



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:54 AM UTC

PDB ID : 4Z76 / pdb_00004z76
Title : Weak TCR binding to an unstable insulin epitope drives type 1 diabetes
Authors : Rizkallah, P.J.; Cole, D.K.
Deposited on : 2015-04-06
Resolution : 1.88 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

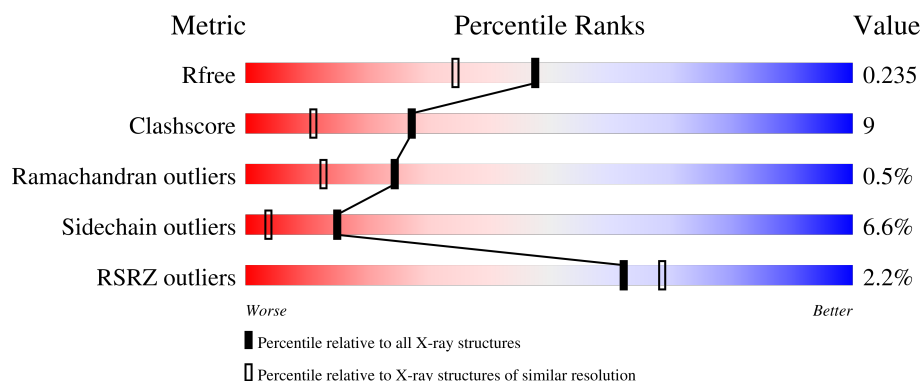
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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.



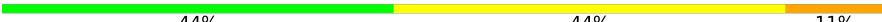
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	277	2% 82% 15% .
1	D	277	4% 81% 16% .
2	B	100	80% 16% .
2	E	100	84% 11% 5%
3	C	9	56% 44%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	9	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (44%), yellow (44%), and orange (11%).

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7048 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 H-2 class I histocompatibility antigen, K-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	2	0
			2304	1460	409	427	8			
1	D	277	Total	C	N	O	S	0	5	0
			2331	1476	417	430	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01902
A	114	HIS	GLN	conflict	UNP P01902
A	276	PRO	-	expression tag	UNP P01902
D	0	MET	-	initiating methionine	UNP P01902
D	114	HIS	GLN	conflict	UNP P01902
D	276	PRO	-	expression tag	UNP P01902

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	0	1	0
			848	539	145	160	4			

There are 2 discrepancies between the modelled and reference sequences:

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

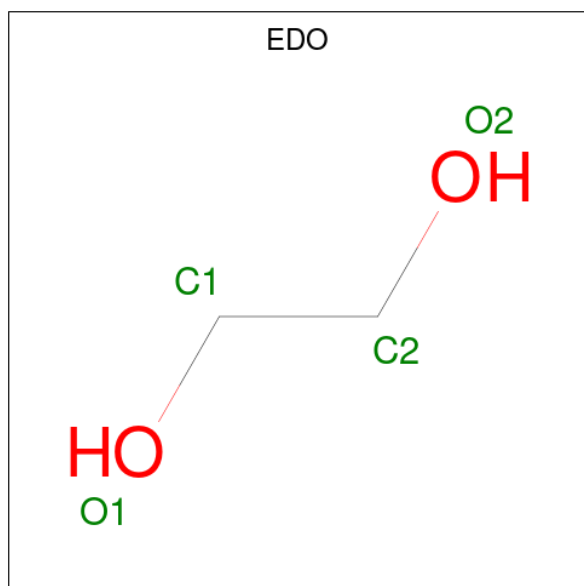
- Molecule 3 is a protein called Insulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total 73	C 47	N 12	O 13	S 1	0	0	0
3	F	9	Total 73	C 47	N 12	O 13	S 1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

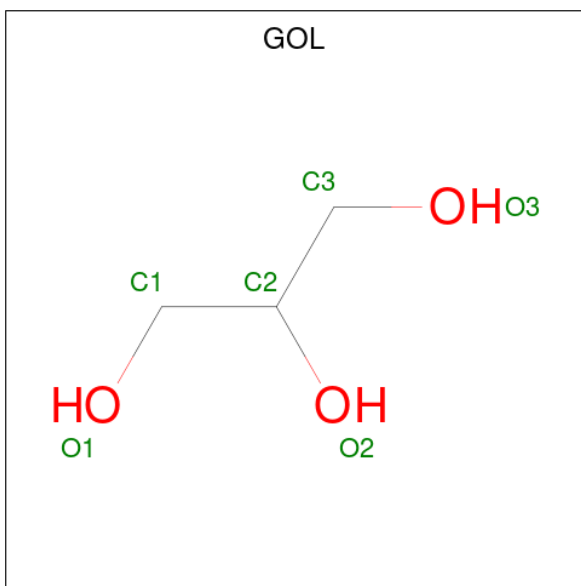
Chain	Residue	Modelled	Actual	Comment	Reference
C	9	VAL	GLY	conflict	UNP P01308
F	9	VAL	GLY	conflict	UNP P01308

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



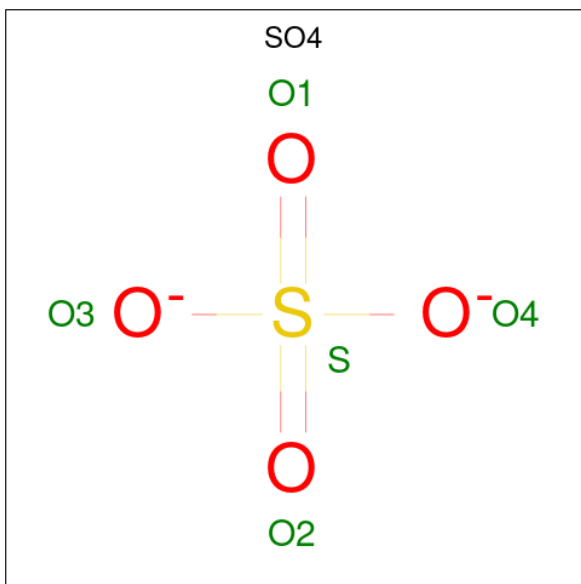
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- 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	A	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	137	Total O 137 137	0	0
7	B	82	Total O 82 82	0	0
7	C	3	Total O 3 3	0	0
7	D	163	Total O 163 163	0	0
7	E	74	Total O 74 74	0	0

Continued on next page...

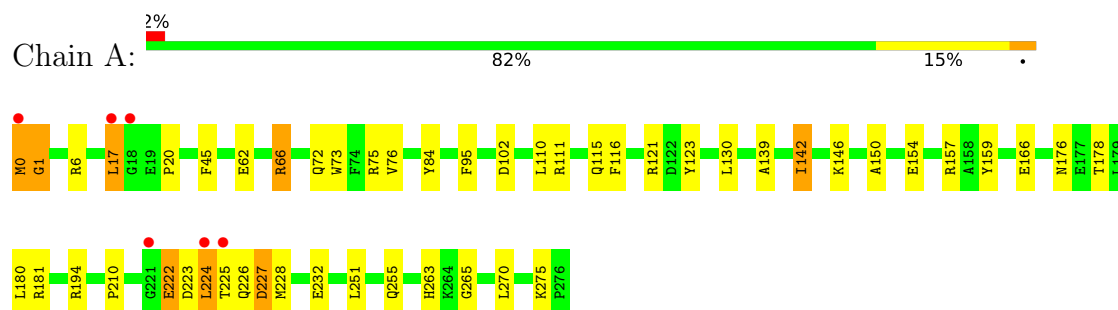
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	6	Total	O	0	0
			6	6		

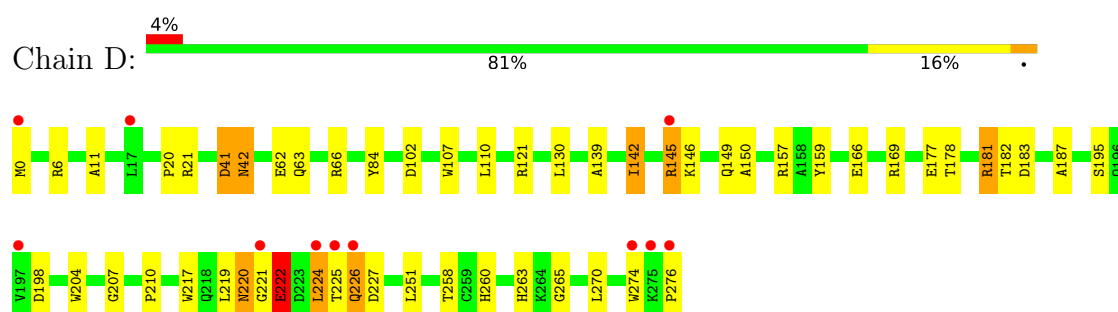
3 Residue-property plots [i](#)

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.

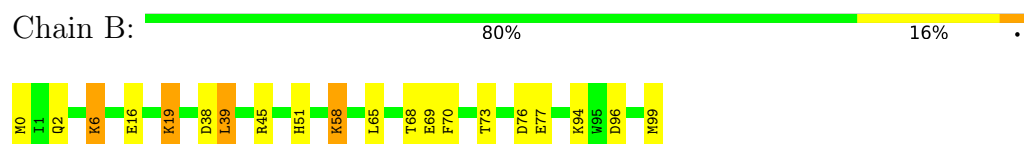
- Molecule 1: H-2 class I histocompatibility antigen, K-D alpha chain



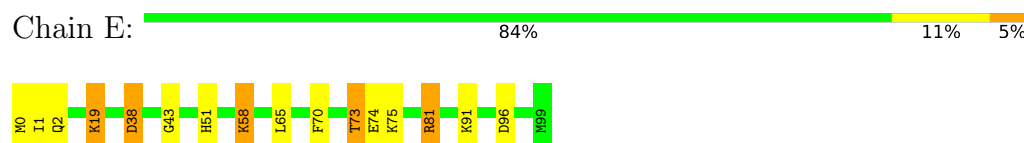
- Molecule 1: H-2 class I histocompatibility antigen, K-D alpha chain



- Molecule 2: Beta-2-microglobulin



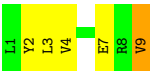
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Insulin



● Molecule 3: Insulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.99Å 62.37Å 72.31Å 69.81° 85.76° 87.05°	Depositor
Resolution (Å)	38.27 – 1.88 38.27 – 1.88	Depositor EDS
% Data completeness (in resolution range)	89.3 (38.27-1.88) 89.3 (38.27-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.184 , 0.230 0.191 , 0.235	Depositor DCC
R_{free} test set	2886 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.2	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	0.95	EDS
Total number of atoms	7048	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.46% 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

5.1 Standard geometry

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

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	0.99	3/2374 (0.1%)	1.01	3/3228 (0.1%)
1	D	0.99	0/2401	0.99	1/3264 (0.0%)
2	B	1.01	0/860	0.95	1/1162 (0.1%)
2	E	0.95	0/871	0.91	0/1176
3	C	1.01	0/73	1.10	0/96
3	F	1.19	0/73	1.21	1/96 (1.0%)
All	All	0.99	3/6652 (0.0%)	0.98	6/9022 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	TYR	CA-C	6.60	1.57	1.52
1	A	76	VAL	N-CA	-5.43	1.40	1.46
1	A	116	PHE	C-O	5.35	1.30	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	GLY	N-CA-C	10.29	133.33	112.34
1	A	115	GLN	N-CA-CB	-6.20	99.99	111.52
1	D	222	GLU	N-CA-C	5.55	122.62	110.80
3	F	9	VAL	N-CA-CB	-5.47	102.20	111.50
1	A	17	LEU	N-CA-C	-5.34	106.95	112.93
2	B	6	LYS	CD-CE-NZ	5.33	128.96	111.90

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	2304	0	2170	34	0
1	D	2331	0	2202	48	0
2	B	837	0	803	15	0
2	E	848	0	815	18	0
3	C	73	0	78	4	0
3	F	73	0	78	4	0
4	A	8	0	12	2	0
4	B	12	0	18	2	0
4	E	4	0	6	2	0
5	A	12	0	16	2	0
5	E	6	0	8	1	0
6	A	5	0	0	1	0
6	B	15	0	0	0	0
6	D	30	0	0	1	0
6	E	25	0	0	3	0
7	A	137	0	0	3	0
7	B	82	0	0	6	0
7	C	3	0	0	0	0
7	D	163	0	0	7	0
7	E	74	0	0	5	0
7	F	6	0	0	0	0
All	All	7048	0	6206	117	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 9.

All (117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142[A]:ILE:HD12	1:D:145[A]:ARG:HH12	1.15	1.05
2:E:81[A]:ARG:HH11	2:E:81[A]:ARG:HG2	1.28	0.95
2:E:1:ILE:HA	6:E:106:SO4:O3	1.72	0.89
1:D:142[A]:ILE:HD12	1:D:145[A]:ARG:NH1	1.91	0.83
1:D:195:SER:HB2	1:D:198:ASP:HB2	1.63	0.80
2:B:38:ASP:OD1	2:B:45:ARG:CZ	2.31	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ARG:NH2	1:D:102:ASP:OD1	2.15	0.76
1:D:181[B]:ARG:NH2	1:D:183:ASP:OD2	2.19	0.75
1:A:227:ASP:N	1:A:227:ASP:OD1	2.19	0.73
2:E:81[A]:ARG:HH11	2:E:81[A]:ARG:CG	2.00	0.72
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.18	0.72
1:A:263:HIS:CD2	1:A:265:GLY:H	2.07	0.72
1:D:263:HIS:CD2	1:D:265:GLY:H	2.08	0.71
1:D:63:GLN:HE22	3:F:2:TYR:H	1.38	0.71
1:D:219:LEU:O	1:D:221:GLY:N	2.25	0.70
1:A:20:PRO:HG3	6:A:305:SO4:O4	1.92	0.69
1:D:20:PRO:HG3	6:D:306:SO4:O3	1.91	0.69
1:A:142[A]:ILE:HD12	1:A:142[A]:ILE:C	2.19	0.68
1:A:154:GLU:OE1	1:A:157:ARG:NH2	2.26	0.67
1:A:263:HIS:HD2	1:A:265:GLY:H	1.41	0.67
1:D:182[B]:THR:OG1	7:D:401:HOH:O	2.07	0.66
1:A:142[A]:ILE:HD12	1:A:142[A]:ILE:O	1.96	0.64
1:D:221:GLY:O	1:D:222:GLU:HB3	1.98	0.64
2:E:2:GLN:OE1	7:E:201:HOH:O	2.15	0.63
1:A:62:GLU:O	1:A:66:ARG:HG2	1.99	0.63
2:B:16:GLU:HB2	2:B:19:LYS:HD3	1.80	0.63
1:A:159:TYR:CG	3:C:3:LEU:HD22	2.35	0.62
2:E:43:GLY:N	6:E:103:SO4:O2	2.33	0.62
1:A:223:ASP:OD1	1:A:223:ASP:C	2.43	0.61
1:D:178:THR:O	1:D:181[B]:ARG:HG3	2.02	0.60
1:D:263:HIS:HD2	1:D:265:GLY:H	1.49	0.60
2:B:2:GLN:NE2	7:B:402:HOH:O	2.33	0.59
7:A:515:HOH:O	1:D:226:GLN:HA	2.01	0.59
1:A:130:LEU:HB2	1:A:157:ARG:HD2	1.84	0.58
1:D:145[A]:ARG:HH11	1:D:146:LYS:HG3	1.69	0.58
5:E:102:GOL:H31	7:E:270:HOH:O	2.02	0.58
1:D:107:TRP:CE2	1:D:169:ARG:HD3	2.38	0.57
1:A:139:ALA:O	1:A:142[A]:ILE:HG23	2.05	0.56
2:B:58:LYS:HB2	2:B:58:LYS:NZ	2.20	0.56
1:A:223:ASP:OD1	1:A:224:LEU:N	2.39	0.56
1:D:220:ASN:ND2	7:D:405:HOH:O	2.32	0.56
1:A:121:ARG:HH11	2:B:0:MET:N	2.04	0.56
1:A:146:LYS:NZ	7:A:401:HOH:O	2.35	0.56
1:D:139:ALA:O	1:D:142[A]:ILE:HG23	2.06	0.55
1:A:159:TYR:CD2	3:C:3:LEU:HD22	2.42	0.55
2:E:38:ASP:CB	7:E:237:HOH:O	2.54	0.55
1:D:159:TYR:CG	3:F:3:LEU:HD22	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:O	1:A:225:THR:C	2.49	0.54
2:B:73:THR:OG1	2:B:76:ASP:OD2	2.20	0.54
1:D:221:GLY:HA3	7:D:560:HOH:O	2.07	0.54
1:D:226:GLN:NE2	7:D:406:HOH:O	2.34	0.54
1:D:274:TRP:CZ2	1:D:276:PRO:HA	2.44	0.53
2:B:16:GLU:CB	2:B:19:LYS:HD3	2.38	0.53
4:B:302:EDO:H12	7:B:439:HOH:O	2.07	0.53
2:E:58:LYS:N	6:E:105:SO4:O3	2.40	0.53
1:D:62:GLU:OE1	1:D:66:ARG:HD2	2.08	0.53
1:D:107:TRP:CZ2	1:D:169:ARG:HD3	2.45	0.51
1:A:111:ARG:NH2	7:A:407:HOH:O	2.44	0.51
1:D:130:LEU:HB2	1:D:157:ARG:HD2	1.92	0.51
1:D:274:TRP:CH2	1:D:276:PRO:HA	2.46	0.50
1:D:121:ARG:HH11	2:E:0:MET:H2	1.59	0.50
5:A:304:GOL:H11	7:D:533:HOH:O	2.11	0.50
2:B:38:ASP:OD1	2:B:45:ARG:NH2	2.44	0.50
2:B:99:MET:O	4:B:302:EDO:H21	2.12	0.50
2:B:39:LEU:HD23	2:B:68:THR:HG22	1.94	0.49
1:D:217:TRP:H	1:D:224:LEU:HD23	1.77	0.49
1:A:84:TYR:CZ	1:A:142[A]:ILE:HG12	2.48	0.48
1:D:207:GLY:O	7:D:402:HOH:O	2.20	0.48
2:E:38:ASP:OD1	2:E:81[A]:ARG:NH1	2.46	0.48
1:A:232:GLU:CG	4:A:301:EDO:H12	2.44	0.48
1:A:62:GLU:OE2	1:A:66:ARG:HD3	2.12	0.48
1:A:73:TRP:CD1	3:C:8:ARG:HD3	2.48	0.48
1:D:177:GLU:O	1:D:181[A]:ARG:CG	2.62	0.48
1:D:178:THR:O	1:D:181[B]:ARG:NE	2.44	0.48
2:E:91:LYS:HD3	4:E:101:EDO:C1	2.44	0.48
1:D:20:PRO:HD2	7:D:467:HOH:O	2.14	0.47
1:D:177:GLU:O	1:D:181[A]:ARG:HG3	2.14	0.47
1:A:72:GLN:HE22	1:A:75:ARG:NH1	2.14	0.47
2:E:73:THR:CG2	2:E:74:GLU:N	2.77	0.47
2:B:94:LYS:NZ	7:B:406:HOH:O	2.47	0.46
2:E:73:THR:HG22	2:E:75:LYS:H	1.79	0.46
2:E:81[A]:ARG:CG	2:E:81[A]:ARG:NH1	2.67	0.46
1:A:222:GLU:N	1:A:222:GLU:OE2	2.49	0.46
2:E:38:ASP:HB2	7:E:237:HOH:O	2.16	0.46
1:A:0:MET:HE3	1:A:180:LEU:O	2.16	0.45
1:D:181[A]:ARG:CD	1:D:181[A]:ARG:C	2.89	0.45
1:A:210:PRO:O	1:A:263:HIS:HE1	2.00	0.45
1:D:84:TYR:CZ	1:D:142[A]:ILE:HG12	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:N	1:A:224:LEU:CD2	2.81	0.44
2:E:51:HIS:HA	2:E:65:LEU:O	2.17	0.44
2:E:91:LYS:HD3	4:E:101:EDO:H12	2.00	0.44
1:D:181[A]:ARG:CZ	1:D:183:ASP:OD1	2.65	0.44
1:D:258:THR:OG1	1:D:260:HIS:HE1	2.01	0.44
1:A:150:ALA:HB2	3:C:7:GLU:HG3	1.99	0.44
4:A:301:EDO:C2	7:B:422:HOH:O	2.65	0.44
1:D:224:LEU:C	1:D:224:LEU:HD22	2.43	0.44
2:B:77:GLU:HG3	7:B:432:HOH:O	2.18	0.43
2:E:19:LYS:CD	7:E:206:HOH:O	2.66	0.43
1:A:142[A]:ILE:C	1:A:142[A]:ILE:CD1	2.83	0.43
1:D:150:ALA:HB2	3:F:7:GLU:HG3	2.01	0.43
1:D:41:ASP:OD1	1:D:41:ASP:N	2.42	0.43
2:E:96:ASP:OD1	2:E:96:ASP:C	2.61	0.43
2:B:51:HIS:HA	2:B:65:LEU:O	2.19	0.43
1:D:150:ALA:CB	3:F:7:GLU:HG3	2.48	0.43
2:B:69:GLU:HG2	7:B:469:HOH:O	2.19	0.42
2:B:96:ASP:OD1	2:B:96:ASP:C	2.62	0.42
1:D:11:ALA:HA	1:D:21:ARG:O	2.19	0.42
1:D:182[A]:THR:HG21	1:D:265:GLY:CA	2.49	0.42
1:D:187:ALA:HA	1:D:204:TRP:O	2.19	0.42
1:D:166:GLU:O	1:D:169:ARG:HB2	2.20	0.41
1:A:178:THR:O	1:A:181:ARG:HG2	2.20	0.41
1:D:210:PRO:O	1:D:263:HIS:HE1	2.03	0.41
1:A:139:ALA:HB2	5:A:304:GOL:H31	2.03	0.41
1:A:176:ASN:HB2	1:A:180:LEU:HD12	2.02	0.41
1:A:222:GLU:N	1:A:222:GLU:CD	2.79	0.41
1:D:42:ASN:O	1:D:42:ASN:CG	2.63	0.41
1:D:107:TRP:CZ2	1:D:169:ARG:CD	3.04	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	277/277 (100%)	266 (96%)	10 (4%)	1 (0%)	30	18
1	D	280/277 (101%)	268 (96%)	9 (3%)	3 (1%)	11	3
2	B	98/100 (98%)	98 (100%)	0	0	100	100
2	E	99/100 (99%)	99 (100%)	0	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	768/772 (100%)	745 (97%)	19 (2%)	4 (0%)	24	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	GLY
1	D	220	ASN
1	D	222	GLU
1	D	225	THR

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	238/236 (101%)	218 (92%)	20 (8%)	10	2
1	D	241/236 (102%)	225 (93%)	16 (7%)	15	4
2	B	95/95 (100%)	90 (95%)	5 (5%)	20	6
2	E	96/95 (101%)	89 (93%)	7 (7%)	13	3
3	C	8/8 (100%)	7 (88%)	1 (12%)	4	0
3	F	8/8 (100%)	6 (75%)	2 (25%)	0	0
All	All	686/678 (101%)	635 (93%)	51 (7%)	15	3

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	17	LEU
1	A	45	PHE
1	A	66	ARG
1	A	95	PHE
1	A	110	LEU
1	A	142[A]	ILE
1	A	142[B]	ILE
1	A	166	GLU
1	A	194	ARG
1	A	222	GLU
1	A	224	LEU
1	A	226	GLN
1	A	227	ASP
1	A	228	MET
1	A	251	LEU
1	A	255[A]	GLN
1	A	255[B]	GLN
1	A	270	LEU
1	A	275	LYS
2	B	6	LYS
2	B	19	LYS
2	B	39	LEU
2	B	58	LYS
2	B	70	PHE
3	C	9	VAL
1	D	0	MET
1	D	41	ASP
1	D	42	ASN
1	D	110	LEU
1	D	142[A]	ILE
1	D	142[B]	ILE
1	D	145[A]	ARG
1	D	145[B]	ARG
1	D	149	GLN
1	D	181[A]	ARG
1	D	181[B]	ARG
1	D	224	LEU
1	D	226	GLN
1	D	227	ASP
1	D	251	LEU
1	D	270	LEU
2	E	19	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	38	ASP
2	E	58	LYS
2	E	70	PHE
2	E	73	THR
2	E	81[A]	ARG
2	E	81[B]	ARG
3	F	4	VAL
3	F	9	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	82	GLN
1	A	86	ASN
1	A	114	HIS
1	A	218	GLN
1	A	220	ASN
1	A	226	GLN
1	A	262	HIS
1	A	263	HIS
1	D	63	GLN
1	D	65	GLN
1	D	72	GLN
1	D	82	GLN
1	D	86	ASN
1	D	114	HIS
1	D	260	HIS
1	D	262	HIS
1	D	263	HIS
2	E	2	GLN
2	E	13	HIS

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

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	A	305	-	4,4,4	0.48	0	6,6,6	0.45	0
6	SO4	D	301	-	4,4,4	0.48	0	6,6,6	0.87	0
4	EDO	B	303	-	3,3,3	0.40	0	2,2,2	0.46	0
6	SO4	B	304	-	4,4,4	0.53	0	6,6,6	0.26	0
6	SO4	B	306	-	4,4,4	0.47	0	6,6,6	0.58	0
6	SO4	E	107	-	4,4,4	0.45	0	6,6,6	0.46	0
6	SO4	B	305	-	4,4,4	0.66	0	6,6,6	0.35	0
4	EDO	E	101	-	3,3,3	0.30	0	2,2,2	0.79	0
6	SO4	D	304	-	4,4,4	0.47	0	6,6,6	0.19	0
6	SO4	E	106	-	4,4,4	0.69	0	6,6,6	0.80	0
4	EDO	B	302	-	3,3,3	0.32	0	2,2,2	0.55	0
6	SO4	E	105	-	4,4,4	0.62	0	6,6,6	1.07	0
6	SO4	D	306	-	4,4,4	0.62	0	6,6,6	0.46	0
4	EDO	B	301	-	3,3,3	0.25	0	2,2,2	0.68	0
6	SO4	E	103	-	4,4,4	0.52	0	6,6,6	0.83	0
6	SO4	E	104	-	4,4,4	0.62	0	6,6,6	0.67	0
5	GOL	A	303	-	5,5,5	0.35	0	5,5,5	0.46	0
6	SO4	D	305	-	4,4,4	0.48	0	6,6,6	0.37	0
4	EDO	A	301	-	3,3,3	0.77	0	2,2,2	0.83	0
4	EDO	A	302	-	3,3,3	0.68	0	2,2,2	0.40	0
5	GOL	E	102	-	5,5,5	0.65	0	5,5,5	0.74	0
5	GOL	A	304	-	5,5,5	0.78	0	5,5,5	1.07	0
6	SO4	D	303	-	4,4,4	0.46	0	6,6,6	0.57	0
6	SO4	D	302	-	4,4,4	0.72	0	6,6,6	0.70	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
4	EDO	B	303	-	-	0/1/1/1	-
4	EDO	E	101	-	-	1/1/1/1	-
4	EDO	A	302	-	-	1/1/1/1	-
5	GOL	E	102	-	-	4/4/4/4	-
4	EDO	B	301	-	-	0/1/1/1	-
5	GOL	A	304	-	-	4/4/4/4	-
5	GOL	A	303	-	-	1/4/4/4	-
4	EDO	A	301	-	-	1/1/1/1	-
4	EDO	B	302	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	304	GOL	O1-C1-C2-C3
5	A	304	GOL	C1-C2-C3-O3
5	E	102	GOL	O1-C1-C2-C3
5	E	102	GOL	C1-C2-C3-O3
5	A	304	GOL	O2-C2-C3-O3
5	A	304	GOL	O1-C1-C2-O2
5	E	102	GOL	O1-C1-C2-O2
5	E	102	GOL	O2-C2-C3-O3
4	A	302	EDO	O1-C1-C2-O2
5	A	303	GOL	O1-C1-C2-C3
4	B	302	EDO	O1-C1-C2-O2
4	E	101	EDO	O1-C1-C2-O2
4	A	301	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	305	SO4	1	0
4	E	101	EDO	2	0
6	E	106	SO4	1	0
4	B	302	EDO	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	105	SO4	1	0
6	D	306	SO4	1	0
6	E	103	SO4	1	0
4	A	301	EDO	2	0
5	E	102	GOL	1	0
5	A	304	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	277/277 (100%)	0.13	6 (2%) 62 68	9, 26, 54, 102	2 (0%)
1	D	277/277 (100%)	0.09	11 (3%) 42 45	7, 25, 54, 92	5 (1%)
2	B	100/100 (100%)	-0.19	0 100 100	14, 21, 33, 43	0
2	E	100/100 (100%)	-0.08	0 100 100	12, 24, 42, 46	1 (1%)
3	C	9/9 (100%)	0.07	0 100 100	25, 26, 32, 33	0
3	F	9/9 (100%)	-0.11	0 100 100	20, 23, 27, 28	0
All	All	772/772 (100%)	0.04	17 (2%) 62 68	7, 25, 48, 102	8 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	LEU	4.5
1	A	17	LEU	4.2
1	A	225	THR	4.0
1	D	224	LEU	4.0
1	D	226	GLN	3.7
1	D	0	MET	3.5
1	D	225	THR	3.4
1	D	276	PRO	3.1
1	A	18	GLY	2.8
1	D	17	LEU	2.8
1	D	221	GLY	2.4
1	A	0	MET	2.3
1	D	274	TRP	2.3
1	A	221	GLY	2.2
1	D	275	LYS	2.2
1	D	197	VAL	2.2
1	D	145[A]	ARG	2.1

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
5	GOL	A	303	6/6	0.70	0.16	61,66,68,70	0
6	SO4	B	304	5/5	0.71	0.19	91,95,103,107	0
6	SO4	E	106	5/5	0.72	0.17	63,68,74,83	0
5	GOL	E	102	6/6	0.77	0.15	43,50,58,65	0
6	SO4	E	107	5/5	0.80	0.18	87,89,97,100	0
4	EDO	A	302	4/4	0.81	0.18	43,44,47,48	0
6	SO4	B	305	5/5	0.81	0.14	72,74,80,81	0
6	SO4	B	306	5/5	0.82	0.17	75,76,82,98	0
6	SO4	D	304	5/5	0.82	0.13	68,72,80,87	0
6	SO4	E	105	5/5	0.85	0.18	22,26,29,30	5
6	SO4	D	302	5/5	0.85	0.14	45,45,57,64	0
6	SO4	D	305	5/5	0.85	0.13	78,80,89,91	0
6	SO4	D	303	5/5	0.87	0.15	50,59,70,78	0
5	GOL	A	304	6/6	0.87	0.13	40,48,50,53	0
6	SO4	D	306	5/5	0.90	0.11	42,42,57,61	0
4	EDO	A	301	4/4	0.91	0.17	22,26,28,29	0
6	SO4	E	104	5/5	0.92	0.11	33,41,56,59	0
6	SO4	D	301	5/5	0.92	0.21	34,34,51,54	0
4	EDO	B	303	4/4	0.93	0.11	22,24,29,33	0
4	EDO	E	101	4/4	0.93	0.10	30,31,32,34	0
4	EDO	B	301	4/4	0.95	0.08	23,25,26,26	0
6	SO4	A	305	5/5	0.96	0.15	27,39,46,48	0
6	SO4	E	103	5/5	0.96	0.16	29,38,48,52	0
4	EDO	B	302	4/4	0.97	0.06	18,24,25,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.