



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2018 – 08:03 PM EST

PDB ID : 5N6B
Title : Human Leukocyte Antigen Class I A02 Carrying LLWNPGMAV
Authors : Rizkallah, P.J.; Cole, D.K.; Fuller, A.; Bulek, A.M.; Bovay, A.
Deposited on : 2017-02-14
Resolution : 1.71 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030736

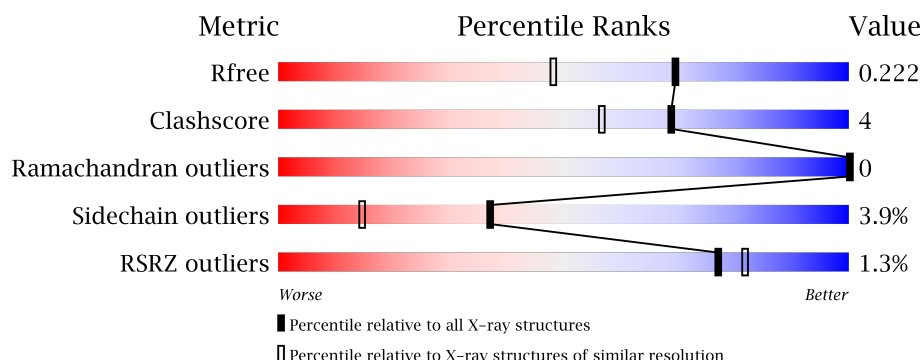
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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.



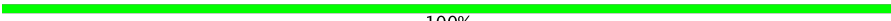
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4385 (1.74-1.70)
Clashscore	112137	4841 (1.74-1.70)
Ramachandran outliers	110173	4771 (1.74-1.70)
Sidechain outliers	110143	4771 (1.74-1.70)
RSRZ outliers	101464	4426 (1.74-1.70)

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>2%</div> <div>87%</div> <div>11%</div> <div>...</div> </div>
1	D	276	<div> <div>%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
2	B	100	<div> <div>%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	E	100	<div> <div>%</div> <div>87%</div> <div>13%</div> </div>
3	C	9	<div> <div>89%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	9	 100%

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	EDO	D	301	-	-	-	X
5	EPE	A	306[A]	-	-	-	X
5	EPE	A	306[B]	-	-	-	X
5	EPE	D	302[A]	-	-	-	X
5	EPE	D	302[B]	-	-	-	X
6	PEG	A	307	-	-	-	X
6	PEG	A	308	-	-	-	X
6	PEG	E	104	-	-	-	X
7	SO4	A	309	-	-	-	X
7	SO4	A	311	-	-	-	X
7	SO4	A	312	-	-	-	X
7	SO4	B	103	-	-	-	X
7	SO4	D	303	-	-	-	X
8	GOL	E	101	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7416 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	8	0
			2313	1445	418	440	10			
1	D	276	Total	C	N	O	S	0	9	0
			2319	1449	419	441	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	5	0
			877	557	148	167	5			
2	E	100	Total	C	N	O	S	0	3	0
			857	546	143	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 NS5.

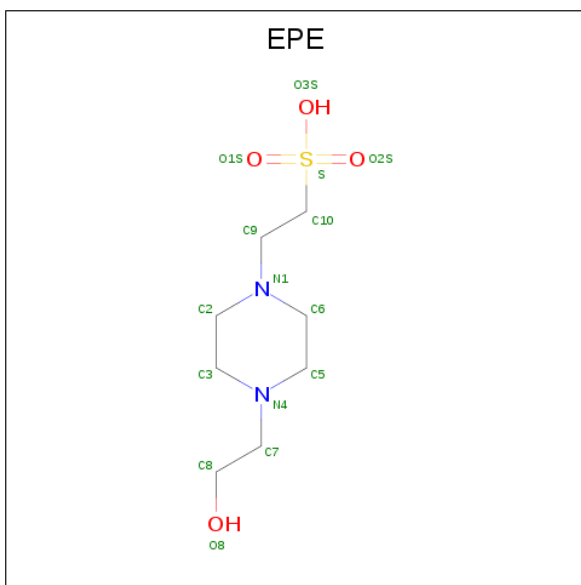
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			70	47	11	11	1			
3	F	9	Total	C	N	O	S	0	0	0
			70	47	11	11	1			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



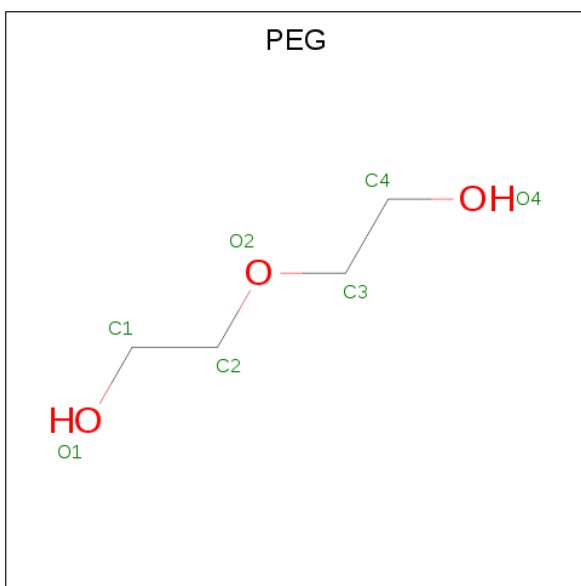
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	1
			30	16	4	8	2		
5	D	1	Total	C	N	O	S	0	1
			30	16	4	8	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		

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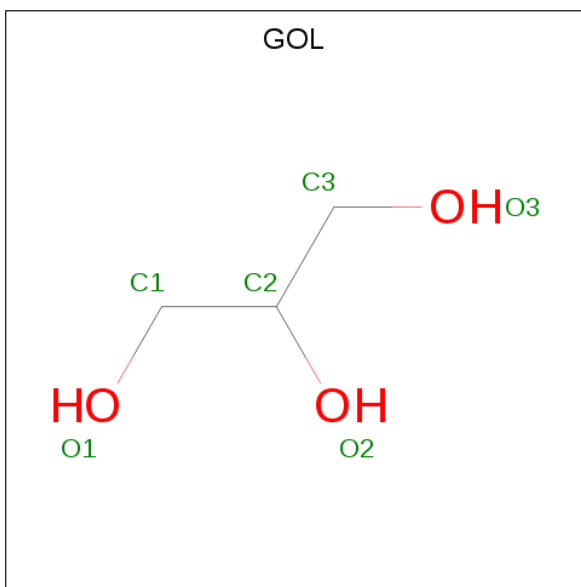
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			7	4	3		

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



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	0
			6	3	3		

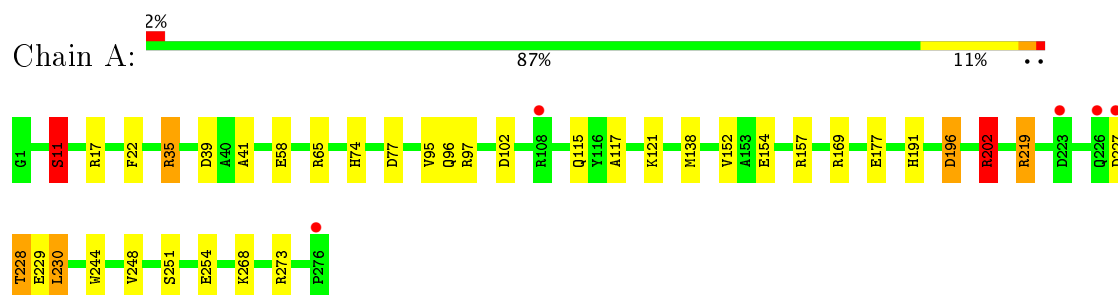
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	243	Total	O	0	0
			243	243		
9	B	125	Total	O	0	0
			125	125		
9	C	9	Total	O	0	0
			9	9		
9	D	268	Total	O	0	0
			268	268		
9	E	97	Total	O	0	0
			97	97		
9	F	7	Total	O	0	0
			7	7		

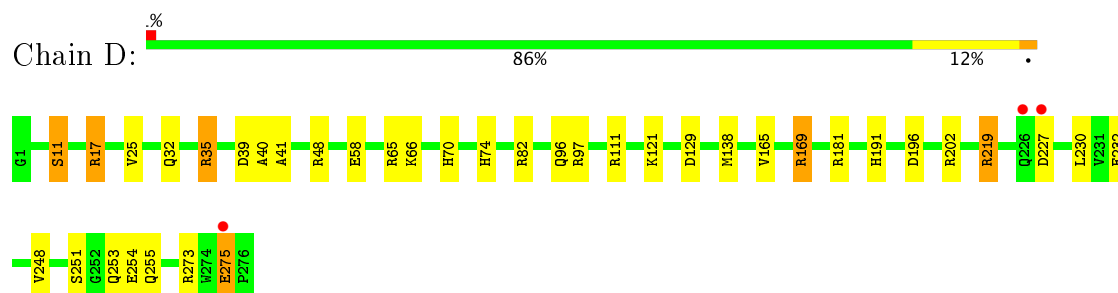
3 Residue-property plots [i](#)

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.

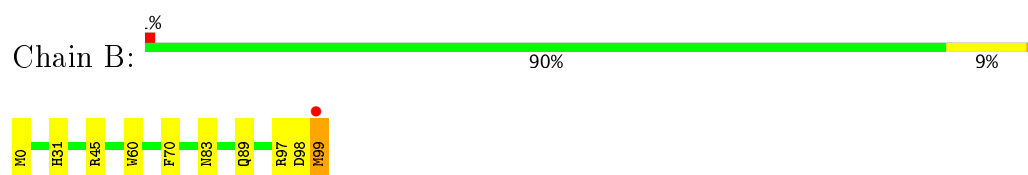
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



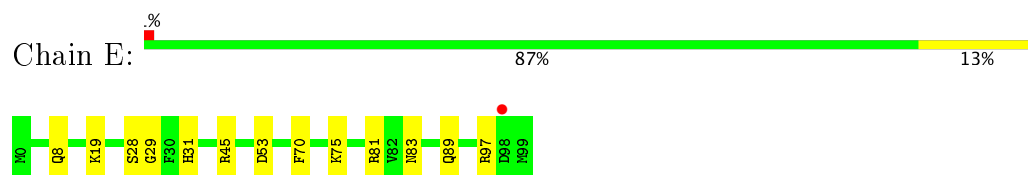
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: NS5





- Molecule 3: NS5

Chain F: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	118.09 Å 168.99 Å 49.15 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.80 – 1.71 96.80 – 1.71	Depositor EDS
% Data completeness (in resolution range)	100.0 (96.80-1.71) 100.0 (96.80-1.71)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.71 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.183 , 0.214 0.192 , 0.222	Depositor DCC
R_{free} test set	5240 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7416	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 41.25 % 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 2.4273e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: EPE, GOL, PEG, 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	0.92	2/2382 (0.1%)	1.21	17/3233 (0.5%)
1	D	0.95	1/2391 (0.0%)	1.04	18/3245 (0.6%)
2	B	1.02	0/903	1.01	4/1219 (0.3%)
2	E	0.93	0/883	1.06	6/1195 (0.5%)
3	C	1.09	0/72	1.15	0/97
3	F	1.15	0/72	1.04	0/97
All	All	0.95	3/6703 (0.0%)	1.10	45/9086 (0.5%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	ARG	CD-NE	-6.95	1.34	1.46
1	D	39	ASP	CG-OD1	6.01	1.39	1.25
1	A	154	GLU	CD-OE2	5.86	1.32	1.25

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ARG	NE-CZ-NH1	-27.97	106.31	120.30
1	A	202	ARG	NE-CZ-NH2	24.36	132.48	120.30
1	D	39	ASP	CB-CG-OD1	10.75	127.98	118.30
1	D	39	ASP	CB-CG-OD2	-10.37	108.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ARG	NE-CZ-NH2	9.79	125.20	120.30
1	D	138[A]	MET	CG-SD-CE	9.42	115.27	100.20
1	D	138[B]	MET	CG-SD-CE	9.42	115.27	100.20
1	A	202	ARG	CD-NE-CZ	8.16	135.02	123.60
1	A	157	ARG	NE-CZ-NH1	-7.77	116.42	120.30
2	E	97	ARG	NE-CZ-NH2	7.47	124.03	120.30
1	D	169	ARG	NE-CZ-NH1	7.13	123.86	120.30
2	B	45	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	39	ASP	CB-CG-OD1	6.98	124.58	118.30
2	E	45	ARG	NE-CZ-NH2	-6.52	117.04	120.30
2	B	99	MET	CG-SD-CE	-6.42	89.92	100.20
1	A	77	ASP	CB-CG-OD1	6.33	123.99	118.30
1	A	138[A]	MET	CG-SD-CE	6.29	110.27	100.20
1	A	138[B]	MET	CG-SD-CE	6.29	110.27	100.20
2	E	81	ARG	CG-CD-NE	-6.27	98.63	111.80
1	A	273	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	B	97	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	A	169	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	65	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	D	82	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	A	230	LEU	CA-CB-CG	5.70	128.40	115.30
1	D	35	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	230	LEU	CA-CB-CG	5.68	128.38	115.30
1	D	219	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	D	17	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	D	111	ARG	NE-CZ-NH2	5.56	123.08	120.30
2	E	53	ASP	CB-CG-OD1	5.51	123.26	118.30
1	D	11	SER	N-CA-CB	-5.46	102.32	110.50
2	E	81	ARG	CD-NE-CZ	5.45	131.22	123.60
1	A	11[A]	SER	N-CA-CB	-5.37	102.45	110.50
1	A	11[B]	SER	N-CA-CB	-5.37	102.45	110.50
1	D	82	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	A	102	ASP	CB-CG-OD1	5.34	123.10	118.30
2	B	99	MET	N-CA-C	5.31	125.33	111.00
1	D	202	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	D	129	ASP	CB-CG-OD1	5.23	123.00	118.30
1	D	65	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	D	273	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	219	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	E	97	ARG	NE-CZ-NH1	-5.13	117.74	120.30
1	D	48	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	ARG	Sidechain

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	2313	0	2157	22	0
1	D	2319	0	2165	21	0
2	B	877	0	842	4	0
2	E	857	0	824	6	0
3	C	70	0	73	1	0
3	F	70	0	73	0	0
4	A	20	0	30	0	0
4	B	8	0	12	0	0
4	D	4	0	6	0	0
4	E	8	0	12	0	0
4	F	4	0	6	0	0
5	A	30	0	35	5	0
5	D	30	0	36	8	0
6	A	14	0	20	1	0
6	E	7	0	10	0	0
7	A	20	0	0	0	0
7	B	5	0	0	0	0
7	D	5	0	0	0	0
8	E	6	0	8	2	0
9	A	243	0	0	5	0
9	B	125	0	0	1	0
9	C	9	0	0	0	0
9	D	268	0	0	3	0
9	E	97	0	0	1	0
9	F	7	0	0	0	0
All	All	7416	0	6309	56	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 4.

All (56) 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:255:GLN:HE22	1:D:275:GLU:HG2	1.43	0.82
2:E:29:GLY:O	8:E:101:GOL:H31	1.91	0.70
5:D:302[A]:EPE:S	5:D:302[A]:EPE:H61	2.33	0.67
1:A:115[B]:GLN:NE2	9:A:403:HOH:O	2.31	0.63
5:D:302[A]:EPE:H62	5:D:302[A]:EPE:O3S	1.99	0.62
1:A:248[A]:VAL:O	1:A:248[A]:VAL:HG13	2.02	0.60
1:A:227:ASP:HB3	1:A:248[A]:VAL:HG12	1.84	0.60
1:D:248[A]:VAL:O	1:D:248[A]:VAL:HG13	2.00	0.60
1:D:248[A]:VAL:O	1:D:248[A]:VAL:CG1	2.51	0.58
1:A:248[A]:VAL:CG1	1:A:248[A]:VAL:O	2.52	0.57
1:D:227:ASP:HB3	1:D:248[A]:VAL:HG12	1.88	0.56
1:A:17:ARG:NH1	9:A:404:HOH:O	2.32	0.55
5:D:302[A]:EPE:O3S	5:D:302[A]:EPE:C6	2.55	0.55
5:D:302[A]:EPE:S	5:D:302[A]:EPE:C6	2.96	0.52
1:D:17:ARG:NH2	9:D:405:HOH:O	2.42	0.51
1:D:74:HIS:CE1	1:D:97:ARG:HE	2.29	0.51
1:A:191:HIS:HD2	9:A:601:HOH:O	1.93	0.51
1:D:121:LYS:NZ	9:D:402:HOH:O	2.31	0.51
1:D:191:HIS:HE1	1:D:254:GLU:OE1	1.93	0.51
1:D:25[B]:VAL:HG13	1:D:32:GLN:NE2	2.26	0.50
2:E:31:HIS:HD2	9:E:212:HOH:O	1.92	0.50
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.46	0.50
1:A:152:VAL:HG22	3:C:7:MET:HG3	1.93	0.50
2:B:31:HIS:HD2	9:B:206:HOH:O	1.95	0.49
1:A:191:HIS:HE1	1:A:254:GLU:OE1	1.96	0.49
5:D:302[B]:EPE:H91	5:D:302[B]:EPE:H31	1.45	0.49
1:A:41:ALA:HB3	5:A:306[A]:EPE:H72	1.95	0.48
1:D:232[B]:GLU:HG2	2:E:8:GLN:NE2	2.28	0.48
1:D:191:HIS:HD2	9:D:625:HOH:O	1.95	0.48
5:D:302[A]:EPE:H51	5:D:302[A]:EPE:H82	1.32	0.48
1:A:11[B]:SER:OG	1:A:22:PHE:HD1	1.97	0.47
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.49	0.47
1:D:96:GLN:OE1	2:E:31:HIS:HE1	1.97	0.47
1:A:96:GLN:OE1	2:B:31:HIS:HE1	1.98	0.47
1:A:74:HIS:CE1	1:A:97:ARG:HE	2.32	0.47
1:D:255:GLN:NE2	1:D:275:GLU:HG2	2.23	0.47
1:D:219:ARG:HH22	1:D:253:GLN:HE22	1.63	0.46
1:A:121:LYS:HB2	6:A:307:PEG:H32	1.98	0.45
1:A:35:ARG:HH22	5:A:306[A]:EPE:H92	1.80	0.45
1:D:232[B]:GLU:OE2	2:E:28:SER:OG	2.27	0.44
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.53	0.44
1:D:41:ALA:H	5:D:302[A]:EPE:H51	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:LYS:O	1:D:70:HIS:HD2	2.00	0.44
5:A:306[B]:EPE:H101	9:A:622:HOH:O	2.18	0.43
2:B:0[B]:MET:HE3	2:B:0[B]:MET:HB2	1.89	0.43
2:E:29:GLY:O	8:E:101:GOL:C3	2.66	0.42
1:A:230:LEU:HD13	9:A:549:HOH:O	2.20	0.42
1:A:41:ALA:H	5:A:306[B]:EPE:C3	2.34	0.41
1:D:255:GLN:OE1	1:D:275:GLU:N	2.40	0.41
5:A:306[A]:EPE:H81	5:A:306[A]:EPE:H51	1.85	0.41
1:A:196:ASP:N	1:A:196:ASP:OD1	2.54	0.41
1:D:40:ALA:HB1	5:D:302[B]:EPE:H51	2.03	0.41
1:D:165[B]:VAL:HG12	1:D:169:ARG:CZ	2.51	0.40
1:D:74:HIS:HE1	1:D:97:ARG:HE	1.67	0.40
1:A:228:THR:HG23	1:A:229:GLU:N	2.37	0.40
1:A:74:HIS:HD2	1:A:95:VAL:HG11	1.87	0.40

There are no symmetry-related clashes.

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	282/276 (102%)	279 (99%)	3 (1%)	0	100	100
1	D	283/276 (102%)	279 (99%)	4 (1%)	0	100	100
2	B	102/100 (102%)	102 (100%)	0	0	100	100
2	E	101/100 (101%)	101 (100%)	0	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	782/770 (102%)	775 (99%)	7 (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	240/232 (103%)	229 (95%)	11 (5%)	31	11
1	D	241/232 (104%)	233 (97%)	8 (3%)	43	20
2	B	100/95 (105%)	95 (95%)	5 (5%)	28	9
2	E	98/95 (103%)	93 (95%)	5 (5%)	28	9
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
All	All	693/668 (104%)	664 (96%)	29 (4%)	37	13

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11[A]	SER
1	A	11[B]	SER
1	A	35	ARG
1	A	58[A]	GLU
1	A	58[B]	GLU
1	A	177	GLU
1	A	196	ASP
1	A	219	ARG
1	A	228	THR
1	A	251	SER
1	A	268	LYS
2	B	70	PHE
2	B	83	ASN
2	B	89	GLN
2	B	98	ASP
2	B	99	MET
1	D	11	SER
1	D	35	ARG
1	D	58[A]	GLU
1	D	58[B]	GLU
1	D	181	ARG
1	D	196	ASP

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Mol	Chain	Res	Type
1	D	251	SER
1	D	275	GLU
2	E	19	LYS
2	E	70	PHE
2	E	75	LYS
2	E	83	ASN
2	E	89	GLN

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

Mol	Chain	Res	Type
1	A	74	HIS
1	A	86	ASN
1	A	141	GLN
1	A	174	ASN
1	A	191	HIS
1	A	226	GLN
1	A	253	GLN
2	B	31	HIS
2	B	83	ASN
1	D	70	HIS
1	D	74	HIS
1	D	86	ASN
1	D	141	GLN
1	D	151	HIS
1	D	174	ASN
1	D	191	HIS
1	D	226	GLN
1	D	253	GLN
2	E	31	HIS
2	E	83	ASN

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 ⓘ

25 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	EDO	A	301	-	3,3,3	0.49	0	2,2,2	0.22	0
4	EDO	A	302	-	3,3,3	0.44	0	2,2,2	0.28	0
4	EDO	A	303	-	3,3,3	0.42	0	2,2,2	0.59	0
4	EDO	A	304	-	3,3,3	0.43	0	2,2,2	0.35	0
4	EDO	A	305	-	3,3,3	0.44	0	2,2,2	0.17	0
5	EPE	A	306[A]	-	15,15,15	2.20	1 (6%)	18,20,20	2.03	7 (38%)
5	EPE	A	306[B]	-	15,15,15	1.87	1 (6%)	18,20,20	2.36	7 (38%)
6	PEG	A	307	-	6,6,6	0.60	0	5,5,5	0.30	0
6	PEG	A	308	-	6,6,6	0.66	0	5,5,5	0.44	0
7	SO4	A	309	-	4,4,4	0.47	0	6,6,6	0.33	0
7	SO4	A	310	-	4,4,4	0.61	0	6,6,6	0.65	0
7	SO4	A	311	-	4,4,4	0.57	0	6,6,6	0.31	0
7	SO4	A	312	-	4,4,4	0.46	0	6,6,6	0.22	0
4	EDO	B	101	-	3,3,3	0.44	0	2,2,2	0.52	0
4	EDO	B	102	-	3,3,3	0.38	0	2,2,2	0.68	0
7	SO4	B	103	-	4,4,4	0.41	0	6,6,6	0.25	0
4	EDO	D	301	-	3,3,3	0.26	0	2,2,2	0.96	0
5	EPE	D	302[A]	-	15,15,15	2.09	2 (13%)	18,20,20	2.40	3 (16%)
5	EPE	D	302[B]	-	15,15,15	2.07	1 (6%)	18,20,20	1.64	4 (22%)
7	SO4	D	303	-	4,4,4	0.48	0	6,6,6	0.35	0
8	GOL	E	101	-	5,5,5	1.29	1 (20%)	5,5,5	1.50	1 (20%)
4	EDO	E	102	-	3,3,3	0.43	0	2,2,2	0.62	0
4	EDO	E	103	-	3,3,3	0.46	0	2,2,2	0.32	0
6	PEG	E	104	-	6,6,6	0.56	0	5,5,5	1.00	0
4	EDO	F	101	-	3,3,3	0.60	0	2,2,2	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	301	-	-	0/1/1/1	0/0/0/0
4	EDO	A	302	-	-	0/1/1/1	0/0/0/0
4	EDO	A	303	-	-	0/1/1/1	0/0/0/0
4	EDO	A	304	-	-	0/1/1/1	0/0/0/0
4	EDO	A	305	-	-	0/1/1/1	0/0/0/0
5	EPE	A	306[A]	-	-	0/9/19/19	0/1/1/1
5	EPE	A	306[B]	-	-	0/9/19/19	0/1/1/1
6	PEG	A	307	-	-	0/4/4/4	0/0/0/0
6	PEG	A	308	-	-	0/4/4/4	0/0/0/0
7	SO4	A	309	-	-	0/0/0/0	0/0/0/0
7	SO4	A	310	-	-	0/0/0/0	0/0/0/0
7	SO4	A	311	-	-	0/0/0/0	0/0/0/0
7	SO4	A	312	-	-	0/0/0/0	0/0/0/0
4	EDO	B	101	-	-	0/1/1/1	0/0/0/0
4	EDO	B	102	-	-	0/1/1/1	0/0/0/0
7	SO4	B	103	-	-	0/0/0/0	0/0/0/0
4	EDO	D	301	-	-	0/1/1/1	0/0/0/0
5	EPE	D	302[A]	-	-	0/9/19/19	0/1/1/1
5	EPE	D	302[B]	-	-	0/9/19/19	0/1/1/1
7	SO4	D	303	-	-	0/0/0/0	0/0/0/0
8	GOL	E	101	-	-	0/4/4/4	0/0/0/0
4	EDO	E	102	-	-	0/1/1/1	0/0/0/0
4	EDO	E	103	-	-	0/1/1/1	0/0/0/0
6	PEG	E	104	-	-	0/4/4/4	0/0/0/0
4	EDO	F	101	-	-	0/1/1/1	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	306[A]	EPE	C10-S	-8.19	1.65	1.77
5	D	302[B]	EPE	C10-S	-7.76	1.65	1.77
5	D	302[A]	EPE	C10-S	-7.61	1.66	1.77
5	A	306[B]	EPE	C10-S	-6.80	1.67	1.77
5	D	302[A]	EPE	O2S-S	2.06	1.51	1.45
8	E	101	GOL	O2-C2	2.52	1.50	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	306[A]	EPE	C6-C5-N4	-3.85	102.84	110.63
5	D	302[A]	EPE	C9-N1-C6	-3.69	101.78	111.26
5	A	306[B]	EPE	C7-N4-C3	-3.47	102.36	111.26
5	D	302[B]	EPE	C3-C2-N1	-3.32	103.93	110.63
5	A	306[B]	EPE	C5-C6-N1	-3.25	104.06	110.63
5	A	306[B]	EPE	C6-N1-C2	-3.22	101.57	108.87
5	D	302[A]	EPE	C7-N4-C5	-2.70	104.32	111.26
5	A	306[B]	EPE	C3-C2-N1	-2.65	105.27	110.63
5	A	306[A]	EPE	O1S-S-C10	-2.57	104.58	106.79
5	A	306[A]	EPE	C5-C6-N1	-2.22	106.14	110.63
5	A	306[A]	EPE	C7-N4-C5	-2.09	105.89	111.26
8	E	101	GOL	O1-C1-C2	2.36	121.94	110.07
5	A	306[A]	EPE	O3S-S-C10	2.56	109.21	106.06
5	A	306[B]	EPE	C2-C3-N4	2.62	115.93	110.63
5	A	306[A]	EPE	C2-C3-N4	2.62	115.94	110.63
5	D	302[B]	EPE	O2S-S-C10	2.68	109.09	106.79
5	D	302[B]	EPE	O3S-S-C10	2.70	109.38	106.06
5	A	306[B]	EPE	O2S-S-C10	3.22	109.56	106.79
5	D	302[B]	EPE	O1S-S-C10	3.48	109.78	106.79
5	A	306[A]	EPE	O2S-S-C10	4.64	110.78	106.79
5	A	306[B]	EPE	O1S-S-C10	5.20	111.26	106.79
5	D	302[A]	EPE	O2S-S-C10	8.07	113.72	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	306[A]	EPE	3	0
5	A	306[B]	EPE	2	0
6	A	307	PEG	1	0
5	D	302[A]	EPE	6	0
5	D	302[B]	EPE	2	0
8	E	101	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	5 (1%) 69 74	15, 27, 53, 71	0
1	D	276/276 (100%)	-0.08	3 (1%) 80 84	14, 27, 48, 64	0
2	B	100/100 (100%)	-0.01	1 (1%) 82 86	15, 24, 47, 60	0
2	E	100/100 (100%)	-0.09	1 (1%) 82 86	14, 27, 50, 70	0
3	C	9/9 (100%)	-0.37	0 100 100	21, 24, 27, 29	0
3	F	9/9 (100%)	-0.09	0 100 100	21, 22, 33, 38	0
All	All	770/770 (100%)	-0.07	10 (1%) 77 82	14, 27, 50, 71	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	ASP	3.9
1	A	226	GLN	3.6
1	A	276	PRO	3.5
1	D	226	GLN	3.3
1	D	227	ASP	3.0
1	A	108	ARG	2.3
1	D	275	GLU	2.3
1	A	223	ASP	2.3
2	E	98	ASP	2.2
2	B	99	MET	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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
7	SO4	A	312	5/5	0.77	0.44	34.18	98,101,106,107	0
5	EPE	A	306[A]	15/15	0.64	0.32	15.17	41,47,55,56	15
7	SO4	A	311	5/5	0.77	0.36	14.28	65,67,81,86	0
7	SO4	B	103	5/5	0.82	0.47	13.76	94,95,100,101	0
5	EPE	A	306[B]	15/15	0.64	0.32	13.10	24,34,47,47	15
5	EPE	D	302[B]	15/15	0.68	0.37	11.18	32,44,58,59	15
5	EPE	D	302[A]	15/15	0.68	0.37	10.22	29,41,50,52	15
8	GOL	E	101	6/6	0.71	0.27	9.98	17,20,21,23	6
6	PEG	E	104	7/7	0.89	0.27	6.86	38,40,42,43	0
7	SO4	D	303	5/5	0.92	0.27	5.10	62,63,65,73	0
6	PEG	A	308	7/7	0.60	0.19	3.46	52,58,60,62	0
7	SO4	A	309	5/5	0.97	0.17	3.01	42,45,49,52	0
4	EDO	D	301	4/4	0.92	0.13	2.47	40,40,41,41	0
6	PEG	A	307	7/7	0.81	0.16	2.20	28,43,55,55	0
4	EDO	B	102	4/4	0.82	0.14	1.86	45,46,48,49	0
4	EDO	A	303	4/4	0.84	0.12	1.31	40,42,44,50	0
4	EDO	F	101	4/4	0.85	0.16	1.11	36,40,42,46	0
4	EDO	A	301	4/4	0.88	0.12	0.28	38,39,40,42	0
4	EDO	E	102	4/4	0.92	0.09	0.13	31,36,39,43	0
4	EDO	B	101	4/4	0.93	0.07	-0.37	31,33,35,38	0
4	EDO	A	305	4/4	0.97	0.10	-0.37	25,26,28,30	0
4	EDO	A	304	4/4	0.79	0.11	-	54,55,56,58	0
4	EDO	E	103	4/4	0.81	0.17	-	58,59,60,61	0
4	EDO	A	302	4/4	0.79	0.22	-	62,63,64,66	0
7	SO4	A	310	5/5	0.95	0.21	-	46,49,53,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.