



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:48 PM GMT

PDB ID : 4Z77
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 : 1.85 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

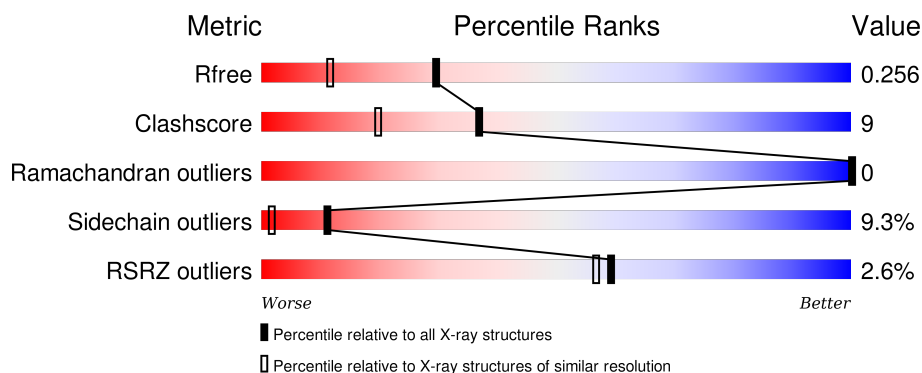
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>5%</div> <div>76%</div> <div>19%</div> <div>•</div> </div>
1	D	277	<div> <div>2%</div> <div>77%</div> <div>17%</div> <div>5%</div> <div>•</div> </div>
2	B	100	<div> <div>80%</div> <div>16%</div> <div>•</div> </div>
2	E	100	<div> <div>2%</div> <div>84%</div> <div>13%</div> <div>•</div> </div>
3	C	9	<div> <div>67%</div> <div>22%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	9	 <div>67% 22% 11%</div>

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	A	301	-	-	X	X
4	GOL	A	302	-	-	-	X
4	GOL	B	302	-	-	-	X
4	GOL	D	301	-	-	-	X
4	GOL	D	302	-	-	-	X
4	GOL	E	101	-	-	-	X
5	15P	D	304	-	-	-	X
6	EDO	A	306	-	-	-	X
6	EDO	B	304	-	-	-	X
6	EDO	B	305	-	-	-	X
7	SO4	A	307	-	-	-	X
7	SO4	D	308	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6964 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	1	0
			2296	1454	407	427	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	0	0
			837	533	141	159	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:

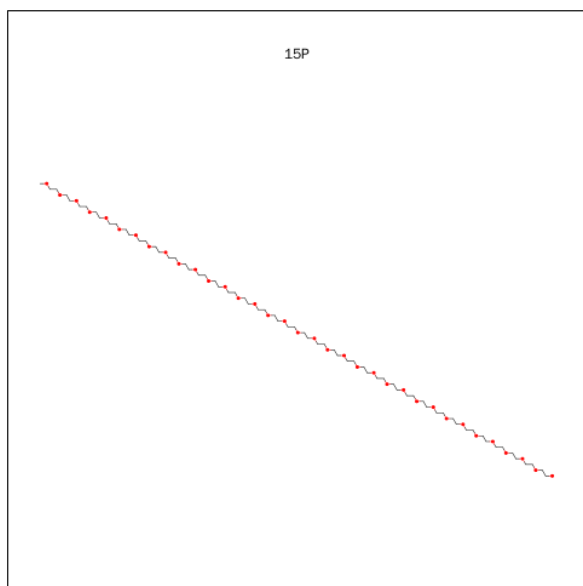
Chain	Residue	Modelled	Actual	Comment	Reference
C	9	VAL	GLY	engineered mutation	UNP P01308
F	9	VAL	GLY	engineered mutation	UNP P01308

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



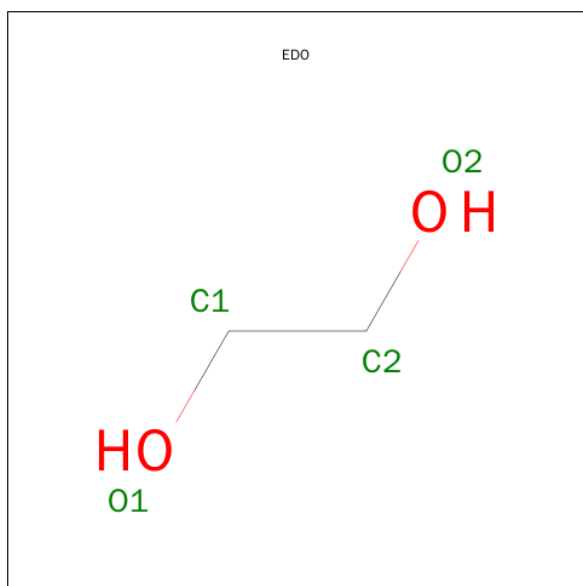
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is POLYETHYLENE GLYCOL (N=34) (three-letter code: 15P) (formula: $C_{69}H_{140}O_{35}$).



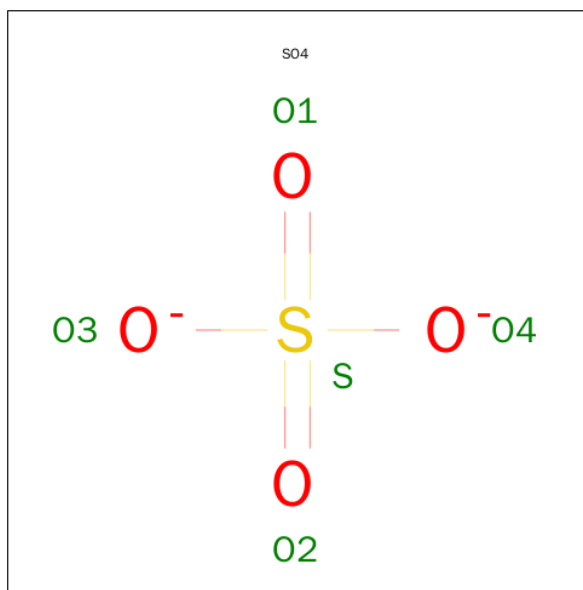
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

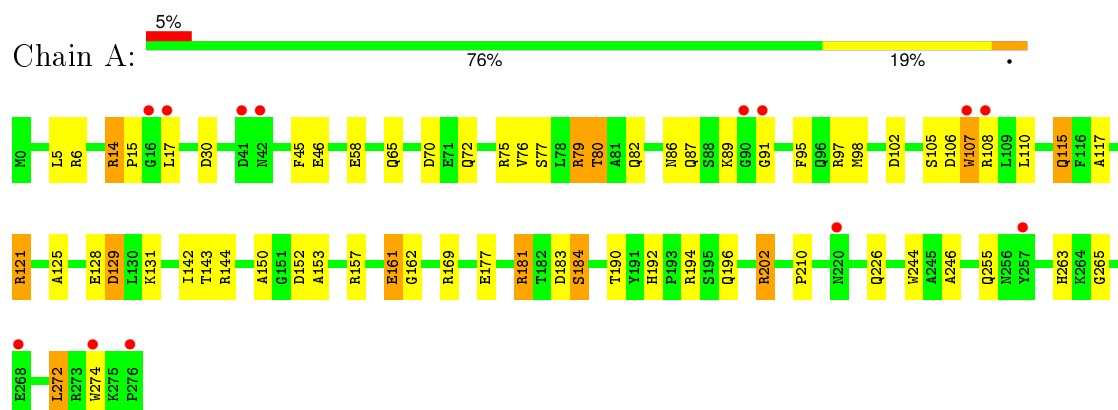
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	117	Total O 117 117	0	0
8	B	71	Total O 71 71	0	0
8	C	4	Total O 4 4	0	0
8	D	147	Total O 147 147	0	0
8	E	65	Total O 65 65	0	0
8	F	7	Total O 7 7	0	0

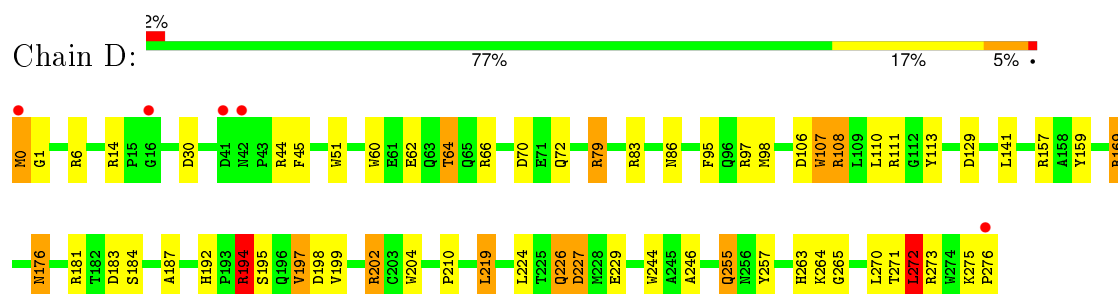
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

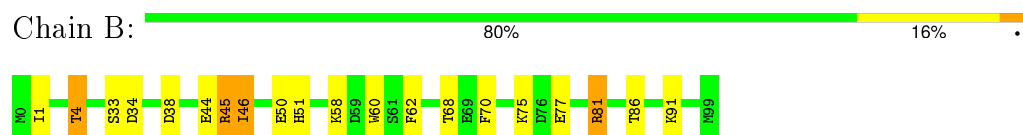
- Molecule 1: H-2 class I histocompatibility antigen, K-D alpha chain



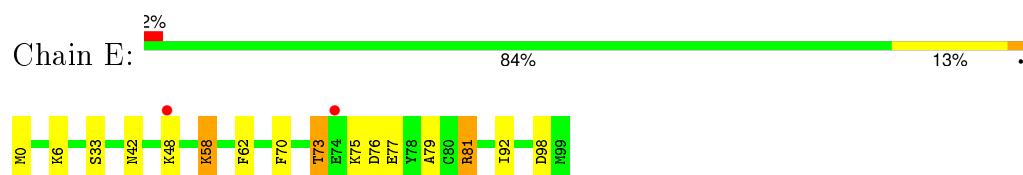
- Molecule 1: H-2 class I histocompatibility antigen, K-D alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: Insulin

Chain C:  67% 22% 11%



- Molecule 3: Insulin

Chain F:  67% 22% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.15Å 84.53Å 72.86Å 90.00° 106.86° 90.00°	Depositor
Resolution (Å)	37.10 – 1.85 37.10 – 1.85	Depositor EDS
% Data completeness (in resolution range)	92.6 (37.10-1.85) 92.6 (37.10-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 1.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.206 , 0.253 0.212 , 0.256	Depositor DCC
R_{free} test set	3073 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 60683 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6964	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, 15P, EDO, 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	0.82	0/2357	0.99	10/3205 (0.3%)
1	D	0.83	2/2366 (0.1%)	1.05	13/3217 (0.4%)
2	B	0.85	0/860	0.99	3/1162 (0.3%)
2	E	0.79	0/860	0.92	1/1162 (0.1%)
3	C	1.27	0/73	1.32	1/96 (1.0%)
3	F	1.10	0/73	1.22	1/96 (1.0%)
All	All	0.84	2/6589 (0.0%)	1.01	29/8938 (0.3%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	227	ASP	CB-CG	6.48	1.65	1.51
1	D	1	GLY	N-CA	5.28	1.53	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	202	ARG	NE-CZ-NH2	-14.15	113.22	120.30
1	A	202	ARG	NE-CZ-NH2	-12.85	113.88	120.30
1	D	202	ARG	NE-CZ-NH1	12.73	126.67	120.30
1	A	202	ARG	NE-CZ-NH1	11.38	125.99	120.30
2	B	81	ARG	NE-CZ-NH1	9.21	124.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	194	ARG	NE-CZ-NH1	8.78	124.69	120.30
2	B	81	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	D	66	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	A	272	LEU	CA-CB-CG	7.01	131.41	115.30
1	D	272	LEU	CA-CB-CG	6.99	131.37	115.30
1	D	194	ARG	NE-CZ-NH2	-6.84	116.88	120.30
2	E	81	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	D	227	ASP	CB-CG-OD1	6.67	124.31	118.30
1	A	97	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	D	129	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	157	ARG	NE-CZ-NH1	6.14	123.37	120.30
3	C	8	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	D	157	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	129	ASP	CB-CG-OD1	6.04	123.73	118.30
1	D	79	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	D	183	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	161	GLU	O-C-N	-5.70	113.50	123.20
1	A	128	GLU	N-CA-CB	-5.70	100.34	110.60
2	B	38	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	D	97	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	D	6	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	161	GLU	CA-C-N	5.14	126.48	116.20
1	A	30	ASP	CB-CG-OD2	5.12	122.91	118.30
3	F	9	VAL	CG1-CB-CG2	5.05	118.99	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	LEU	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	2287	0	2153	46	1
1	D	2296	0	2158	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	837	0	803	15	1
2	E	837	0	803	11	0
3	C	73	0	78	3	0
3	F	73	0	78	2	0
4	A	12	0	16	5	0
4	B	12	0	16	3	0
4	D	12	0	16	1	0
4	E	6	0	8	0	0
5	A	10	0	13	3	0
5	D	20	0	26	5	0
6	A	12	0	17	3	0
6	B	12	0	18	0	0
6	C	4	0	6	0	0
6	D	12	0	18	1	0
6	E	8	0	12	1	0
7	A	10	0	0	0	0
7	D	5	0	0	4	0
7	E	15	0	0	0	0
8	A	117	0	0	10	0
8	B	71	0	0	4	0
8	C	4	0	0	0	0
8	D	147	0	0	9	0
8	E	65	0	0	1	0
8	F	7	0	0	0	0
All	All	6964	0	6239	120	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 9.

All (120) 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)
8:A:455:HOH:O	1:D:227:ASP:HB2	1.67	0.95
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.07	0.90
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.08	0.88
1:A:75:ARG:O	1:A:79:ARG:NH1	2.08	0.86
1:D:86:ASN:ND2	7:D:308:SO4:O3	2.12	0.83
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.16	0.78
1:A:202:ARG:HD2	1:A:244:TRP:CE3	2.22	0.75
1:D:255:GLN:O	1:D:273:ARG:NH1	2.22	0.72
2:B:51:HIS:HE1	4:B:302:GOL:H32	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:ARG:HH11	1:D:194:ARG:HG2	1.55	0.71
2:B:81:ARG:NH1	8:B:402:HOH:O	2.26	0.69
1:D:202:ARG:HD2	1:D:244:TRP:CE3	2.26	0.69
1:A:263:HIS:CD2	1:A:265:GLY:H	2.11	0.68
1:A:115:GLN:HG2	1:A:125:ALA:HB1	1.77	0.67
8:D:430:HOH:O	2:E:58:LYS:HD3	1.95	0.66
1:D:86:ASN:ND2	7:D:308:SO4:S	2.67	0.65
1:D:62[A]:GLU:HG3	8:D:517:HOH:O	1.96	0.65
1:D:263:HIS:CD2	1:D:265:GLY:H	2.16	0.63
1:A:121:ARG:HD3	8:A:478:HOH:O	1.98	0.63
1:D:108:ARG:HA	1:D:108:ARG:HE	1.63	0.63
1:A:5:LEU:HD21	6:A:306:EDO:H22	1.79	0.63
1:A:115:GLN:HG2	1:A:125:ALA:CB	2.30	0.62
8:D:430:HOH:O	2:E:58:LYS:CD	2.48	0.61
1:D:106:ASP:O	1:D:107:TRP:HB2	2.01	0.60
5:D:304:15P:C4	5:D:304:15P:OXT	2.48	0.60
1:D:51:TRP:HA	4:D:301:GOL:H2	1.82	0.60
1:D:108:ARG:HA	1:D:108:ARG:NE	2.17	0.60
5:D:303:15P:C3	3:F:7:GLU:OE1	2.50	0.60
1:A:131:LYS:HA	1:A:153:ALA:HB1	1.83	0.59
2:B:51:HIS:CE1	4:B:302:GOL:H32	2.37	0.59
1:A:150:ALA:HB1	4:A:301:GOL:H32	1.84	0.59
2:B:34:ASP:HB2	8:B:453:HOH:O	2.02	0.59
1:A:150:ALA:CB	4:A:301:GOL:H12	2.31	0.59
1:A:202:ARG:CD	1:A:244:TRP:CE3	2.85	0.59
1:D:60:TRP:O	1:D:64:THR:HG23	2.03	0.59
2:E:42:ASN:OD1	2:E:77:GLU:HG2	2.03	0.58
1:D:62[A]:GLU:CG	8:D:517:HOH:O	2.52	0.58
2:B:51:HIS:HE1	4:B:302:GOL:C3	2.16	0.58
2:B:46:ILE:HD13	2:B:68:THR:HG21	1.84	0.58
1:D:192:HIS:CE1	2:E:98:ASP:HB3	2.39	0.58
6:A:306:EDO:H12	3:C:1:LEU:C	2.25	0.57
2:B:46:ILE:CD1	2:B:68:THR:HG21	2.36	0.56
1:A:14:ARG:NH2	8:A:404:HOH:O	2.39	0.56
1:A:263:HIS:HD2	1:A:265:GLY:H	1.53	0.55
1:A:106:ASP:O	1:A:107:TRP:HB2	2.05	0.55
2:E:79:ALA:HB3	6:E:103:EDO:H21	1.88	0.54
1:A:77:SER:HA	1:A:80:THR:CG2	2.38	0.54
1:D:202:ARG:CD	1:D:244:TRP:CE3	2.91	0.53
1:A:150:ALA:HB1	4:A:301:GOL:H12	1.91	0.53
1:D:275:LYS:O	1:D:276:PRO:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:PRO:O	1:D:263:HIS:HE1	1.92	0.52
1:D:195:SER:OG	1:D:198:ASP:HB2	2.10	0.52
1:D:270:LEU:HD23	1:D:271:THR:N	2.26	0.51
1:A:210:PRO:O	1:A:263:HIS:HE1	1.93	0.51
1:D:226:GLN:H	1:D:226:GLN:HE21	1.59	0.51
1:A:58:GLU:OE2	1:D:226:GLN:HA	2.10	0.50
1:D:229:GLU:OE2	8:D:401:HOH:O	2.20	0.50
1:A:115:GLN:HG3	8:A:431:HOH:O	2.10	0.50
1:A:161:GLU:O	1:A:162:GLY:C	2.50	0.50
1:D:86:ASN:ND2	7:D:308:SO4:O2	2.45	0.50
1:A:46:GLU:HG2	5:A:303:15P:C2	2.42	0.50
1:D:202:ARG:HD3	1:D:246:ALA:HB2	1.95	0.49
1:D:30:ASP:OD1	6:D:305:EDO:H12	2.11	0.49
2:E:0:MET:N	8:E:205:HOH:O	2.45	0.49
5:D:304:15P:O3	5:D:304:15P:H14	2.12	0.49
1:D:219:LEU:HG	1:D:257:TYR:CE2	2.47	0.49
1:D:219:LEU:HG	1:D:257:TYR:CZ	2.48	0.48
1:D:270:LEU:HD22	1:D:272:LEU:CD1	2.44	0.48
1:D:159:TYR:CD2	3:F:3:LEU:HD22	2.48	0.48
1:A:76:VAL:O	1:A:80:THR:HG22	2.13	0.48
1:A:91:GLY:HA3	8:A:423:HOH:O	2.13	0.48
1:D:0:MET:HG2	1:D:264:LYS:HZ1	1.79	0.48
1:D:169:ARG:O	1:D:169:ARG:HD2	2.14	0.48
1:D:60:TRP:O	1:D:64:THR:CG2	2.62	0.48
1:A:194:ARG:HD3	8:A:489:HOH:O	2.13	0.48
1:A:181:ARG:HD2	1:A:183:ASP:OD1	2.13	0.47
1:A:177:GLU:OE2	2:E:6:LYS:NZ	2.48	0.47
1:D:83:ARG:O	7:D:308:SO4:S	2.72	0.47
1:A:121:ARG:HG3	8:A:478:HOH:O	2.14	0.47
2:B:50:GLU:OE1	8:B:401:HOH:O	2.20	0.47
1:A:190:THR:OG1	1:A:192:HIS:HE1	1.98	0.47
6:A:306:EDO:H12	3:C:1:LEU:O	2.14	0.47
2:B:81:ARG:HH11	2:B:81:ARG:HG2	1.79	0.46
1:D:195:SER:HG	1:D:198:ASP:HB2	1.80	0.46
1:A:255:GLN:CD	1:A:255:GLN:H	2.18	0.46
1:D:0:MET:HG2	1:D:264:LYS:NZ	2.31	0.46
1:D:111:ARG:HG2	1:D:113:TYR:CZ	2.51	0.45
1:D:263:HIS:HD2	1:D:265:GLY:H	1.63	0.45
2:B:4:THR:HB	2:B:86:THR:OG1	2.16	0.45
1:A:121:ARG:HB3	2:B:1:ILE:HD12	1.98	0.45
5:D:304:15P:OXT	5:D:304:15P:H14	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ALA:O	4:A:301:GOL:O2	2.20	0.45
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.52	0.45
5:D:304:15P:H25	8:D:485:HOH:O	2.17	0.44
1:D:83:ARG:NH1	8:D:405:HOH:O	2.40	0.44
1:D:0:MET:HG3	1:D:264:LYS:HE2	1.99	0.44
1:D:197:VAL:O	1:D:197:VAL:CG2	2.65	0.44
1:A:202:ARG:HD3	1:A:246:ALA:HB2	1.99	0.44
1:A:46:GLU:HG2	5:A:303:15P:H12	2.00	0.44
2:B:46:ILE:HD11	2:B:68:THR:OG1	2.18	0.44
1:A:196:GLN:H	1:A:196:GLN:CD	2.22	0.43
1:A:144:ARG:CZ	8:A:427:HOH:O	2.66	0.43
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.54	0.42
2:B:91:LYS:HE2	8:B:439:HOH:O	2.20	0.42
2:E:73:THR:HG23	2:E:76:ASP:OD2	2.20	0.42
2:E:81:ARG:HG3	2:E:92:ILE:CD1	2.49	0.42
1:D:176:ASN:ND2	8:D:402:HOH:O	2.32	0.42
1:A:82:GLN:NE2	8:A:412:HOH:O	2.52	0.42
1:D:255:GLN:H	1:D:255:GLN:NE2	2.17	0.42
1:A:115:GLN:HE21	1:A:115:GLN:HB2	1.33	0.42
1:A:46:GLU:HG2	5:A:303:15P:H22	2.00	0.42
1:A:143:THR:OG1	3:C:9:VAL:HG13	2.20	0.42
1:A:184:SER:HB2	2:E:0:MET:O	2.21	0.41
2:E:33:SER:HB3	2:E:62:PHE:CE2	2.55	0.41
1:D:192:HIS:O	1:D:199:VAL:HG23	2.20	0.41
1:A:87:GLN:NE2	8:A:414:HOH:O	2.53	0.41
1:A:14:ARG:HA	1:A:15:PRO:HD3	2.00	0.41
1:A:152:ASP:OD1	4:A:301:GOL:H32	2.21	0.40
1:D:187:ALA:HA	1:D:204:TRP:O	2.20	0.40
1:D:14:ARG:NH2	8:D:414:HOH:O	2.55	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)
1:A:129:ASP:O	2:B:45:ARG:NH1[2_645]	2.19	0.01

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	275/277 (99%)	268 (98%)	7 (2%)	0	100	100
1	D	276/277 (100%)	268 (97%)	8 (3%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	E	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	761/772 (99%)	743 (98%)	18 (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	236/236 (100%)	212 (90%)	24 (10%)	9	1
1	D	237/236 (100%)	213 (90%)	24 (10%)	9	1
2	B	95/95 (100%)	87 (92%)	8 (8%)	14	2
2	E	95/95 (100%)	90 (95%)	5 (5%)	28	10
3	C	8/8 (100%)	7 (88%)	1 (12%)	6	0
3	F	8/8 (100%)	7 (88%)	1 (12%)	6	0
All	All	679/678 (100%)	616 (91%)	63 (9%)	11	2

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	45	PHE
1	A	65	GLN
1	A	70	ASP
1	A	72	GLN
1	A	79	ARG
1	A	80	THR
1	A	86	ASN
1	A	89	LYS
1	A	95	PHE
1	A	98	MET
1	A	105	SER
1	A	107	TRP
1	A	108	ARG
1	A	110	LEU
1	A	115	GLN
1	A	121	ARG
1	A	142	ILE
1	A	169	ARG
1	A	181	ARG
1	A	184	SER
1	A	226	GLN
1	A	272	LEU
1	A	274	TRP
2	B	4	THR
2	B	44	GLU
2	B	45	ARG
2	B	46	ILE
2	B	58	LYS
2	B	70	PHE
2	B	75	LYS
2	B	77	GLU
3	C	1	LEU
1	D	0	MET
1	D	44	ARG
1	D	45	PHE
1	D	64	THR
1	D	70	ASP
1	D	72	GLN
1	D	79	ARG
1	D	95	PHE
1	D	98	MET

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Mol	Chain	Res	Type
1	D	107	TRP
1	D	108	ARG
1	D	110	LEU
1	D	141	LEU
1	D	169	ARG
1	D	176	ASN
1	D	181	ARG
1	D	184	SER
1	D	194	ARG
1	D	197	VAL
1	D	219	LEU
1	D	224	LEU
1	D	226	GLN
1	D	255	GLN
1	D	272	LEU
2	E	48	LYS
2	E	58	LYS
2	E	70	PHE
2	E	73	THR
2	E	75	LYS
3	F	9	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	115	GLN
1	A	192	HIS
1	A	263	HIS
2	B	51	HIS
1	D	86	ASN
1	D	220	ASN
1	D	226	GLN
1	D	255	GLN
1	D	263	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

28 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	$\# Z > 2$
4	GOL	A	301	-	5,5,5	1.03	0	5,5,5	2.05	2 (40%)
4	GOL	A	302	-	5,5,5	0.39	0	5,5,5	0.44	0
5	15P	A	303	-	9,9,103	0.51	0	8,8,102	0.49	0
6	EDO	A	304	-	3,3,3	0.51	0	2,2,2	0.46	0
6	EDO	A	305	-	3,3,3	0.46	0	2,2,2	0.40	0
6	EDO	A	306	-	3,3,3	0.74	0	2,2,2	0.70	0
7	SO4	A	307	-	4,4,4	0.49	0	6,6,6	0.55	0
7	SO4	A	308	-	4,4,4	0.49	0	6,6,6	0.14	0
4	GOL	B	301	-	5,5,5	1.18	0	5,5,5	1.23	0
4	GOL	B	302	-	5,5,5	0.32	0	5,5,5	0.95	0
6	EDO	B	303	-	3,3,3	0.55	0	2,2,2	0.26	0
6	EDO	B	304	-	3,3,3	0.72	0	2,2,2	0.15	0
6	EDO	B	305	-	3,3,3	0.72	0	2,2,2	0.39	0
6	EDO	C	101	-	3,3,3	0.39	0	2,2,2	0.44	0
4	GOL	D	301	-	5,5,5	0.36	0	5,5,5	0.62	0
4	GOL	D	302	-	5,5,5	0.31	0	5,5,5	0.69	0
5	15P	D	303	-	9,9,103	0.74	0	8,8,102	0.90	0
5	15P	D	304	-	9,9,103	1.17	1 (11%)	8,8,102	1.23	1 (12%)
6	EDO	D	305	-	3,3,3	0.53	0	2,2,2	0.54	0
6	EDO	D	306	-	3,3,3	0.61	0	2,2,2	0.51	0
6	EDO	D	307	-	3,3,3	0.41	0	2,2,2	0.40	0
7	SO4	D	308	-	4,4,4	0.73	0	6,6,6	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	E	101	-	5,5,5	0.66	0	5,5,5	0.54	0
6	EDO	E	102	-	3,3,3	0.21	0	2,2,2	0.69	0
6	EDO	E	103	-	3,3,3	0.40	0	2,2,2	0.68	0
7	SO4	E	104	-	4,4,4	0.44	0	6,6,6	0.23	0
7	SO4	E	105	-	4,4,4	0.35	0	6,6,6	0.23	0
7	SO4	E	106	-	4,4,4	0.40	0	6,6,6	0.15	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	GOL	A	301	-	-	0/4/4/4	0/0/0/0
4	GOL	A	302	-	-	0/4/4/4	0/0/0/0
5	15P	A	303	-	-	0/7/7/101	0/0/0/0
6	EDO	A	304	-	-	0/1/1/1	0/0/0/0
6	EDO	A	305	-	-	0/1/1/1	0/0/0/0
6	EDO	A	306	-	-	0/1/1/1	0/0/0/0
7	SO4	A	307	-	-	0/0/0/0	0/0/0/0
7	SO4	A	308	-	-	0/0/0/0	0/0/0/0
4	GOL	B	301	-	-	0/4/4/4	0/0/0/0
4	GOL	B	302	-	-	0/4/4/4	0/0/0/0
6	EDO	B	303	-	-	0/1/1/1	0/0/0/0
6	EDO	B	304	-	-	0/1/1/1	0/0/0/0
6	EDO	B	305	-	-	0/1/1/1	0/0/0/0
6	EDO	C	101	-	-	0/1/1/1	0/0/0/0
4	GOL	D	301	-	-	0/4/4/4	0/0/0/0
4	GOL	D	302	-	-	0/4/4/4	0/0/0/0
5	15P	D	303	-	-	0/7/7/101	0/0/0/0
5	15P	D	304	-	-	0/7/7/101	0/0/0/0
6	EDO	D	305	-	-	0/1/1/1	0/0/0/0
6	EDO	D	306	-	-	0/1/1/1	0/0/0/0
6	EDO	D	307	-	-	0/1/1/1	0/0/0/0
7	SO4	D	308	-	-	0/0/0/0	0/0/0/0
4	GOL	E	101	-	-	0/4/4/4	0/0/0/0
6	EDO	E	102	-	-	0/1/1/1	0/0/0/0
6	EDO	E	103	-	-	0/1/1/1	0/0/0/0
7	SO4	E	104	-	-	0/0/0/0	0/0/0/0
7	SO4	E	105	-	-	0/0/0/0	0/0/0/0
7	SO4	E	106	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	304	15P	O2-C4	-2.03	1.33	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	GOL	O2-C2-C3	-2.73	95.34	108.47
5	D	304	15P	O1-C3-C4	-2.04	101.36	110.40
4	A	301	GOL	C3-C2-C1	2.91	123.31	111.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	GOL	5	0
5	A	303	15P	3	0
6	A	306	EDO	3	0
4	B	302	GOL	3	0
4	D	301	GOL	1	0
5	D	303	15P	1	0
5	D	304	15P	4	0
6	D	305	EDO	1	0
7	D	308	SO4	4	0
6	E	103	EDO	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%)	0.16	13 (4%) 35 33	15, 29, 55, 72	0
1	D	277/277 (100%)	-0.05	5 (1%) 71 71	16, 26, 45, 66	0
2	B	100/100 (100%)	-0.13	0 100 100	15, 26, 44, 52	0
2	E	100/100 (100%)	0.00	2 (2%) 68 67	16, 27, 46, 52	0
3	C	9/9 (100%)	0.05	0 100 100	20, 23, 30, 31	0
3	F	9/9 (100%)	-0.14	0 100 100	22, 24, 27, 28	0
All	All	772/772 (100%)	0.02	20 (2%) 59 57	15, 27, 48, 72	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	LEU	6.7
1	D	41	ASP	4.0
1	A	90	GLY	3.3
1	A	276	PRO	3.2
1	D	42	ASN	3.2
1	A	108	ARG	2.8
1	D	0	MET	2.7
1	A	257	TYR	2.6
1	D	16	GLY	2.6
1	A	220	ASN	2.6
1	A	41	ASP	2.5
1	A	42	ASN	2.4
2	E	48	LYS	2.4
1	A	16	GLY	2.4
1	A	274	TRP	2.3
1	A	107	TRP	2.2
1	D	276	PRO	2.1
2	E	74	GLU	2.1
1	A	91	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	268	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	EDO	B	305	4/4	0.53	0.17	8.17	38,39,42,43	0
5	15P	D	304	10/104	0.84	0.15	6.34	20,25,36,37	0
4	GOL	A	302	6/6	0.52	0.32	5.43	52,63,65,68	0
4	GOL	E	101	6/6	0.28	0.28	5.40	49,56,57,57	0
4	GOL	B	302	6/6	0.82	0.17	5.14	32,36,38,40	0
4	GOL	D	301	6/6	0.76	0.23	4.94	45,48,50,50	0
6	EDO	A	306	4/4	0.92	0.16	4.62	8,9,13,16	0
6	EDO	B	304	4/4	0.78	0.18	4.20	37,44,45,48	0
7	SO4	A	307	5/5	0.94	0.20	3.90	57,59,62,63	0
4	GOL	D	302	6/6	0.63	0.24	3.01	49,53,53,56	0
4	GOL	A	301	6/6	0.89	0.15	2.93	27,28,29,32	0
7	SO4	E	106	5/5	0.86	0.28	1.89	76,79,95,96	0
6	EDO	D	305	4/4	0.84	0.16	1.71	38,39,40,40	0
4	GOL	B	301	6/6	0.88	0.13	1.38	24,32,37,41	0
5	15P	D	303	10/104	0.82	0.14	1.19	36,41,44,47	0
5	15P	A	303	10/104	0.73	0.21	0.87	50,55,59,60	0
7	SO4	E	105	5/5	0.94	0.14	0.75	76,76,80,81	0
6	EDO	D	306	4/4	0.93	0.09	0.58	32,35,35,36	0
6	EDO	C	101	4/4	0.90	0.12	0.57	33,33,34,34	0
7	SO4	D	308	5/5	0.89	0.19	0.46	18,21,25,28	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	EDO	D	307	4/4	0.91	0.10	-0.40	30,32,33,36	0
6	EDO	E	102	4/4	0.91	0.08	-0.70	18,20,20,24	0
6	EDO	E	103	4/4	0.91	0.08	-1.60	33,33,34,37	0
7	SO4	A	308	5/5	0.84	0.34	-	80,90,92,98	0
7	SO4	E	104	5/5	0.79	0.22	-	39,40,42,43	5
6	EDO	B	303	4/4	0.78	0.14	-	43,47,48,48	0
6	EDO	A	304	4/4	0.85	0.12	-	48,48,48,50	0
6	EDO	A	305	4/4	0.81	0.15	-	47,48,49,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.