



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:49 PM UTC

PDB ID : 4JFP / pdb_00004jfp
Title : A2 HLA complex with G4A heteroclitic variant of Melanoma peptide
Authors : Rizkallah, P.J.; Cole, D.K.; Madura, F.; Sewell, A.K.
Deposited on : 2013-02-28
Resolution : 1.91 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

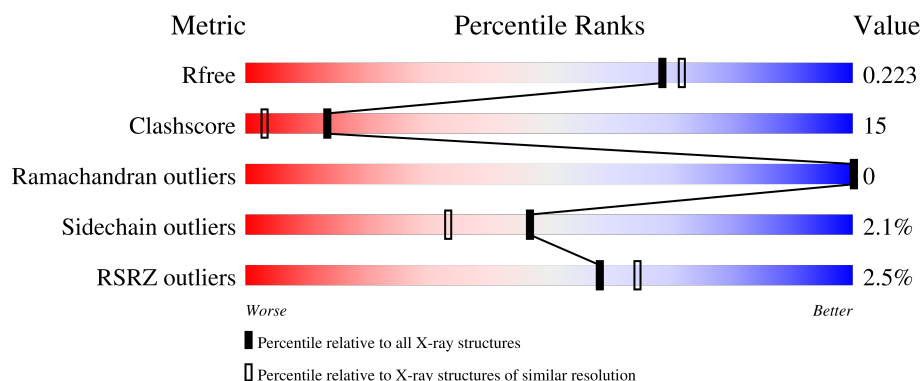
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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.



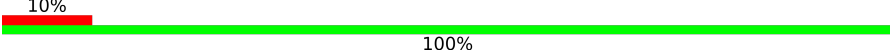
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	276	2% 75% 22% .
1	D	276	3% 77% 22% .
2	B	100	% 84% 16%
2	E	100	4% 83% 16% .
3	C	10	80% 20%

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Mol	Chain	Length	Quality of chain
3	F	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
4	GOL	B	303	-	-	X	-
4	GOL	B	304	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7089 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	13	0
			2364	1479	427	449	9			
1	D	276	Total	C	N	O	S	0	11	0
			2332	1456	422	444	10			

- 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	2	0
			857	545	147	161	4			
2	E	100	Total	C	N	O	S	0	4	0
			868	554	146	164	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 G4A heteroclitic Melanoma peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			70	46	10	14			
3	F	10	Total	C	N	O	0	0	0
			70	46	10	14			

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



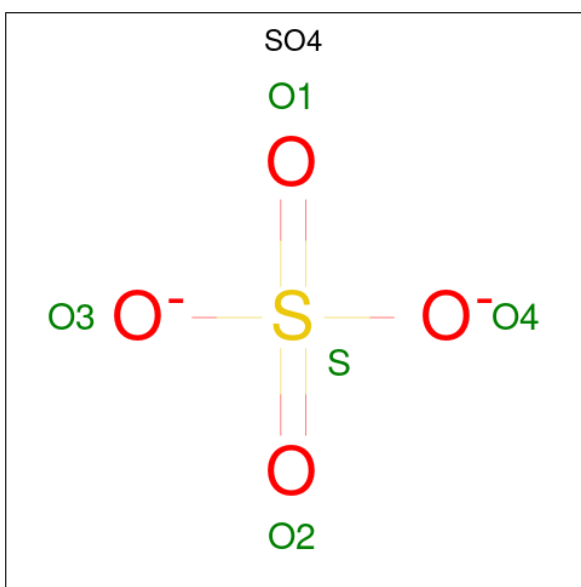
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



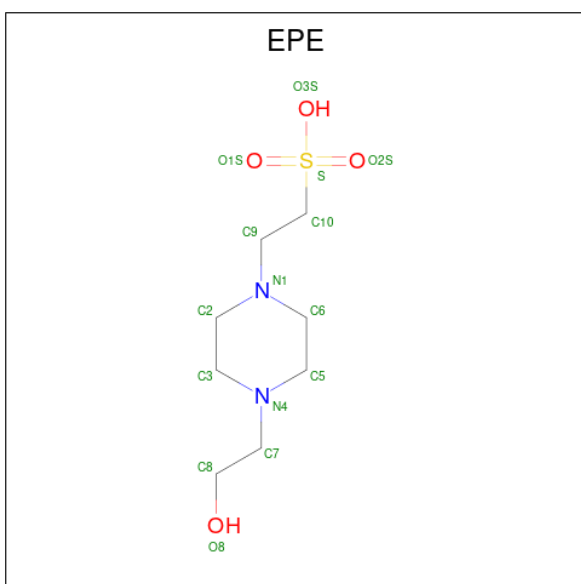
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

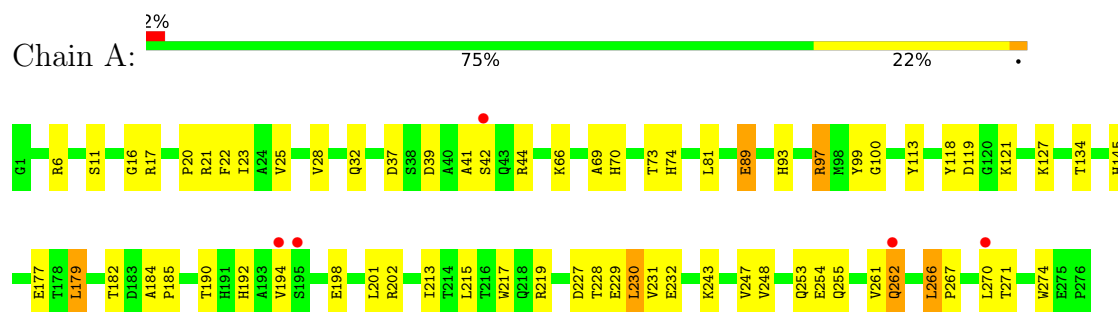
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	147	Total	O	0	0
			147	147		
8	B	89	Total	O	0	0
			89	89		
8	C	8	Total	O	0	0
			8	8		
8	D	109	Total	O	0	0
			109	109		
8	E	71	Total	O	0	0
			71	71		
8	F	3	Total	O	0	0
			3	3		

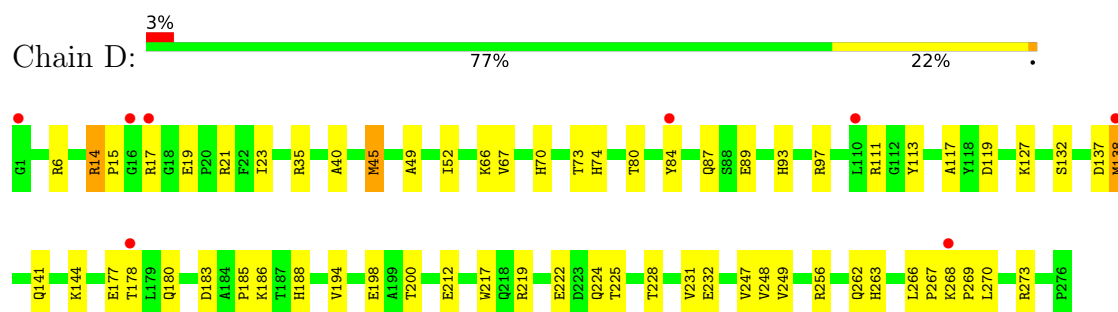
3 Residue-property plots

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.

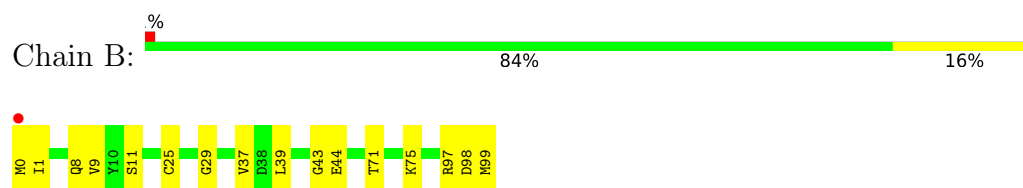
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



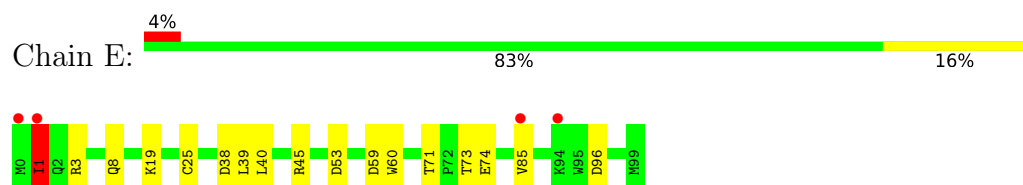
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



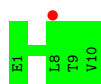
- Molecule 3: G4A heteroclitic Melanoma peptide

Chain C:  80% 20%



- Molecule 3: G4A heteroclitic Melanoma peptide

Chain F:  10% 100%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	202.59Å 49.11Å 117.60Å 90.00° 123.02° 90.00°	Depositor
Resolution (Å)	39.71 – 1.91 39.71 – 1.91	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.71-1.91) 97.8 (39.71-1.91)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.228 0.192 , 0.223	Depositor DCC
R_{free} test set	3730 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.042 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7089	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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: EDO, GOL, EPE, 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	1.26	6/2431 (0.2%)	0.79	1/3301 (0.0%)
1	D	1.19	2/2398 (0.1%)	0.78	3/3258 (0.1%)
2	B	1.44	2/880 (0.2%)	0.83	0/1187
2	E	1.25	1/891 (0.1%)	0.82	1/1205 (0.1%)
3	C	1.32	0/69	0.70	0/92
3	F	1.13	0/69	0.76	0/92
All	All	1.26	11/6738 (0.2%)	0.80	5/9135 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	VAL	CA-CB	-6.72	1.46	1.54
1	A	97	ARG	N-CA	-6.19	1.38	1.46
1	A	213	ILE	CA-CB	6.08	1.62	1.55
2	E	1	ILE	CA-CB	6.03	1.61	1.54
2	B	44	GLU	N-CA	5.75	1.52	1.46
1	A	271	THR	C-O	-5.48	1.17	1.24
1	D	188	HIS	C-O	5.38	1.30	1.23
1	A	179	LEU	CA-C	5.29	1.59	1.52
1	A	100	GLY	CA-C	-5.26	1.46	1.52
1	D	249	VAL	CA-C	5.04	1.56	1.52
1	A	20	PRO	C-O	5.01	1.29	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	249	VAL	N-CA-C	6.35	116.07	108.45
1	A	179	LEU	N-CA-C	6.24	119.06	111.82
2	E	1	ILE	N-CA-C	5.42	116.05	108.89
1	D	45	MET	N-CA-C	-5.24	102.53	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	186	LYS	N-CA-C	-5.12	100.89	109.24

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	2364	0	2205	81	0
1	D	2332	0	2173	67	0
2	B	857	0	827	33	0
2	E	868	0	840	20	0
3	C	70	0	81	4	0
3	F	70	0	81	0	0
4	A	6	0	8	1	0
4	B	24	0	30	16	0
4	E	12	0	15	3	0
5	A	8	0	12	1	0
5	B	4	0	6	0	0
5	D	8	0	12	0	0
5	E	4	0	6	0	0
6	A	10	0	0	0	0
6	B	10	0	0	0	0
7	D	15	0	18	1	0
8	A	147	0	0	3	0
8	B	89	0	0	2	0
8	C	8	0	0	1	0
8	D	109	0	0	5	0
8	E	71	0	0	5	0
8	F	3	0	0	0	0
All	All	7089	0	6314	191	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 15.

All (191) 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:225:THR:O	1:D:228:THR:HG22	1.49	1.13
2:B:97[B]:ARG:HD2	2:B:97[B]:ARG:N	1.66	1.11
2:B:97[B]:ARG:H	2:B:97[B]:ARG:CD	1.61	1.10
2:B:11:SER:H	4:B:303:GOL:H31	1.15	1.09
1:A:261[A]:VAL:HG22	1:A:270:LEU:HB2	1.40	1.00
2:E:85[B]:VAL:HG23	8:E:433:HOH:O	1.62	0.98
2:B:97[B]:ARG:HD2	2:B:97[B]:ARG:H	0.81	0.96
1:D:138:MET:N	1:D:138:MET:HE3	1.84	0.92
1:D:266:LEU:CD2	1:D:270[A]:LEU:HD23	2.01	0.90
1:D:266:LEU:HD23	1:D:270[A]:LEU:HD23	1.54	0.90
2:E:1:ILE:HD11	2:E:3:ARG:HG3	1.55	0.88
1:A:261[A]:VAL:CG2	1:A:270:LEU:HB2	2.04	0.88
1:A:127:LYS:NZ	1:A:134:THR:OG1	2.08	0.86
2:B:11:SER:N	4:B:303:GOL:H31	1.92	0.85
1:A:190[A]:THR:HG21	2:B:98:ASP:OD2	1.75	0.84
4:B:303:GOL:H32	8:B:434:HOH:O	1.77	0.83
1:A:231[A]:VAL:HG11	2:B:8:GLN:OE1	1.78	0.83
1:A:69:ALA:O	1:A:73:THR:HG23	1.82	0.79
1:D:194:VAL:CG1	1:D:200[A]:THR:HG23	2.12	0.79
1:A:121:LYS:CG	2:B:1:ILE:HD11	2.13	0.78
1:D:194:VAL:HG11	1:D:200[A]:THR:HG23	1.63	0.78
1:D:70:HIS:O	1:D:73[A]:THR:HG22	1.85	0.77
1:D:225:THR:O	1:D:228:THR:CG2	2.33	0.75
2:E:1:ILE:O	2:E:1:ILE:HD13	1.85	0.75
1:D:266:LEU:HD23	1:D:270[A]:LEU:CD2	2.17	0.75
1:A:39:ASP:OD1	5:A:303:EDO:O1	2.02	0.74
1:A:192:HIS:HE1	2:B:98:ASP:OD2	1.70	0.74
2:E:71[A]:THR:HG23	8:E:455:HOH:O	1.87	0.74
1:D:231[A]:VAL:HG11	2:E:8:GLN:OE1	1.88	0.73
1:A:121:LYS:HG2	2:B:1:ILE:HD11	1.71	0.73
2:B:11:SER:H	4:B:303:GOL:C3	1.99	0.72
2:E:1:ILE:HD13	2:E:1:ILE:C	2.14	0.72
1:A:121:LYS:HG3	2:B:1:ILE:CD1	2.19	0.72
1:A:93:HIS:HD2	1:A:119:ASP:OD1	1.71	0.72
3:C:8:LEU:HD23	3:C:9:THR:N	2.05	0.72
1:A:230:LEU:HD21	1:A:243:LYS:HE3	1.72	0.71
1:A:21:ARG:NH2	1:A:23:ILE:HD11	2.05	0.70
1:D:266:LEU:CD2	1:D:270[A]:LEU:CD2	2.69	0.70
3:C:8:LEU:HD21	8:C:103:HOH:O	1.91	0.70
2:B:99:MET:O	4:B:304:GOL:H32	1.91	0.70
1:A:227:ASP:HB3	1:A:248:VAL:HG12	1.75	0.68
1:A:190[A]:THR:HG22	1:A:202:ARG:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:73:THR:HG22	2:E:74:GLU:H	1.58	0.68
1:A:267:PRO:HB3	1:D:177:GLU:HB2	1.77	0.67
1:D:21:ARG:NH2	1:D:23:ILE:HD11	2.10	0.67
1:D:267:PRO:O	1:D:268:LYS:HD2	1.95	0.67
1:D:270[A]:LEU:HD22	1:D:270[A]:LEU:N	2.08	0.67
1:A:261[A]:VAL:HG23	1:A:261[A]:VAL:O	1.95	0.66
1:A:93:HIS:HE1	8:A:422:HOH:O	1.79	0.66
2:E:73:THR:HG22	2:E:74:GLU:N	2.11	0.66
1:D:217:TRP:CD1	1:D:247[B]:VAL:HG23	2.31	0.65
1:A:266:LEU:CD2	1:A:270:LEU:HD23	2.27	0.65
1:D:185:PRO:HD2	1:D:266:LEU:CD1	2.26	0.65
1:D:267:PRO:C	1:D:268:LYS:HD2	2.22	0.65
1:D:200[A]:THR:HG21	8:D:481:HOH:O	1.97	0.64
1:D:87:GLN:HG2	7:D:303:EPE:H31	1.79	0.64
1:A:230:LEU:HD21	1:A:243:LYS:CE	2.27	0.64
1:A:121:LYS:CG	2:B:1:ILE:CD1	2.77	0.63
1:A:190[A]:THR:CG2	1:A:202:ARG:HB3	2.29	0.63
1:A:266:LEU:HG	1:A:270:LEU:CD2	2.29	0.63
1:A:217:TRP:CD1	1:A:247:VAL:HG13	2.33	0.63
2:B:99:MET:HE2	4:B:304:GOL:H31	1.80	0.62
1:D:266:LEU:HG	1:D:270[A]:LEU:HD21	1.81	0.62
2:E:85[A]:VAL:HG13	8:E:433:HOH:O	1.99	0.62
1:D:15:PRO:HB3	1:D:89:GLU:O	1.99	0.61
1:D:137:ASP:C	1:D:138:MET:HE3	2.25	0.61
1:A:230:LEU:C	1:A:230:LEU:HD23	2.25	0.61
2:B:11:SER:OG	4:B:303:GOL:C3	2.49	0.61
1:D:194:VAL:HG11	1:D:200[A]:THR:CG2	2.31	0.60
1:D:74:HIS:HE1	1:D:97:ARG:HE	1.48	0.59
1:D:266:LEU:HD21	1:D:270[A]:LEU:HD23	1.84	0.59
1:A:121:LYS:HG3	2:B:1:ILE:HD12	1.86	0.58
1:D:185:PRO:HD2	1:D:266:LEU:HD13	1.87	0.57
1:A:230:LEU:HD23	1:A:231[A]:VAL:N	2.19	0.57
2:B:99:MET:HB3	4:B:304:GOL:H32	1.87	0.57
1:A:266:LEU:HG	1:A:270:LEU:HD21	1.87	0.56
1:D:49:ALA:O	1:D:52:ILE:HG22	2.05	0.56
1:A:266:LEU:HD23	1:A:270:LEU:HD23	1.88	0.56
2:B:43:GLY:HA2	4:B:301:GOL:H12	1.88	0.55
1:A:230:LEU:HD23	1:A:231[B]:VAL:O	2.07	0.55
1:A:230:LEU:HD23	1:A:231[B]:VAL:N	2.21	0.55
1:A:121:LYS:HG3	2:B:1:ILE:HD11	1.84	0.55
1:A:230:LEU:HD21	1:A:243:LYS:NZ	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:VAL:HG13	1:A:248:VAL:O	2.06	0.55
1:A:255:GLN:NE2	1:A:274:TRP:O	2.37	0.55
1:A:41:ALA:H	4:A:301:GOL:HO2	1.53	0.55
1:D:178:THR:HG22	8:D:495:HOH:O	2.07	0.54
2:B:11:SER:OG	4:B:303:GOL:H31	2.06	0.54
1:D:231[A]:VAL:HG12	1:D:232:GLU:O	2.08	0.53
1:D:194:VAL:HG13	1:D:200[A]:THR:HG23	1.88	0.53
1:A:25[A]:VAL:HG23	1:A:32:GLN:OE1	2.07	0.53
1:D:180:GLN:OE1	1:D:183:ASP:OD1	2.27	0.53
1:D:231[A]:VAL:CG1	2:E:8:GLN:OE1	2.56	0.53
2:E:1:ILE:HD11	2:E:3:ARG:CG	2.34	0.53
1:A:219:ARG:HH12	1:A:253:GLN:NE2	2.07	0.53
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.44	0.52
1:A:89:GLU:H	1:A:89:GLU:CD	2.18	0.52
1:A:261[A]:VAL:CG2	1:A:261[A]:VAL:O	2.58	0.52
1:A:192:HIS:CE1	2:B:98:ASP:OD2	2.59	0.52
1:A:194:VAL:HG12	1:A:198:GLU:O	2.10	0.52
1:A:230:LEU:C	1:A:230:LEU:CD2	2.83	0.52
1:A:227:ASP:HB3	1:A:248:VAL:CG1	2.39	0.51
1:D:21:ARG:HH21	1:D:23:ILE:HD11	1.75	0.51
1:A:228:THR:HG22	1:A:229:GLU:N	2.26	0.51
2:B:11:SER:OG	4:B:303:GOL:H32	2.10	0.51
1:D:185:PRO:HD2	1:D:266:LEU:HD11	1.92	0.50
1:D:270[A]:LEU:CD2	1:D:270[A]:LEU:N	2.73	0.50
1:A:74:HIS:HE1	1:A:97:ARG:HE	1.59	0.50
1:D:217:TRP:CD1	1:D:247[B]:VAL:CG2	2.95	0.50
1:A:11:SER:OG	1:A:22:PHE:HD1	1.95	0.50
2:B:29:GLY:HA3	4:B:302:GOL:H11	1.94	0.50
1:D:219:ARG:O	1:D:222:GLU:HG2	2.12	0.50
1:A:177[A]:GLU:H	1:A:177[A]:GLU:CD	2.19	0.50
3:C:8:LEU:HD22	3:C:9:THR:O	2.12	0.50
1:A:6:ARG:NE	1:A:113[B]:TYR:OH	2.29	0.49
2:B:99:MET:HB3	4:B:304:GOL:C3	2.41	0.49
1:D:141:GLN:NE2	1:D:144:LYS:HD3	2.27	0.49
1:A:6:ARG:HD3	1:A:113[B]:TYR:HE1	1.77	0.49
1:A:21:ARG:NH2	1:A:37:ASP:OD1	2.46	0.49
1:D:40:ALA:HB3	8:D:499:HOH:O	2.12	0.49
1:D:200[A]:THR:CG2	8:D:481:HOH:O	2.58	0.49
1:D:14:ARG:HB2	1:D:17:ARG:HB2	1.94	0.49
1:D:127:LYS:HD2	1:D:132:SER:HB2	1.95	0.49
1:A:74:HIS:CE1	1:A:97:ARG:HE	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:NE	1:A:39:ASP:OD2	2.46	0.48
2:E:38:ASP:OD1	2:E:45:ARG:NH2	2.44	0.48
1:A:185:PRO:HD2	1:A:266:LEU:HD13	1.96	0.48
1:A:201[A]:LEU:HD11	1:A:254:GLU:HG3	1.95	0.48
1:D:80:THR:HG22	1:D:84:TYR:CE2	2.49	0.48
1:A:182:THR:O	1:A:182:THR:HG23	2.13	0.48
1:A:217:TRP:CD1	1:A:247:VAL:CG1	2.97	0.48
1:A:266:LEU:HG	1:A:270:LEU:HD23	1.96	0.47
2:E:25:CYS:HB2	2:E:39:LEU:HD21	1.96	0.47
1:D:93:HIS:HD2	1:D:119:ASP:OD1	1.97	0.47
2:E:96:ASP:HA	4:E:102:GOL:H31	1.95	0.47
1:A:230:LEU:HD23	1:A:231[A]:VAL:O	2.15	0.46
1:D:217:TRP:CG	1:D:247[B]:VAL:CG2	2.98	0.46
4:E:101:GOL:C1	8:E:432:HOH:O	2.63	0.46
1:A:184:ALA:HB1	1:A:266:LEU:CD1	2.46	0.46
1:D:93:HIS:HE1	8:D:420:HOH:O	1.98	0.46
1:D:35:ARG:HD3	2:E:53:ASP:OD2	2.15	0.46
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.50	0.46
3:C:8:LEU:CD2	3:C:9:THR:O	2.64	0.46
1:D:138:MET:HE3	1:D:138:MET:CA	2.46	0.46
1:A:255:GLN:NE2	1:A:255:GLN:HA	2.30	0.45
2:B:9:VAL:O	4:B:304:GOL:H2	2.15	0.45
1:D:217:TRP:CD1	1:D:247[A]:VAL:HG13	2.51	0.45
1:A:219:ARG:HH22	1:A:253:GLN:HE22	1.65	0.45
1:D:66:LYS:O	1:D:70:HIS:HD2	1.99	0.45
1:A:231[A]:VAL:CG1	2:B:8:GLN:CD	2.90	0.45
2:B:99:MET:CB	4:B:304:GOL:H32	2.46	0.45
2:B:99:MET:C	4:B:304:GOL:H32	2.42	0.45
1:D:141:GLN:HE22	1:D:144:LYS:HD3	1.81	0.45
1:A:231[A]:VAL:CG1	2:B:8:GLN:OE1	2.56	0.45
1:A:66:LYS:O	1:A:70:HIS:HD2	2.00	0.44
1:A:145:HIS:ND1	8:A:512:HOH:O	2.35	0.44
1:D:19:GLU:N	1:D:19:GLU:OE2	2.50	0.44
1:D:45:MET:HE2	1:D:67:VAL:HB	1.99	0.44
2:B:25:CYS:HB2	2:B:39:LEU:HD21	2.00	0.44
1:D:74:HIS:CE1	1:D:97:ARG:HE	2.33	0.44
1:D:262[A]:GLN:HE21	1:D:263:HIS:N	2.15	0.43
4:E:101:GOL:H12	8:E:432:HOH:O	2.16	0.43
1:A:255:GLN:HA	1:A:255:GLN:HE21	1.84	0.43
2:B:0:MET:HE2	8:B:489:HOH:O	2.19	0.43
1:A:266:LEU:CG	1:A:270:LEU:HD23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262[A]:GLN:HE21	1:A:262[A]:GLN:CA	2.31	0.43
1:D:262[A]:GLN:HE21	1:D:262[A]:GLN:HA	1.84	0.43
1:D:219:ARG:CZ	1:D:256:ARG:HH11	2.32	0.42
2:E:59:ASP:O	2:E:60:TRP:HB2	2.20	0.42
1:A:16:GLY:C	1:A:17[B]:ARG:HG2	2.45	0.42
1:D:6:ARG:NE	1:D:113:TYR:OH	2.47	0.42
1:D:217:TRP:CG	1:D:247[B]:VAL:HG21	2.54	0.42
2:E:40:LEU:HD23	2:E:45:ARG:HA	2.01	0.42
1:D:14:ARG:HD3	1:D:19:GLU:O	2.19	0.42
1:A:127:LYS:HE2	8:A:493:HOH:O	2.20	0.42
1:D:269:PRO:C	1:D:270[A]:LEU:HD22	2.45	0.42
1:A:42:SER:OG	1:A:44:ARG:HB2	2.20	0.41
2:B:0:MET:HE2	2:B:0:MET:HB2	1.86	0.41
2:E:1:ILE:C	2:E:1:ILE:CD1	2.85	0.41
1:A:231[A]:VAL:CG1	1:A:232:GLU:N	2.82	0.41
1:A:93:HIS:CD2	1:A:119:ASP:OD1	2.61	0.41
1:A:217:TRP:CG	1:A:247:VAL:HG11	2.56	0.41
1:D:70:HIS:C	1:D:73[A]:THR:HG22	2.43	0.41
1:A:28:VAL:HG11	1:A:179:LEU:HD13	2.02	0.41
2:E:19:LYS:HE3	2:E:19:LYS:HB2	1.89	0.41
1:A:70:HIS:HE1	1:A:99:TYR:OH	2.04	0.41
1:D:89:GLU:OE1	1:D:89:GLU:N	2.46	0.41
1:D:198:GLU:HG2	1:D:248[A]:VAL:CG2	2.50	0.41
1:A:230:LEU:CD2	1:A:231[B]:VAL:O	2.68	0.40
1:A:6:ARG:HD3	1:A:113[B]:TYR:CE1	2.54	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	287/276 (104%)	284 (99%)	3 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	285/276 (103%)	280 (98%)	5 (2%)	0	100	100
2	B	100/100 (100%)	100 (100%)	0	0	100	100
2	E	102/100 (102%)	101 (99%)	1 (1%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
3	F	8/10 (80%)	8 (100%)	0	0	100	100
All	All	790/772 (102%)	781 (99%)	9 (1%)	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	245/232 (106%)	239 (98%)	6 (2%)	43	28
1	D	243/232 (105%)	237 (98%)	6 (2%)	42	26
2	B	97/95 (102%)	95 (98%)	2 (2%)	47	33
2	E	99/95 (104%)	98 (99%)	1 (1%)	68	64
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
All	All	698/668 (104%)	683 (98%)	15 (2%)	47	33

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	215	LEU
1	A	230	LEU
1	A	262[A]	GLN
1	A	262[B]	GLN
1	A	266	LEU
2	B	71	THR
2	B	75	LYS

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Mol	Chain	Res	Type
1	D	14	ARG
1	D	111	ARG
1	D	138	MET
1	D	212	GLU
1	D	224	GLN
1	D	273	ARG
2	E	1	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	74	HIS
1	A	86	ASN
1	A	93	HIS
1	A	141	GLN
1	A	174	ASN
1	A	180	GLN
1	A	192	HIS
1	A	226	GLN
1	A	253	GLN
1	A	255	GLN
2	B	13	HIS
2	B	83	ASN
1	D	54	GLN
1	D	70	HIS
1	D	74	HIS
1	D	86	ASN
1	D	87	GLN
1	D	93	HIS
1	D	141	GLN
1	D	174	ASN
1	D	224	GLN
1	D	226	GLN
2	E	13	HIS
2	E	83	ASN
2	E	89	GLN

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 ⓘ

18 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	B	302	-	5,5,5	0.61	0	5,5,5	0.42	0
5	EDO	A	303	-	3,3,3	0.31	0	2,2,2	0.46	0
6	SO4	A	304	-	4,4,4	0.23	0	6,6,6	0.15	0
4	GOL	E	102	-	5,5,5	0.69	0	5,5,5	0.20	0
5	EDO	D	302	-	3,3,3	0.41	0	2,2,2	0.33	0
4	GOL	E	101	-	5,5,5	1.66	1 (20%)	5,5,5	0.63	0
5	EDO	D	301	-	3,3,3	0.60	0	2,2,2	0.35	0
6	SO4	A	305	-	4,4,4	0.35	0	6,6,6	0.08	0
6	SO4	B	307	-	4,4,4	0.23	0	6,6,6	0.10	0
4	GOL	A	301	-	5,5,5	0.61	0	5,5,5	0.26	0
7	EPE	D	303	-	15,15,15	0.76	1 (6%)	19,20,20	0.88	0
6	SO4	B	306	-	4,4,4	0.46	0	6,6,6	0.27	0
4	GOL	B	303	-	5,5,5	1.97	1 (20%)	5,5,5	0.74	0
5	EDO	B	305	-	3,3,3	0.64	0	2,2,2	0.32	0
4	GOL	B	304	-	5,5,5	3.04	1 (20%)	5,5,5	0.61	0
4	GOL	B	301	-	5,5,5	0.62	0	5,5,5	0.22	0
5	EDO	A	302	-	3,3,3	0.31	0	2,2,2	0.47	0
5	EDO	E	103	-	3,3,3	0.42	0	2,2,2	0.51	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	B	302	-	-	0/4/4/4	-
5	EDO	A	303	-	-	0/1/1/1	-
4	GOL	E	102	-	-	2/4/4/4	-
5	EDO	D	302	-	-	0/1/1/1	-
4	GOL	E	101	-	-	3/4/4/4	-
5	EDO	D	301	-	-	1/1/1/1	-
7	EPE	D	303	-	-	5/9/19/19	0/1/1/1
4	GOL	A	301	-	-	4/4/4/4	-
4	GOL	B	303	-	-	1/4/4/4	-
5	EDO	B	305	-	-	0/1/1/1	-
4	GOL	B	304	-	-	2/4/4/4	-
4	GOL	B	301	-	-	3/4/4/4	-
5	EDO	A	302	-	-	1/1/1/1	-
5	EDO	E	103	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	304	GOL	O2-C2	-6.33	1.25	1.43
4	B	303	GOL	O2-C2	-4.27	1.31	1.43
4	E	101	GOL	O2-C2	-3.35	1.33	1.43
7	D	303	EPE	C10-S	2.14	1.80	1.77

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GOL	O1-C1-C2-C3
4	A	301	GOL	C1-C2-C3-O3
4	B	301	GOL	O1-C1-C2-C3
4	E	101	GOL	C1-C2-C3-O3
7	D	303	EPE	C10-C9-N1-C2
7	D	303	EPE	C10-C9-N1-C6
7	D	303	EPE	S-C10-C9-N1
4	B	301	GOL	O1-C1-C2-O2
4	B	304	GOL	O1-C1-C2-C3
4	E	102	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	301	GOL	O2-C2-C3-O3
4	E	101	GOL	O2-C2-C3-O3
4	A	301	GOL	O1-C1-C2-O2
4	B	304	GOL	O1-C1-C2-O2
4	E	102	GOL	O1-C1-C2-O2
5	E	103	EDO	O1-C1-C2-O2
4	E	101	GOL	O1-C1-C2-O2
5	A	302	EDO	O1-C1-C2-O2
5	D	301	EDO	O1-C1-C2-O2
7	D	303	EPE	C9-C10-S-O1S
7	D	303	EPE	C9-C10-S-O2S
4	B	301	GOL	C1-C2-C3-O3
4	B	303	GOL	O2-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	302	GOL	1	0
5	A	303	EDO	1	0
4	E	102	GOL	1	0
4	E	101	GOL	2	0
4	A	301	GOL	1	0
7	D	303	EPE	1	0
4	B	303	GOL	7	0
4	B	304	GOL	7	0
4	B	301	GOL	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	276/276 (100%)	0.11	5 (1%) 67 74	11, 34, 58, 76	13 (4%)
1	D	276/276 (100%)	0.37	8 (2%) 53 60	12, 42, 67, 81	11 (3%)
2	B	100/100 (100%)	-0.20	1 (1%) 79 85	13, 27, 40, 53	2 (2%)
2	E	100/100 (100%)	0.14	4 (4%) 42 47	12, 36, 62, 74	4 (4%)
3	C	10/10 (100%)	-0.05	0 100 100	30, 33, 36, 41	0
3	F	10/10 (100%)	0.84	1 (10%) 12 16	37, 41, 56, 64	0
All	All	772/772 (100%)	0.18	19 (2%) 58 64	11, 36, 62, 81	30 (3%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	VAL	3.8
2	E	1	ILE	3.0
1	D	1	GLY	2.9
2	B	0	MET	2.8
2	E	0	MET	2.8
1	A	270	LEU	2.7
2	E	94[A]	LYS	2.6
1	D	16	GLY	2.4
1	A	195	SER	2.3
2	E	85[A]	VAL	2.3
1	D	17	ARG	2.3
1	D	268	LYS	2.3
1	D	110	LEU	2.2
3	F	8	LEU	2.2
1	D	138	MET	2.1
1	A	42	SER	2.1
1	D	84	TYR	2.0
1	A	262[A]	GLN	2.0
1	D	178	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EPE	D	303	15/15	0.66	0.25	89,91,98,99	0
4	GOL	E	102	6/6	0.73	0.21	61,63,65,67	0
6	SO4	A	304	5/5	0.79	0.18	98,99,99,102	0
4	GOL	B	302	6/6	0.80	0.17	50,57,58,61	0
4	GOL	B	301	6/6	0.80	0.15	34,50,52,54	0
4	GOL	B	304	6/6	0.83	0.21	13,16,21,22	6
4	GOL	A	301	6/6	0.84	0.17	48,55,57,59	0
4	GOL	B	303	6/6	0.84	0.24	10,23,27,30	6
6	SO4	B	307	5/5	0.85	0.15	110,110,111,111	0
5	EDO	A	302	4/4	0.85	0.17	52,52,54,56	0
6	SO4	A	305	5/5	0.87	0.14	86,87,88,89	0
4	GOL	E	101	6/6	0.89	0.12	25,40,45,51	0
5	EDO	A	303	4/4	0.91	0.10	40,44,44,45	0
5	EDO	D	301	4/4	0.91	0.11	40,41,42,42	0
5	EDO	B	305	4/4	0.92	0.10	41,42,42,43	0
5	EDO	E	103	4/4	0.93	0.10	26,36,38,40	0
5	EDO	D	302	4/4	0.95	0.09	48,48,49,50	0
6	SO4	B	306	5/5	0.96	0.11	37,40,43,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.