRO:HD3	4:H:144:LEU:HG	2.01	0.43
1:A:116:GLY:O	2:B:3:ARG:NH2	2.51	0.43
3:G:108[A]:LYS:HB3	3:G:139:SER:HB3	1.99	0.43
3:D:29:PHE:HB3	3:D:66[B]:ARG:HH21	1.83	0.43
1:A:28:VAL:HG23	1:A:33:ILE:HD13	1.99	0.43
1:C:149:GLU:OE1	4:E:101:SER:OG	2.32	0.42
1:A:1[A]:ARG:HD2	8:A:729:HOH:O	2.18	0.42
1:A:4:SER:HB3	1:A:99:GLU:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LYS:HE3	1:A:173:LYS:HB2	1.68	0.42
1:C:127:LEU:HD11	1:C:154:LYS:HD2	2.02	0.41
1:C:144:GLU:HA	1:C:150:LEU:HD11	2.03	0.41
3:D:66[B]:ARG:HH11	3:D:66[B]:ARG:HB3	1.86	0.41
4:H:154:ASP:CG	4:H:177:PRO:HG3	2.45	0.41
4:H:31:SER:HA	4:H:49:SER:O	2.21	0.41
1:A:14:ASP:HB3	1:A:89:SER:HB2	2.02	0.41
3:D:1:GLY:H1	3:D:27:SER:H	1.69	0.41
4:E:131:PRO:HD2	4:E:202:TRP:CZ2	2.56	0.41
4:E:154[A]:ASP:CG	4:E:177:PRO:HG2	2.46	0.41
1:C:49:TRP:CD1	1:C:49:TRP:H	2.38	0.41
3:G:132:CYS:SG	3:G:182[B]:CYS:HB3	2.59	0.41
4:E:46:ILE:HG22	4:E:47:TYR:HD1	1.86	0.40
3:G:125:LYS:HB3	3:G:125:LYS:HE2	1.90	0.40
4:E:181:GLN:O	4:E:187:SER:HB2	2.20	0.40
1:A:188:ARG:HG2	1:A:198:LEU:HD23	2.04	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	270/271 (100%)	265 (98%)	5 (2%)	0	100	100
1	C	267/271 (98%)	261 (98%)	6 (2%)	0	100	100
2	B	96/100 (96%)	96 (100%)	0	0	100	100
2	F	98/100 (98%)	98 (100%)	0	0	100	100
3	D	194/204 (95%)	186 (96%)	8 (4%)	0	100	100
3	G	207/204 (102%)	204 (99%)	3 (1%)	0	100	100
4	E	244/246 (99%)	239 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	253/246 (103%)	250 (99%)	3 (1%)	0	100	100
All	All	1629/1642 (99%)	1599 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	237/240 (99%)	230 (97%)	7 (3%)	36	38
1	C	235/240 (98%)	226 (96%)	9 (4%)	29	29
2	B	83/95 (87%)	79 (95%)	4 (5%)	23	21
2	F	89/95 (94%)	89 (100%)	0	100	100
3	D	160/181 (88%)	156 (98%)	4 (2%)	42	45
3	G	183/181 (101%)	178 (97%)	5 (3%)	39	42
4	E	198/212 (93%)	192 (97%)	6 (3%)	36	38
4	H	210/212 (99%)	202 (96%)	8 (4%)	29	29
All	All	1395/1456 (96%)	1352 (97%)	43 (3%)	39	37

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1[A]	ARG
1	A	1[B]	ARG
1	A	16[A]	ILE
1	A	16[B]	ILE
1	A	57	ASP
1	A	221	ILE
1	A	244	ILE
2	B	16	GLU
2	B	88	SER
2	B	89	GLN

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Mol	Chain	Res	Type
2	B	97	ARG
1	C	14	ASP
1	C	72	MET
1	C	73	PHE
1	C	127	LEU
1	C	221	ILE
1	C	246	LEU
1	C	253	LEU
1	C	261	SER
1	C	268	GLN
3	D	93[A]	SER
3	D	93[B]	SER
3	D	96	GLN
3	D	150	ASP
4	E	19	MET
4	E	79	GLU
4	E	97	THR
4	E	195	LEU
4	E	220	GLU
4	E	221	ASN
3	G	93[A]	SER
3	G	93[B]	SER
3	G	162	ARG
3	G	164	MET
3	G	199	SER
4	H	19[A]	MET
4	H	19[B]	MET
4	H	65[A]	ASN
4	H	65[B]	ASN
4	H	112	LEU
4	H	132	SER
4	H	184	LEU
4	H	212	GLN

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

Mol	Chain	Res	Type
1	A	17	HIS
1	A	42	GLN
1	A	64	GLN
2	B	17	ASN
1	C	123	ASN

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Mol	Chain	Res	Type
1	C	137	HIS
1	C	217	ASN
3	D	37	GLN
3	D	38	HIS
3	D	96	GLN
4	E	37	GLN
2	F	13	HIS
3	G	19	GLN
3	G	36	GLN
3	G	79	GLN
3	G	94	ASN
4	H	22	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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$
1	LLP	C	43	1	23,24,25	1.21	1 (4%)	25,32,34	2.26	4 (16%)
1	LLP	A	43	1	23,24,25	1.42	3 (13%)	25,32,34	3.47	3 (12%)

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
1	LLP	C	43	1	-	2/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	43	1	-	7/16/17/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	43	LLP	C4'-NZ	4.89	1.43	1.27
1	A	43	LLP	C4'-NZ	4.84	1.43	1.27
1	A	43	LLP	C3-C2	2.60	1.43	1.41
1	A	43	LLP	C2'-C2	-2.34	1.46	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	LLP	CE-NZ-C4'	-14.67	71.73	118.72
1	C	43	LLP	CE-NZ-C4'	-9.73	87.54	118.72
1	A	43	LLP	OP4-C5'-C5	6.59	121.70	109.36
1	A	43	LLP	C4-C4'-NZ	-4.75	102.12	124.04
1	C	43	LLP	C4-C4'-NZ	-3.22	109.18	124.04
1	C	43	LLP	C4-C3-C2	-2.42	118.78	120.14
1	C	43	LLP	OP4-C5'-C5	2.39	113.84	109.36

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	43	LLP	C5'-OP4-P-OP2
1	A	43	LLP	C5'-OP4-P-OP3
1	A	43	LLP	N-CA-CB-CG
1	A	43	LLP	C-CA-CB-CG
1	A	43	LLP	CA-CB-CG-CD
1	C	43	LLP	CA-CB-CG-CD
1	A	43	LLP	C5'-OP4-P-OP1
1	C	43	LLP	CG-CD-CE-NZ
1	A	43	LLP	C4-C4'-NZ-CE

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	43	LLP	3	0
1	A	43	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
5	GOL	A	501	-	5,5,5	0.36	0	5,5,5	0.53	0
6	ACY	A	502	-	3,3,3	1.14	0	3,3,3	1.21	0
5	GOL	F	201	-	5,5,5	0.41	0	5,5,5	0.35	0
6	ACY	F	202	-	3,3,3	1.12	0	3,3,3	1.19	0
5	GOL	H	301	-	5,5,5	0.39	0	5,5,5	0.40	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
5	GOL	A	501	-	-	3/4/4/4	-
5	GOL	H	301	-	-	0/4/4/4	-
5	GOL	F	201	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GOL	C1-C2-C3-O3
5	A	501	GOL	O2-C2-C3-O3
5	A	501	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GOL	2	0
6	A	502	ACY	1	0
6	F	202	ACY	1	0
5	H	301	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	265/271 (97%)	-0.07	2 (0%) 82 82	18, 41, 78, 100	15 (5%)
1	C	266/271 (98%)	-0.01	8 (3%) 52 51	24, 41, 68, 88	14 (5%)
2	B	98/100 (98%)	0.22	0 100 100	34, 59, 90, 95	2 (2%)
2	F	100/100 (100%)	-0.17	0 100 100	30, 45, 67, 72	1 (1%)
3	D	194/204 (95%)	0.34	6 (3%) 51 50	24, 56, 98, 123	10 (5%)
3	G	200/204 (98%)	-0.12	1 (0%) 87 87	21, 38, 64, 79	16 (8%)
4	E	242/246 (98%)	0.29	7 (2%) 53 52	21, 56, 93, 111	8 (3%)
4	H	245/246 (99%)	-0.13	2 (0%) 82 82	22, 39, 63, 96	15 (6%)
All	All	1610/1642 (98%)	0.04	26 (1%) 70 70	18, 44, 83, 123	81 (5%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	96	TRP	3.4
1	C	221	ILE	3.4
1	A	195	VAL	3.3
4	H	245	ASP	2.9
3	D	131	VAL	2.8
1	C	18	GLY	2.8
4	E	244	ALA	2.8
3	D	159	LEU	2.6
3	D	1	GLY	2.6
1	C	222	VAL	2.5
3	G	200	PRO	2.4
1	C	72	MET	2.3
1	C	69[A]	TRP	2.3
4	E	136	ILE	2.2
1	A	270	PRO	2.2
4	E	200	THR	2.2

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Mol	Chain	Res	Type	RSRZ
4	E	167	VAL	2.2
1	C	246	LEU	2.1
4	H	99	GLU	2.1
1	C	17	HIS	2.1
1	C	253	LEU	2.1
3	D	119	TYR	2.1
3	D	118	VAL	2.1
4	E	241	TRP	2.1
4	E	3	GLY	2.0
3	D	124	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	C	43	24/25	0.93	0.10	36,46,61,74	0
1	LLP	A	43	24/25	0.94	0.10	35,38,61,68	1

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
5	GOL	H	301	6/6	0.89	0.10	33,47,54,63	0
6	ACY	F	202	4/4	0.89	0.12	27,45,55,57	0
5	GOL	A	501	6/6	0.90	0.12	47,54,61,63	0
6	ACY	A	502	4/4	0.92	0.10	40,58,60,66	0
5	GOL	F	201	6/6	0.96	0.08	35,35,38,39	0
7	NA	H	302	1/1	0.98	0.05	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.