



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:45 PM EDT

PDB ID : 4Z78 / pdb_00004z78
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 : 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

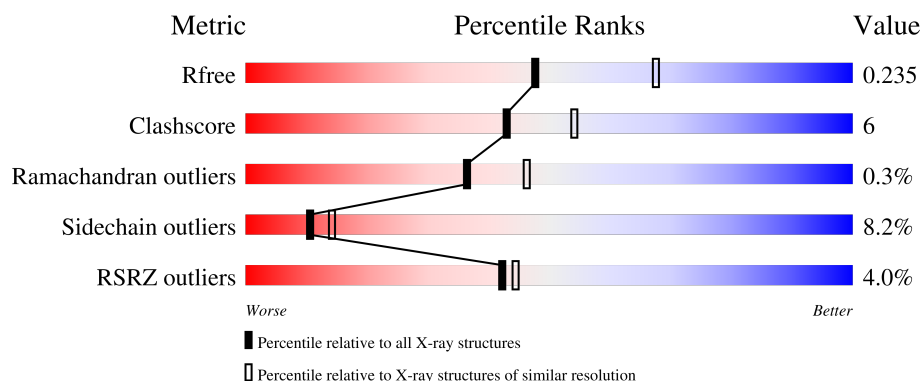
1 Overall quality at a glance

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	277	% 81% 17%
1	D	277	% 83% 15%
1	G	277	4% 83% 15%
2	B	100	% 85% 12%
2	E	100	3% 86% 12%

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Mol	Chain	Length	Quality of chain
2	H	100	
3	C	10	
3	F	10	
3	I	10	

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
5	GOL	A	305	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10098 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	0	0
			2287	1449	406	424	8			
1	D	277	Total	C	N	O	S	0	0	0
			2287	1449	406	424	8			
1	G	277	Total	C	N	O	S	0	1	0
			2298	1455	410	425	8			

There are 9 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
G	0	MET	-	initiating methionine	UNP P01902
G	114	HIS	GLN	conflict	UNP P01902
G	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
			844	538	142	160	4			
2	H	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

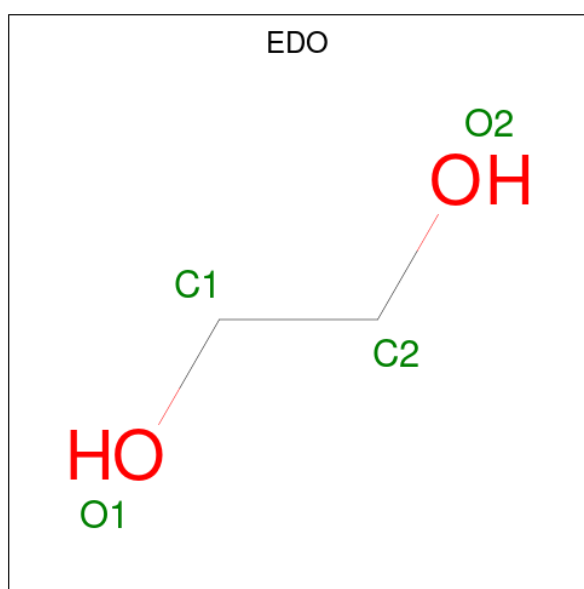
There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called Insulin.

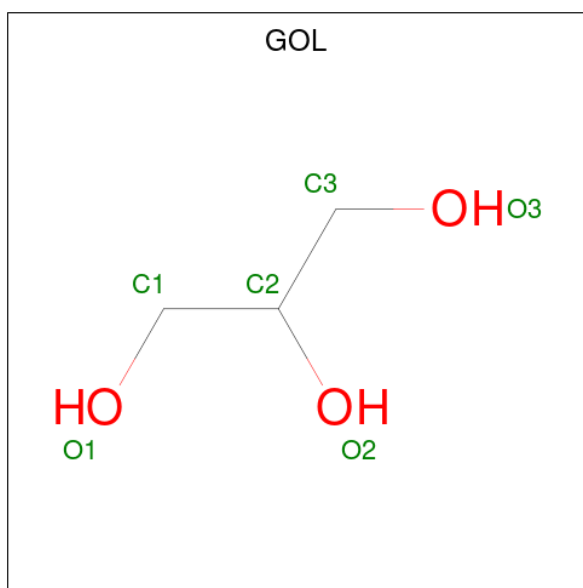
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	S	0	0	0
			81	53	13	14	1			
3	F	10	Total	C	N	O	S	0	0	0
			81	53	13	14	1			
3	I	10	Total	C	N	O	S	0	0	0
			81	53	13	14	1			

- 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	A	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	H	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	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	H	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	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	100	Total	O	0	0
			100	100		
7	B	46	Total	O	0	0
			46	46		
7	D	87	Total	O	0	0
			87	87		

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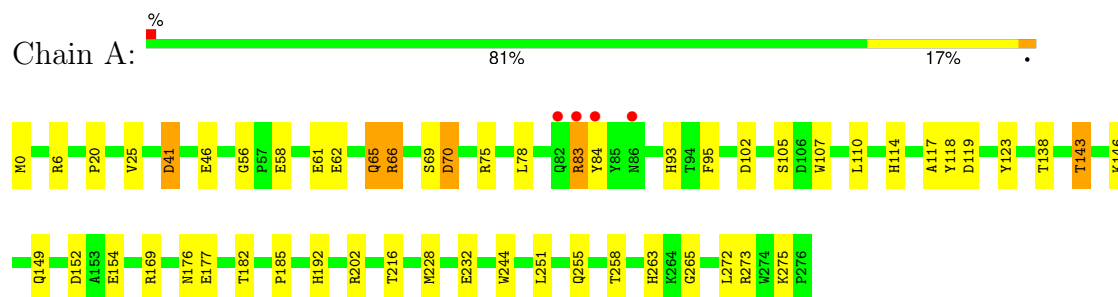
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	27	Total 27	O 27	0	0
7	G	63	Total 63	O 63	0	0
7	H	41	Total 41	O 41	0	0

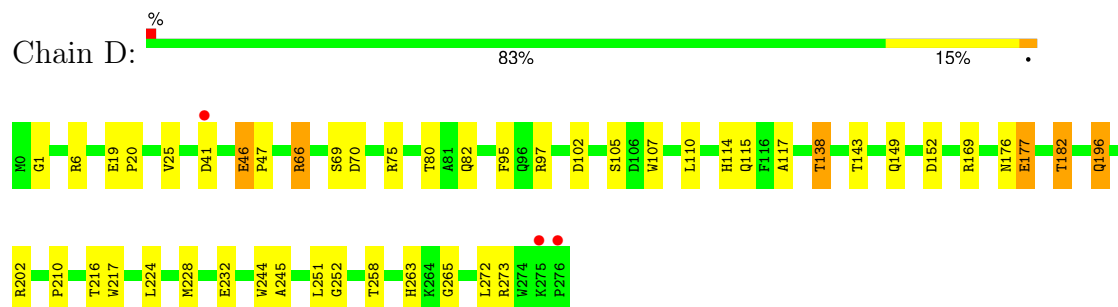
3 Residue-property plots

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.

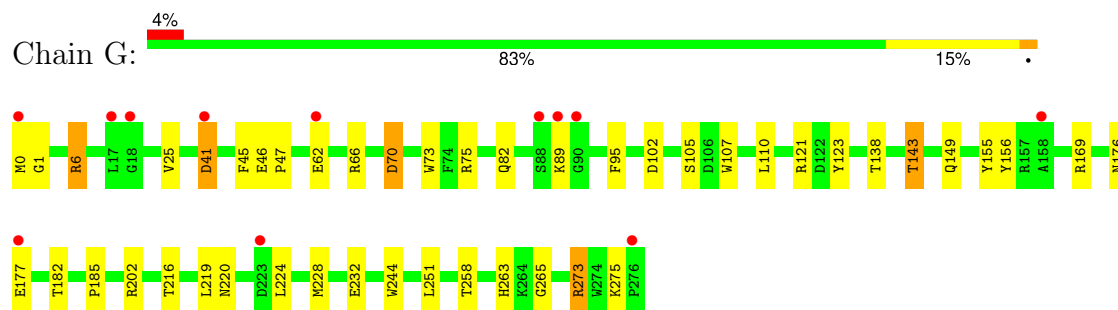
- Molecule 1: H-2 class I histocompatibility antigen, K-D alpha chain



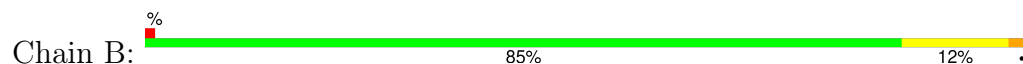
- Molecule 1: H-2 class I histocompatibility antigen, K-D alpha chain



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

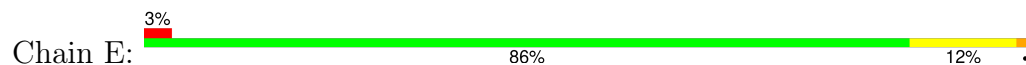


- Molecule 2: Beta-2-microglobulin

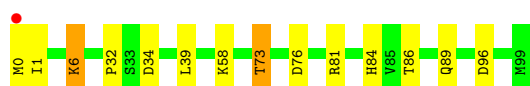
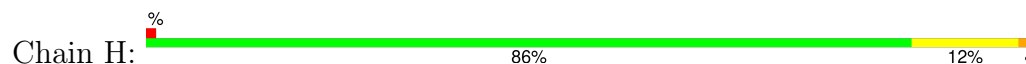




● Molecule 2: Beta-2-microglobulin



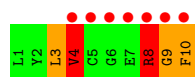
● Molecule 2: Beta-2-microglobulin



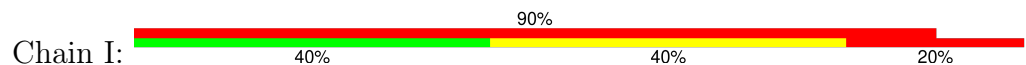
● Molecule 3: Insulin



● Molecule 3: Insulin



● Molecule 3: Insulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.17Å 151.57Å 182.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.09 – 2.30 78.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (78.09-2.30) 99.9 (78.09-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.188 , 0.233 0.193 , 0.235	Depositor DCC
R_{free} test set	2925 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10098	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.7426e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	1.05	0/2357	1.00	2/3205 (0.1%)
1	D	1.03	0/2357	1.01	5/3205 (0.2%)
1	G	0.99	0/2368	1.01	3/3219 (0.1%)
2	B	0.94	0/860	0.91	2/1162 (0.2%)
2	E	0.82	0/867	0.86	0/1172
2	H	0.95	0/860	0.87	0/1162
3	C	1.04	0/82	1.48	1/107 (0.9%)
3	F	1.32	1/82 (1.2%)	1.48	2/107 (1.9%)
3	I	0.92	0/82	1.74	3/107 (2.8%)
All	All	1.00	1/9915 (0.0%)	0.99	18/13446 (0.1%)

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
1	A	0	1
3	C	0	1
3	I	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	LEU	CA-C	5.43	1.59	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	9	GLY	N-CA-C	-8.72	96.32	112.37
3	I	4	VAL	CB-CA-C	-8.13	102.35	111.45
3	F	4	VAL	N-CA-C	7.54	121.15	108.86
1	D	1	GLY	N-CA-C	-6.94	98.18	112.34
3	I	4	VAL	N-CA-C	6.81	117.91	110.21
1	G	1	GLY	N-CA-C	-6.46	99.15	112.34
1	A	46	GLU	N-CA-C	6.02	115.23	108.25
1	D	46	GLU	N-CA-C	5.99	115.19	108.25
3	F	4	VAL	CB-CA-C	-5.85	101.33	110.69
3	C	9	GLY	N-CA-C	5.75	120.75	112.81
1	G	176	ASN	N-CA-C	5.64	117.43	111.28
2	B	1	ILE	N-CA-CB	5.46	120.04	110.49
1	D	115	GLN	N-CA-CB	-5.42	101.33	111.13
2	B	1	ILE	CB-CA-C	-5.28	104.34	111.63
1	A	176	ASN	N-CA-C	5.20	116.95	111.28
1	G	45	PHE	N-CA-C	-5.19	102.17	109.96
1	D	182	THR	CB-CA-C	5.17	118.41	110.14
1	D	41	ASP	N-CA-C	-5.07	101.70	109.76

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	HIS	Peptide
3	C	8	ARG	Peptide
3	I	4	VAL	Peptide
3	I	8	ARG	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	2287	0	2153	39	0
1	D	2287	0	2153	34	0
1	G	2298	0	2165	28	0
2	B	837	0	803	9	0
2	E	844	0	811	6	0
2	H	837	0	803	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	81	0	81	8	0
3	F	81	0	81	9	0
3	I	81	0	81	8	0
4	A	12	0	18	1	0
4	D	4	0	6	0	0
4	H	4	0	6	0	0
5	A	12	0	16	4	0
5	D	6	0	8	0	0
5	E	6	0	8	1	0
5	H	12	0	16	2	0
6	A	20	0	0	0	0
6	D	20	0	0	0	0
6	G	5	0	0	1	0
7	A	100	0	0	2	0
7	B	46	0	0	0	0
7	D	87	0	0	1	1
7	E	27	0	0	0	0
7	G	63	0	0	1	1
7	H	41	0	0	2	0
All	All	10098	0	9209	117	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 6.

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:217:TRP:CD1	1:D:228:MET:HE3	2.06	0.91
1:A:152:ASP:OD2	3:C:8:ARG:NE	2.05	0.87
1:D:217:TRP:HD1	1:D:228:MET:HE3	1.42	0.82
1:A:70:ASP:OD1	3:C:4:VAL:HG23	1.80	0.82
1:A:143:THR:HG22	3:C:10:PHE:HB3	1.60	0.82
1:A:58:GLU:OE2	1:D:138:THR:HG23	1.80	0.82
1:A:143:THR:CG2	3:C:10:PHE:HB3	2.09	0.82
1:A:66:ARG:HG2	3:C:4:VAL:HG12	1.64	0.80
1:G:156:TYR:OH	3:I:4:VAL:O	2.00	0.77
1:D:143:THR:HG23	3:F:9:GLY:CA	2.19	0.72
1:A:84:TYR:C	1:A:84:TYR:CD1	2.69	0.71
2:B:73:THR:HG22	2:B:76:ASP:H	1.55	0.71
2:H:73:THR:HG22	2:H:76:ASP:H	1.56	0.71
1:G:73:TRP:HE1	3:I:8:ARG:HB2	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:HG2	1:A:84:TYR:N	2.09	0.68
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.76	0.68
1:D:228:MET:HE2	1:D:245:ALA:HB1	1.75	0.68
1:A:93:HIS:HB2	5:A:305:GOL:H12	1.77	0.67
1:D:6:ARG:NH2	1:D:102:ASP:OD1	2.29	0.66
1:D:143:THR:HG23	3:F:9:GLY:HA3	1.78	0.65
1:D:176:ASN:ND2	1:D:177:GLU:OE2	2.32	0.62
1:G:73:TRP:HE1	3:I:8:ARG:CB	2.11	0.62
1:G:75[B]:ARG:HD3	6:G:301:SO4:O3	1.98	0.62
1:D:196:GLN:HE21	1:D:196:GLN:HA	1.64	0.62
1:A:41:ASP:OD1	1:A:41:ASP:N	2.33	0.62
2:H:84:HIS:HD2	2:H:86:THR:OG1	1.83	0.61
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.33	0.61
1:A:78:LEU:HB3	5:A:305:GOL:H11	1.82	0.61
1:A:232:GLU:OE2	2:B:6:LYS:NZ	2.31	0.61
1:D:143:THR:HG23	3:F:9:GLY:HA2	1.81	0.61
1:A:118:TYR:HD2	5:A:304:GOL:H31	1.66	0.60
2:E:48:LYS:HE3	2:E:48:LYS:HA	1.83	0.60
2:B:48:LYS:HA	2:B:48:LYS:HE3	1.84	0.59
1:G:263:HIS:CD2	1:G:265:GLY:H	2.20	0.59
1:G:216:THR:HA	1:G:228:MET:HE1	1.85	0.59
2:E:84:HIS:HD2	2:E:86:THR:OG1	1.84	0.59
1:G:232:GLU:OE2	2:H:6:LYS:NZ	2.36	0.59
2:B:84:HIS:HD2	2:B:86:THR:OG1	1.86	0.59
1:A:192:HIS:CE1	2:B:98:ASP:HB3	2.39	0.57
1:G:70:ASP:OD1	3:I:5:CYS:N	2.36	0.57
1:D:228:MET:HE2	1:D:245:ALA:CB	2.34	0.57
1:G:107:TRP:CZ3	1:G:169:ARG:HG2	2.39	0.57
1:D:263:HIS:CD2	1:D:265:GLY:H	2.22	0.56
1:G:41:ASP:OD1	1:G:41:ASP:N	2.31	0.56
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.40	0.56
1:A:216:THR:HA	1:A:228:MET:HE1	1.88	0.55
1:A:263:HIS:CD2	1:A:265:GLY:H	2.24	0.55
1:D:19:GLU:HB3	1:D:75:ARG:NH1	2.22	0.54
1:G:6:ARG:NH2	1:G:102:ASP:OD1	2.40	0.54
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.43	0.53
1:G:219:LEU:O	1:G:220:ASN:HB2	2.09	0.53
2:H:81:ARG:HG2	7:H:427:HOH:O	2.09	0.53
1:D:216:THR:HA	1:D:228:MET:HE1	1.90	0.52
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.44	0.52
1:D:80:THR:HG21	3:F:10:PHE:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.45	0.51
1:D:202:ARG:HD3	1:D:244:TRP:CE3	2.45	0.51
3:I:3:LEU:HD22	3:I:4:VAL:H	1.75	0.51
2:E:99:MET:OXT	5:E:101:GOL:H32	2.10	0.51
1:A:84:TYR:CD1	1:A:84:TYR:O	2.64	0.51
2:H:96:ASP:H	5:H:302:GOL:H12	1.75	0.50
1:A:118:TYR:HD2	5:A:304:GOL:C3	2.25	0.50
1:A:107:TRP:CZ3	1:A:169:ARG:HG2	2.47	0.50
1:D:80:THR:HG21	3:F:10:PHE:CG	2.47	0.50
1:D:82:GLN:HG3	7:D:479:HOH:O	2.12	0.50
1:G:66:ARG:CZ	3:I:3:LEU:HD23	2.42	0.49
1:G:123:TYR:OH	1:G:143:THR:CG2	2.60	0.49
3:F:3:LEU:HD12	3:F:4:VAL:H	1.76	0.49
1:A:123:TYR:OH	1:A:143:THR:CG2	2.60	0.49
2:H:96:ASP:H	5:H:302:GOL:C1	2.26	0.49
1:D:252:GLY:O	1:G:89:LYS:HE3	2.14	0.48
1:G:258:THR:HG22	1:G:273:ARG:HG3	1.96	0.48
1:D:107:TRP:CZ3	1:D:169:ARG:HG2	2.48	0.48
1:G:107:TRP:CH2	1:G:169:ARG:HG2	2.49	0.48
1:A:61:GLU:OE2	1:A:65:GLN:NE2	2.47	0.48
1:G:143:THR:HB	3:I:8:ARG:NH2	2.29	0.47
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.50	0.47
1:G:62:GLU:OE1	1:G:66:ARG:NE	2.48	0.47
1:G:202:ARG:HD3	1:G:244:TRP:CE3	2.50	0.47
1:G:185:PRO:HD3	1:G:263:HIS:CD2	2.50	0.46
1:D:232:GLU:OE2	2:E:6:LYS:HE2	2.16	0.46
1:G:46:GLU:HB2	1:G:47:PRO:HD2	1.98	0.46
1:A:185:PRO:HD3	1:A:263:HIS:CD2	2.52	0.45
2:H:32:PRO:O	2:H:84:HIS:HE1	2.00	0.45
1:A:20:PRO:HG2	1:A:75:ARG:HG3	1.99	0.44
1:G:155:TYR:CE2	3:I:3:LEU:HD11	2.53	0.44
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.52	0.44
1:A:143:THR:HG22	3:C:10:PHE:CB	2.40	0.44
1:D:66:ARG:CA	3:F:4:VAL:HG11	2.49	0.43
1:A:119:ASP:HB3	2:B:0:MET:HA	2.00	0.43
1:A:123:TYR:OH	1:A:143:THR:HG21	2.17	0.43
1:D:152:ASP:OD2	3:F:8:ARG:NH1	2.51	0.43
1:D:216:THR:CA	1:D:228:MET:HE1	2.49	0.43
2:H:34:ASP:HB2	7:H:441:HOH:O	2.18	0.43
1:D:97:ARG:HH21	1:D:114:HIS:CD2	2.37	0.42
1:G:123:TYR:OH	1:G:143:THR:HG21	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLU:HG3	7:A:497:HOH:O	2.20	0.42
1:A:56:GLY:H	4:A:302:EDO:H21	1.85	0.42
1:A:69:SER:OG	3:C:4:VAL:HG21	2.19	0.42
1:A:258:THR:HG22	1:A:273:ARG:HG3	2.01	0.42
1:D:258:THR:HG22	1:D:273:ARG:HG3	2.01	0.42
2:E:32:PRO:O	2:E:84:HIS:HE1	2.02	0.42
1:D:46:GLU:HB2	1:D:47:PRO:HD2	2.01	0.42
1:D:143:THR:HA	3:F:9:GLY:HA2	2.02	0.42
1:A:62:GLU:OE2	1:A:66:ARG:CD	2.68	0.42
1:A:202:ARG:NH2	7:A:401:HOH:O	2.34	0.41
2:B:32:PRO:O	2:B:84:HIS:HE1	2.02	0.41
1:A:62:GLU:OE2	1:A:66:ARG:HD2	2.20	0.41
1:A:146:LYS:HE2	3:C:10:PHE:HD2	1.84	0.41
1:D:202:ARG:CD	1:D:244:TRP:CE3	3.04	0.41
2:B:48:LYS:HA	2:B:48:LYS:CE	2.47	0.41
1:D:196:GLN:HA	1:D:196:GLN:NE2	2.35	0.41
1:D:210:PRO:O	1:D:263:HIS:HE1	2.04	0.41
1:G:202:ARG:NH2	7:G:401:HOH:O	2.32	0.41
1:G:258:THR:HG22	1:G:273:ARG:CG	2.51	0.41
1:G:121:ARG:HD3	2:H:0:MET:H1	1.86	0.40
1:D:20:PRO:HD2	1:D:75:ARG:HG3	2.02	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:D:435:HOH:O	7:G:431:HOH:O[3_745]	2.04	0.16

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	275/277 (99%)	271 (98%)	4 (2%)	0	100	100
1	D	275/277 (99%)	270 (98%)	5 (2%)	0	100	100
1	G	276/277 (100%)	270 (98%)	6 (2%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	E	99/100 (99%)	96 (97%)	3 (3%)	0	100	100
2	H	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	8/10 (80%)	6 (75%)	1 (12%)	1 (12%)	0	0
3	F	8/10 (80%)	4 (50%)	2 (25%)	2 (25%)	0	0
3	I	8/10 (80%)	5 (62%)	2 (25%)	1 (12%)	0	0
All	All	1145/1161 (99%)	1116 (98%)	25 (2%)	4 (0%)	36	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	8	ARG
3	I	8	ARG
3	C	7	GLU
3	F	9	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/236 (100%)	217 (92%)	19 (8%)	11	14
1	D	236/236 (100%)	221 (94%)	15 (6%)	16	23
1	G	237/236 (100%)	219 (92%)	18 (8%)	12	16
2	B	95/95 (100%)	88 (93%)	7 (7%)	13	17
2	E	96/95 (101%)	87 (91%)	9 (9%)	8	11
2	H	95/95 (100%)	89 (94%)	6 (6%)	16	23
3	C	8/8 (100%)	4 (50%)	4 (50%)	0	0
3	F	8/8 (100%)	5 (62%)	3 (38%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	8/8 (100%)	6 (75%)	2 (25%)	0	0
All	All	1019/1017 (100%)	936 (92%)	83 (8%)	10	14

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	25	VAL
1	A	41	ASP
1	A	65	GLN
1	A	66	ARG
1	A	70	ASP
1	A	83	ARG
1	A	95	PHE
1	A	105	SER
1	A	110	LEU
1	A	138	THR
1	A	143	THR
1	A	149	GLN
1	A	177	GLU
1	A	182	THR
1	A	251	LEU
1	A	255	GLN
1	A	272	LEU
1	A	275	LYS
2	B	6	LYS
2	B	39	LEU
2	B	47	GLU
2	B	48	LYS
2	B	58	LYS
2	B	73	THR
2	B	89	GLN
3	C	3	LEU
3	C	4	VAL
3	C	5	CYS
3	C	8	ARG
1	D	25	VAL
1	D	66	ARG
1	D	69	SER
1	D	70	ASP
1	D	95	PHE
1	D	105	SER

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Mol	Chain	Res	Type
1	D	110	LEU
1	D	138	THR
1	D	149	GLN
1	D	177	GLU
1	D	182	THR
1	D	196	GLN
1	D	224	LEU
1	D	251	LEU
1	D	272	LEU
2	E	0	MET
2	E	1	ILE
2	E	6	LYS
2	E	39	LEU
2	E	44	GLU
2	E	47	GLU
2	E	48	LYS
2	E	69	GLU
2	E	89	GLN
3	F	4	VAL
3	F	8	ARG
3	F	10	PHE
1	G	0	MET
1	G	6	ARG
1	G	25	VAL
1	G	41	ASP
1	G	70	ASP
1	G	82	GLN
1	G	95	PHE
1	G	105	SER
1	G	110	LEU
1	G	138	THR
1	G	143	THR
1	G	149	GLN
1	G	177	GLU
1	G	182	THR
1	G	224	LEU
1	G	251	LEU
1	G	273	ARG
1	G	275	LYS
2	H	1	ILE
2	H	6	LYS
2	H	39	LEU

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Mol	Chain	Res	Type
2	H	58	LYS
2	H	73	THR
2	H	89	GLN
3	I	4	VAL
3	I	10	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	86	ASN
1	A	87	GLN
1	A	93	HIS
1	A	114	HIS
1	A	149	GLN
1	A	196	GLN
1	A	226	GLN
1	A	263	HIS
2	B	84	HIS
1	D	82	GLN
1	D	86	ASN
1	D	114	HIS
1	D	149	GLN
1	D	196	GLN
1	D	226	GLN
1	D	255	GLN
1	D	263	HIS
2	E	84	HIS
1	G	65	GLN
1	G	86	ASN
1	G	149	GLN
1	G	220	ASN
1	G	263	HIS
2	H	84	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 ⓘ

20 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	$\# Z > 2$
5	GOL	H	302	-	5,5,5	0.84	0	5,5,5	0.83	0
5	GOL	D	302	-	5,5,5	0.76	0	5,5,5	1.42	1 (20%)
6	SO4	D	303	-	4,4,4	0.52	0	6,6,6	0.88	0
4	EDO	A	303	-	3,3,3	0.31	0	2,2,2	0.46	0
6	SO4	D	305	-	4,4,4	0.53	0	6,6,6	0.40	0
5	GOL	E	101	-	5,5,5	1.00	0	5,5,5	1.36	1 (20%)
4	EDO	H	301	-	3,3,3	0.20	0	2,2,2	1.00	0
4	EDO	D	301	-	3,3,3	0.49	0	2,2,2	0.29	0
5	GOL	A	305	-	5,5,5	0.82	0	5,5,5	1.73	2 (40%)
5	GOL	H	303	-	5,5,5	1.38	0	5,5,5	1.49	1 (20%)
6	SO4	A	307	-	4,4,4	0.49	0	6,6,6	0.41	0
6	SO4	A	306	-	4,4,4	0.53	0	6,6,6	0.89	0
6	SO4	A	309	-	4,4,4	0.53	0	6,6,6	0.40	0
6	SO4	D	304	-	4,4,4	0.59	0	6,6,6	0.50	0
6	SO4	A	308	-	4,4,4	0.45	0	6,6,6	0.51	0
4	EDO	A	302	-	3,3,3	1.23	0	2,2,2	1.02	0
5	GOL	A	304	-	5,5,5	0.73	0	5,5,5	2.25	2 (40%)
6	SO4	G	301	-	4,4,4	0.62	0	6,6,6	0.80	0
4	EDO	A	301	-	3,3,3	0.45	0	2,2,2	0.53	0
6	SO4	D	306	-	4,4,4	0.63	0	6,6,6	0.61	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	H	302	-	-	4/4/4/4	-
5	GOL	H	303	-	-	1/4/4/4	-
4	EDO	A	303	-	-	0/1/1/1	-
4	EDO	A	302	-	-	0/1/1/1	-
5	GOL	A	304	-	-	2/4/4/4	-
4	EDO	A	301	-	-	0/1/1/1	-
5	GOL	D	302	-	-	0/4/4/4	-
5	GOL	E	101	-	-	3/4/4/4	-
4	EDO	H	301	-	-	1/1/1/1	-
4	EDO	D	301	-	-	0/1/1/1	-
5	GOL	A	305	-	-	4/4/4/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	304	GOL	O3-C3-C2	3.13	124.48	110.38
5	A	304	GOL	C3-C2-C1	2.68	121.64	111.80
5	E	101	GOL	O3-C3-C2	2.66	122.34	110.38
5	H	303	GOL	O1-C1-C2	2.47	121.51	110.38
5	A	305	GOL	O1-C1-C2	2.42	121.27	110.38
5	D	302	GOL	O3-C3-C2	2.18	120.21	110.38
5	A	305	GOL	O2-C2-C1	-2.09	100.53	109.18

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	304	GOL	O1-C1-C2-C3
5	A	305	GOL	O1-C1-C2-C3
5	E	101	GOL	O1-C1-C2-C3
5	A	305	GOL	C1-C2-C3-O3
5	H	302	GOL	O1-C1-C2-C3
5	H	302	GOL	C1-C2-C3-O3
5	A	304	GOL	O1-C1-C2-O2
5	A	305	GOL	O1-C1-C2-O2
5	A	305	GOL	O2-C2-C3-O3

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

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	302	GOL	2	0
5	E	101	GOL	1	0
5	A	305	GOL	2	0
4	A	302	EDO	1	0
5	A	304	GOL	2	0
6	G	301	SO4	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	277/277 (100%)	-0.21	4 (1%) 73 75	17, 32, 55, 83	0
1	D	277/277 (100%)	-0.15	3 (1%) 78 79	18, 36, 62, 93	0
1	G	277/277 (100%)	0.17	12 (4%) 40 41	15, 41, 72, 97	1 (0%)
2	B	100/100 (100%)	-0.27	1 (1%) 79 80	19, 35, 58, 68	0
2	E	100/100 (100%)	0.00	3 (3%) 52 54	13, 44, 78, 95	1 (1%)
2	H	100/100 (100%)	-0.26	1 (1%) 79 80	23, 37, 56, 70	0
3	C	10/10 (100%)	4.18	7 (70%) 0 0	21, 31, 36, 47	7 (70%)
3	F	10/10 (100%)	4.94	7 (70%) 0 0	23, 31, 38, 47	7 (70%)
3	I	10/10 (100%)	5.22	9 (90%) 0 0	26, 30, 46, 66	7 (70%)
All	All	1161/1161 (100%)	0.03	47 (4%) 42 44	13, 37, 67, 97	23 (1%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	6	GLY	10.1
3	I	4	VAL	9.4
3	F	10	PHE	8.3
3	F	4	VAL	7.9
3	I	9	GLY	7.6
3	C	4	VAL	7.2
3	C	10	PHE	6.9
3	I	5	CYS	6.6
3	C	6	GLY	6.5
3	I	6	GLY	6.2
3	I	10	PHE	6.1
3	F	5	CYS	6.0
3	F	9	GLY	5.9
3	F	7	GLU	5.6
3	C	5	CYS	5.2

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Mol	Chain	Res	Type	RSRZ
3	I	7	GLU	4.8
3	F	8	ARG	4.8
3	I	8	ARG	4.8
3	C	7	GLU	4.6
3	C	9	GLY	4.4
3	C	8	ARG	4.3
2	E	99	MET	3.5
1	A	86	ASN	3.0
1	A	83	ARG	2.9
1	A	82	GLN	2.8
3	I	3	LEU	2.8
2	B	0	MET	2.7
2	E	75	LYS	2.6
1	G	90	GLY	2.6
1	G	223	ASP	2.6
2	H	0	MET	2.5
1	A	84	TYR	2.4
1	D	275	LYS	2.4
1	G	88	SER	2.4
1	D	41	ASP	2.4
1	G	89	LYS	2.3
1	G	276	PRO	2.3
1	G	18	GLY	2.3
1	G	17	LEU	2.2
2	E	0	MET	2.2
3	I	2	TYR	2.1
1	G	41	ASP	2.1
1	G	177	GLU	2.1
1	D	276	PRO	2.1
1	G	0	MET	2.0
1	G	158	ALA	2.0
1	G	62	GLU	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(Å ²)	Q<0.9
6	SO4	D	304	5/5	0.67	0.14	70,85,91,94	0
5	GOL	H	303	6/6	0.69	0.21	53,58,69,69	0
6	SO4	A	307	5/5	0.75	0.14	78,90,101,104	0
6	SO4	D	306	5/5	0.76	0.17	71,88,103,110	0
4	EDO	A	302	4/4	0.80	0.19	39,51,52,53	0
6	SO4	A	309	5/5	0.80	0.15	87,90,97,107	0
6	SO4	A	308	5/5	0.81	0.16	84,94,108,113	0
5	GOL	E	101	6/6	0.84	0.15	44,52,56,59	0
5	GOL	D	302	6/6	0.86	0.15	46,51,57,59	0
5	GOL	A	305	6/6	0.87	0.24	38,47,50,50	0
6	SO4	A	306	5/5	0.89	0.26	51,57,79,83	0
6	SO4	D	305	5/5	0.89	0.12	75,82,93,101	0
5	GOL	A	304	6/6	0.89	0.14	34,38,40,47	0
6	SO4	G	301	5/5	0.89	0.16	65,74,99,112	0
5	GOL	H	302	6/6	0.91	0.22	32,43,48,60	0
4	EDO	D	301	4/4	0.92	0.11	52,55,55,58	0
4	EDO	A	301	4/4	0.94	0.08	46,46,48,48	0
4	EDO	A	303	4/4	0.95	0.13	39,39,41,42	0
6	SO4	D	303	5/5	0.95	0.16	48,57,72,75	0
4	EDO	H	301	4/4	0.96	0.08	35,36,38,47	0

6.5 Other polymers

There are no such residues in this entry.