



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 06:48 pm GMT

PDB ID : 4JFP
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

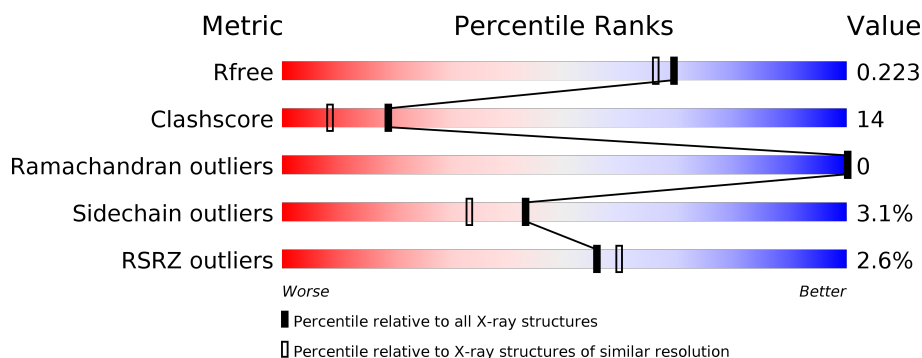
1 Overall quality at a glance

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}	111664	6904 (1.94-1.90)
Clashscore	122126	7577 (1.94-1.90)
Ramachandran outliers	120053	7491 (1.94-1.90)
Sidechain outliers	120020	7491 (1.94-1.90)
RSRZ outliers	108989	6759 (1.94-1.90)

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	276	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>21%</div> <div>.</div> </div> </div>
1	D	276	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>.</div> </div> </div>
2	B	100	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>17%</div> </div> </div>
2	E	100	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>19%</div> <div>.</div> </div> </div>
3	C	10	<div> <div></div> <div> <div></div> <div>80%</div> <div>20%</div> </div> </div>
3	F	10	<div> <div>10%</div> <div> <div></div> <div>100%</div> </div> </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	B	303	-	-	X	-
4	GOL	B	304	-	-	X	-

2 Entry composition [i](#)

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 (three-letter code: 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 (three-letter code: EDO) (formula: C₂H₆O₂).



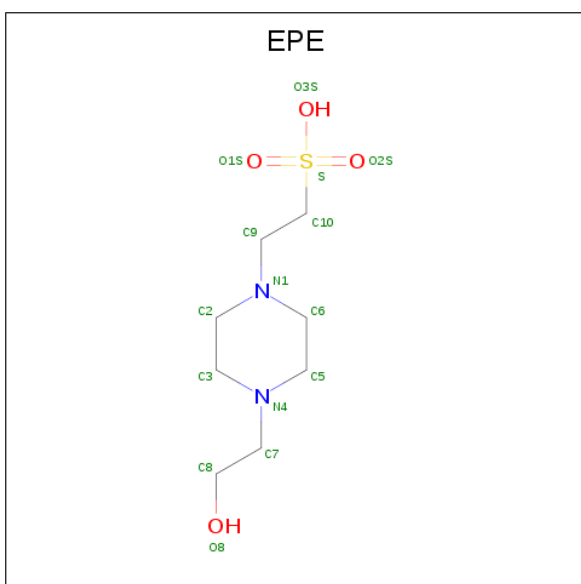
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is SULFATE ION (three-letter code: 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 (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



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

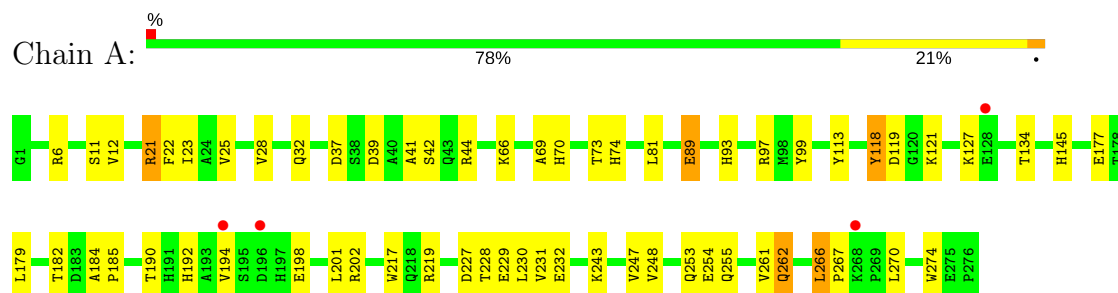
- Molecule 8 is water.

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		

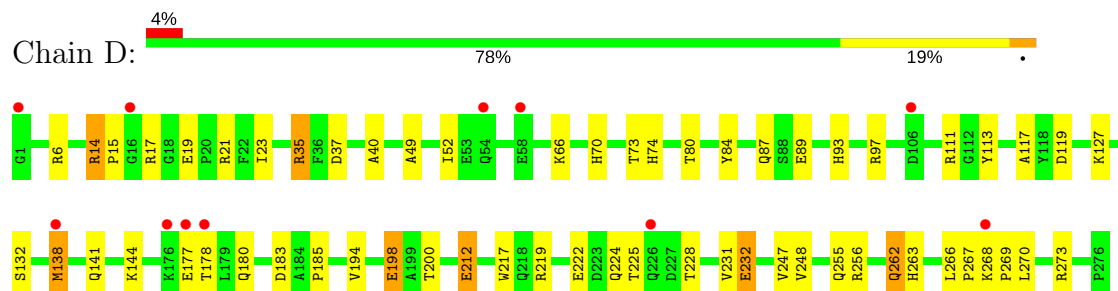
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

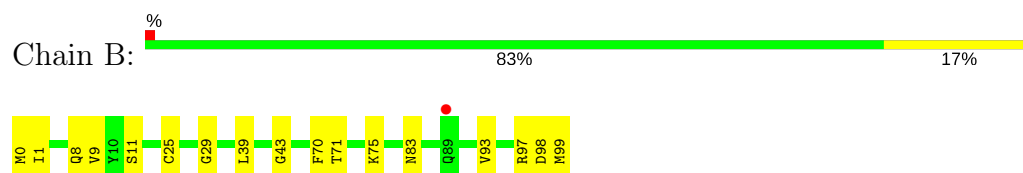
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



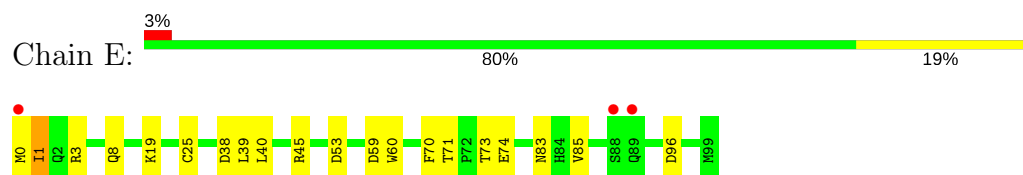
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



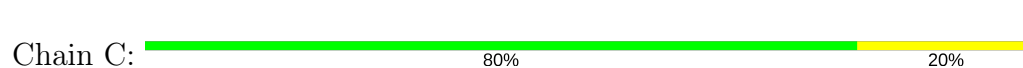
- Molecule 2: Beta-2-microglobulin

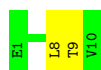


- Molecule 2: Beta-2-microglobulin



- Molecule 3: G4A heteroclitic Melanoma peptide





- 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)	0.33 , 47.4	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: GOL, EPE, SO4, EDO

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	1.07	4/2431 (0.2%)	0.61	0/3301
1	D	1.01	4/2398 (0.2%)	0.59	0/3258
2	B	1.23	1/880 (0.1%)	0.67	0/1187
2	E	1.05	0/891	0.64	0/1205
3	C	1.14	0/69	0.75	0/92
3	F	1.05	0/69	0.69	0/92
All	All	1.07	9/6738 (0.1%)	0.62	0/9135

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	232	GLU	CG-CD	7.85	1.63	1.51
1	D	198	GLU	CB-CG	-6.78	1.39	1.52
1	A	118	TYR	CD1-CE1	6.56	1.49	1.39
1	A	12	VAL	CB-CG2	5.71	1.64	1.52
1	A	89	GLU	CG-CD	5.68	1.60	1.51
1	A	118	TYR	CD2-CE2	5.43	1.47	1.39
1	D	37	ASP	CB-CG	5.27	1.62	1.51
1	D	212	GLU	CG-CD	5.07	1.59	1.51
2	B	93	VAL	CB-CG2	5.05	1.63	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2364	0	2205	80	0
1	D	2332	0	2173	64	0
2	B	857	0	827	30	0
2	E	868	0	840	19	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	14	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	183	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 14.

All (183) 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:CD	2:B:97[B]:ARG:H	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:E:1:ILE:HD13	2:E:1:ILE:C	2.14	0.68
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:N	1:D:270[A]:LEU:HD22	2.08	0.67
1:A:261[A]:VAL:O	1:A:261[A]:VAL:HG23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:190[A]:THR:CG2	1:A:202:ARG:HB3	2.29	0.63
1:A:121:LYS:CG	2:B:1:ILE:CD1	2.77	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
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
2:B:11:SER:OG	4:B:303:GOL:C3	2.49	0.61
1:D:267:PRO:C	1:D:268:LYS:HD2	2.22	0.60
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:A:230:LEU:C	1:A:230:LEU:HD23	2.25	0.57
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:261[A]:VAL:CG2	1:A:261[A]:VAL:O	2.58	0.52
1:A:194:VAL:HG12	1:A:198:GLU:O	2.10	0.52
1:A:192:HIS:CE1	2:B:98:ASP:OD2	2.59	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:N	1:D:270[A]:LEU:CD2	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
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:200[A]:THR:CG2	8:D:481:HOH:O	2.58	0.49
1:D:40:ALA:HB3	8:D:499:HOH:O	2.12	0.49
1:D:127:LYS:HD2	1:D:132:SER:HB2	1.95	0.49
1:D:138:MET:HE3	1:D:138:MET:N	2.28	0.49
1:D:14:ARG:HB2	1:D:17:ARG:HB2	1.94	0.49
1:A:74:HIS:CE1	1:A:97:ARG:HE	2.32	0.48
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:D:138:MET:N	1:D:138:MET:CE	2.77	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:HG23	1:A:182:THR:O	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
1:A:230:LEU:C	1:A:230:LEU:CD2	2.83	0.47
1:A:89:GLU:CD	1:A:89:GLU:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:138:MET:HE2	1:D:138:MET:HA	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:A:255:GLN:HA	1:A:255:GLN:NE2	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:177[A]:GLU:CD	1:A:177[A]:GLU:H	2.19	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
2:B:99:MET:CB	4:B:304:GOL:H32	2.46	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:145:HIS:ND1	8:A:512:HOH:O	2.35	0.44
1:A:66:LYS:O	1:A:70:HIS:HD2	2.00	0.44
1:D:19:GLU:OE2	1:D:19:GLU:N	2.50	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
1:A:266:LEU:CG	1:A:270:LEU:HD23	2.48	0.43
1:A:231[A]:VAL:CG1	1:A:232:GLU:N	2.82	0.43
1:A:262[A]:GLN:HE21	1:A:262[A]:GLN:CA	2.31	0.43
1:D:262[A]:GLN:HA	1:D:262[A]:GLN:HE21	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: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:A:42:SER:OG	1:A:44:ARG:HB2	2.20	0.41
2:B:0:MET:HE2	8:B:489:HOH:O	2.18	0.41
1:A:93:HIS:CD2	1:A:119:ASP:OD1	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:TRP:CG	1:A:247:VAL:HG11	2.56	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:198:GLU:HG2	1:D:248[A]:VAL:CG2	2.50	0.41
1:D:89:GLU:N	1:D:89:GLU:OE1	2.46	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
1:A:231[A]:VAL:CG1	2:B:8:GLN:CD	2.90	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
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%)	241 (98%)	4 (2%)	65	61
1	D	243/232 (105%)	232 (96%)	11 (4%)	30	19
2	B	97/95 (102%)	93 (96%)	4 (4%)	33	22
2	E	99/95 (104%)	95 (96%)	4 (4%)	34	23
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%)	675 (97%)	23 (3%)	43	30

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	262[A]	GLN
1	A	262[B]	GLN
1	A	266	LEU
2	B	70	PHE
2	B	71	THR
2	B	75	LYS
2	B	83	ASN
1	D	14	ARG
1	D	35	ARG
1	D	111	ARG
1	D	138	MET
1	D	212	GLU
1	D	224	GLN
1	D	255	GLN
1	D	262[A]	GLN
1	D	262[B]	GLN
1	D	269	PRO
1	D	273	ARG
2	E	0	MET
2	E	1	ILE
2	E	70	PHE
2	E	83	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) 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	83	ASN
1	D	54	GLN
1	D	70	HIS
1	D	74	HIS
1	D	86	ASN
1	D	93	HIS
1	D	141	GLN
1	D	174	ASN
1	D	224	GLN
1	D	226	GLN
2	E	83	ASN
2	E	89	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	A	301	-	5,5,5	0.61	0	5,5,5	0.23	0
5	EDO	A	302	-	3,3,3	0.36	0	2,2,2	0.46	0
5	EDO	A	303	-	3,3,3	0.35	0	2,2,2	0.46	0
6	SO4	A	304	-	4,4,4	0.17	0	6,6,6	0.13	0
6	SO4	A	305	-	4,4,4	0.29	0	6,6,6	0.10	0
4	GOL	B	301	-	5,5,5	0.59	0	5,5,5	0.20	0
4	GOL	B	302	-	5,5,5	0.60	0	5,5,5	0.40	0
4	GOL	B	303	-	5,5,5	1.95	1 (20%)	5,5,5	0.70	0
4	GOL	B	304	-	5,5,5	3.00	1 (20%)	5,5,5	0.59	0
5	EDO	B	305	-	3,3,3	0.66	0	2,2,2	0.30	0
6	SO4	B	306	-	4,4,4	0.40	0	6,6,6	0.30	0
6	SO4	B	307	-	4,4,4	0.16	0	6,6,6	0.08	0
5	EDO	D	301	-	3,3,3	0.65	0	2,2,2	0.34	0
5	EDO	D	302	-	3,3,3	0.45	0	2,2,2	0.31	0
7	EPE	D	303	-	15,15,15	0.75	1 (6%)	18,20,20	1.01	2 (11%)
4	GOL	E	101	-	5,5,5	1.64	1 (20%)	5,5,5	0.61	0
4	GOL	E	102	-	5,5,5	0.65	0	5,5,5	0.21	0
5	EDO	E	103	-	3,3,3	0.41	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	A	301	-	-	0/4/4/4	0/0/0/0
5	EDO	A	302	-	-	0/1/1/1	0/0/0/0
5	EDO	A	303	-	-	0/1/1/1	0/0/0/0
6	SO4	A	304	-	-	0/0/0/0	0/0/0/0
6	SO4	A	305	-	-	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
4	GOL	B	303	-	-	0/4/4/4	0/0/0/0
4	GOL	B	304	-	-	0/4/4/4	0/0/0/0
5	EDO	B	305	-	-	0/1/1/1	0/0/0/0
6	SO4	B	306	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	B	307	-	-	0/0/0/0	0/0/0/0
5	EDO	D	301	-	-	0/1/1/1	0/0/0/0
5	EDO	D	302	-	-	0/1/1/1	0/0/0/0
7	EPE	D	303	-	-	0/9/19/19	0/1/1/1
4	GOL	E	101	-	-	0/4/4/4	0/0/0/0
4	GOL	E	102	-	-	0/4/4/4	0/0/0/0
5	EDO	E	103	-	-	0/1/1/1	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	304	GOL	O2-C2	-6.27	1.25	1.43
4	B	303	GOL	O2-C2	-4.24	1.31	1.43
4	E	101	GOL	O2-C2	-3.33	1.33	1.43
7	D	303	EPE	C10-S	2.16	1.80	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	303	EPE	O2S-S-C10	2.22	109.58	106.92
7	D	303	EPE	O3S-S-C10	2.35	109.57	105.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	GOL	1	0
5	A	303	EDO	1	0
4	B	301	GOL	1	0
4	B	302	GOL	1	0
4	B	303	GOL	7	0
4	B	304	GOL	5	0
7	D	303	EPE	1	0
4	E	101	GOL	2	0
4	E	102	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%)	0.06	4 (1%) 75 78	18, 34, 59, 76	0
1	D	276/276 (100%)	0.19	11 (3%) 38 42	23, 42, 67, 81	0
2	B	100/100 (100%)	-0.11	1 (1%) 82 84	18, 27, 40, 53	0
2	E	100/100 (100%)	0.07	3 (3%) 50 54	22, 36, 62, 74	0
3	C	10/10 (100%)	0.01	0 100 100	30, 33, 36, 41	0
3	F	10/10 (100%)	0.62	1 (10%) 7 8	37, 41, 56, 64	0
All	All	772/772 (100%)	0.09	20 (2%) 56 60	18, 37, 62, 81	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	GLY	3.6
1	D	106	ASP	3.4
1	D	178	THR	3.2
1	D	16	GLY	3.1
1	A	268	LYS	2.9
1	A	196	ASP	2.8
3	F	10	VAL	2.8
1	D	138	MET	2.7
2	E	0	MET	2.7
2	E	89	GLN	2.5
1	D	268	LYS	2.5
1	A	194	VAL	2.5
1	D	58[A]	GLU	2.5
1	D	226	GLN	2.4
1	D	176	LYS	2.2
2	E	88	SER	2.2
1	D	54	GLN	2.2
2	B	89	GLN	2.1
1	A	128	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	177	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. 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
4	GOL	E	102	6/6	0.26	0.32	61,63,65,67	0
7	EPE	D	303	15/15	0.45	0.33	89,91,98,99	0
4	GOL	B	302	6/6	0.72	0.22	50,57,58,61	0
6	SO4	A	304	5/5	0.79	0.38	98,99,99,102	0
4	GOL	B	301	6/6	0.81	0.26	34,50,52,54	0
4	GOL	A	301	6/6	0.82	0.17	48,55,57,59	0
4	GOL	B	303	6/6	0.83	0.40	10,23,27,30	6
4	GOL	B	304	6/6	0.84	0.32	13,16,21,22	6
6	SO4	B	307	5/5	0.85	0.26	110,110,111,111	0
6	SO4	A	305	5/5	0.86	0.17	86,87,88,89	0
5	EDO	A	302	4/4	0.89	0.15	52,52,54,56	0
5	EDO	D	301	4/4	0.92	0.12	40,41,42,42	0
4	GOL	E	101	6/6	0.92	0.23	25,40,45,51	0
5	EDO	A	303	4/4	0.93	0.13	40,44,44,45	0
5	EDO	D	302	4/4	0.94	0.10	48,48,49,50	0
5	EDO	B	305	4/4	0.95	0.11	41,42,42,43	0
5	EDO	E	103	4/4	0.95	0.10	26,36,38,40	0
6	SO4	B	306	5/5	0.98	0.07	37,40,43,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.