



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 10:24 pm BST

PDB ID : 6R2L
Title : NYBR1-A2-SLSKILDTV
Authors : Rizkallah, P.J.; Cole, D.K.; Sami, M.
Deposited on : 2019-03-18
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

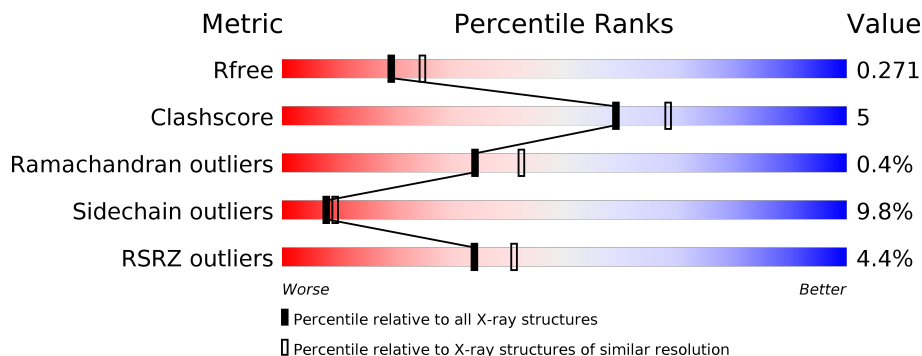
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	B	100	
3	C	9	
4	D	194	
5	E	247	

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
8	GOL	A	304	-	-	X	-
9	SO4	A	308	-	-	-	X
9	SO4	B	303	-	-	-	X
9	SO4	E	302	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7152 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
			Total	C	N	O	S			
1	A	276	2263	1413	411	430	9	0	1	0

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	837	533	141	159	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called SER-LEU-SER-LYS-ILE-LEU-ASP-THR-VAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	68	43	10	15	0	0	0

- Molecule 4 is a protein called T cell receptor alpha variable 22,Human nkt tcr alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	194	1535	959	258	309	9	0	2	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP A0A0B4J277
D	54	TRP	THR	conflict	UNP A0A0B4J277
D	57	GLU	ASN	conflict	UNP A0A0B4J277

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Chain	Residue	Modelled	Actual	Comment	Reference
D	91	GLY	-	linker	UNP A0A0B4J277
D	92	GLY	-	linker	UNP A0A0B4J277
D	93	ASN	-	linker	UNP A0A0B4J277
D	94	ASP	-	linker	UNP A0A0B4J277
D	95	TRP	-	linker	UNP A0A0B4J277
D	96	ASN	-	linker	UNP A0A0B4J277
D	97	THR	-	linker	UNP A0A0B4J277
D	98	ASP	-	linker	UNP A0A0B4J277
D	99	LYS	-	linker	UNP A0A0B4J277
D	100	LEU	-	linker	UNP A0A0B4J277
D	101	ILE	-	linker	UNP A0A0B4J277
D	102	PHE	-	linker	UNP A0A0B4J277
D	103	GLY	-	linker	UNP A0A0B4J277
D	104	THR	-	linker	UNP A0A0B4J277
D	105	GLY	-	linker	UNP A0A0B4J277
D	106	THR	-	linker	UNP A0A0B4J277
D	107	ARG	-	linker	UNP A0A0B4J277
D	108	LEU	-	linker	UNP A0A0B4J277
D	109	GLN	-	linker	UNP A0A0B4J277
D	110	VAL	-	linker	UNP A0A0B4J277
D	111	PHE	-	linker	UNP A0A0B4J277
D	112	PRO	-	linker	UNP A0A0B4J277
D	113	ASN	-	linker	UNP A0A0B4J277

- Molecule 5 is a protein called T cell receptor beta variable 11-2,Human nkt tcr beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	247	1981	1264	339	373	5	0	1	0

There are 22 discrepancies between the modelled and reference sequences:

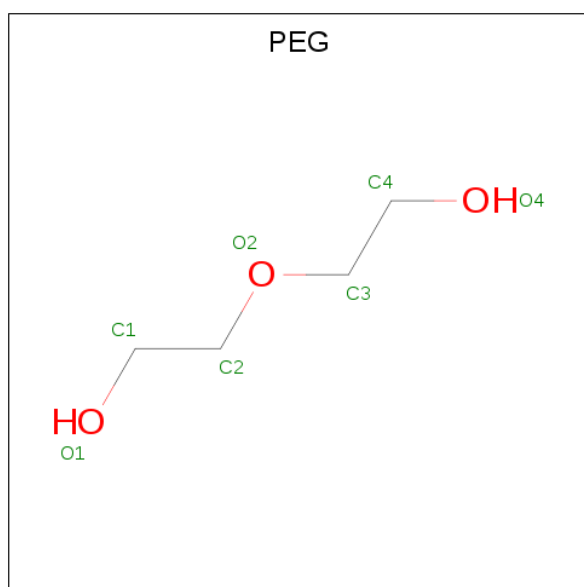
Chain	Residue	Modelled	Actual	Comment	Reference
E	28	PHE	SER	conflict	UNP A0A584
E	29	SER	GLY	conflict	UNP A0A584
E	31	PRO	ALA	conflict	UNP A0A584
E	51	GLY	GLN	conflict	UNP A0A584
E	52	GLY	ASN	conflict	UNP A0A584
E	53	TRP	ASN	conflict	UNP A0A584
E	54	PRO	GLY	conflict	UNP A0A584
E	55	GLY	VAL	conflict	UNP A0A584
E	90	LEU	VAL	conflict	UNP A0A584

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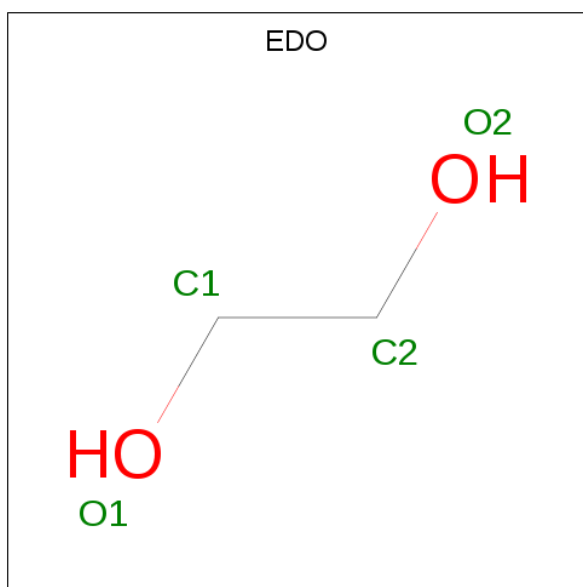
Chain	Residue	Modelled	Actual	Comment	Reference
E	97	PRO	-	linker	UNP A0A584
E	98	LEU	-	linker	UNP A0A584
E	99	ASP	-	linker	UNP A0A584
E	100	VAL	-	linker	UNP A0A584
E	101	SER	-	linker	UNP A0A584
E	102	ILE	-	linker	UNP A0A584
E	103	SER	-	linker	UNP A0A584
E	104	SER	-	linker	UNP A0A584
E	105	TYR	-	linker	UNP A0A584
E	106	ASN	-	linker	UNP A0A584
E	109	PHE	TYR	conflict	UNP K7N5M4
E	119	LEU	THR	conflict	UNP K7N5M4
E	208	ASP	ASN	conflict	UNP K7N5M4

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



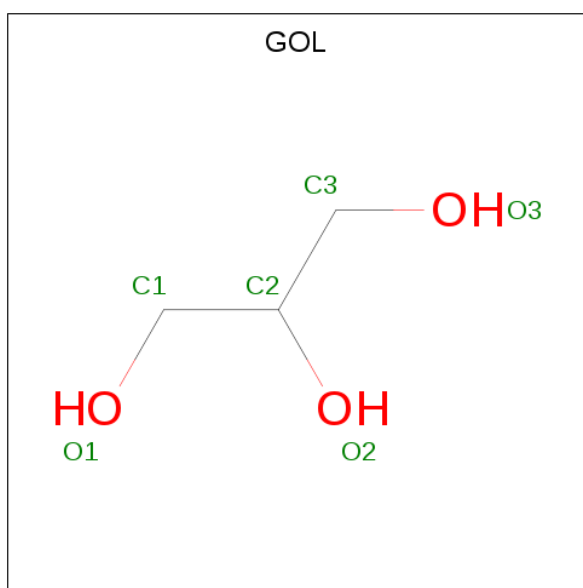
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	7	4	3	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

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



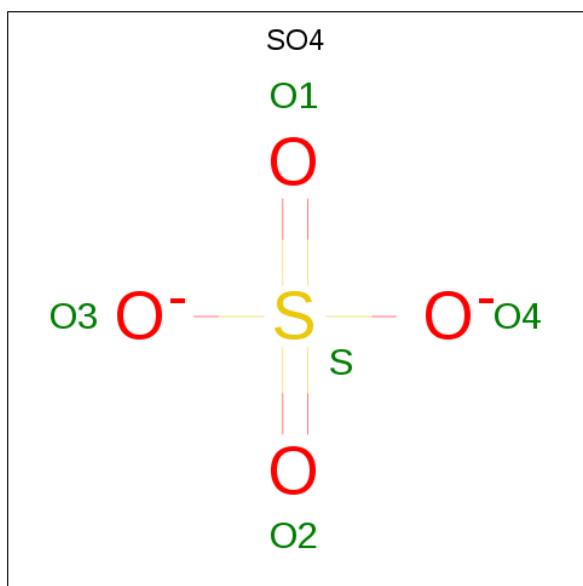
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

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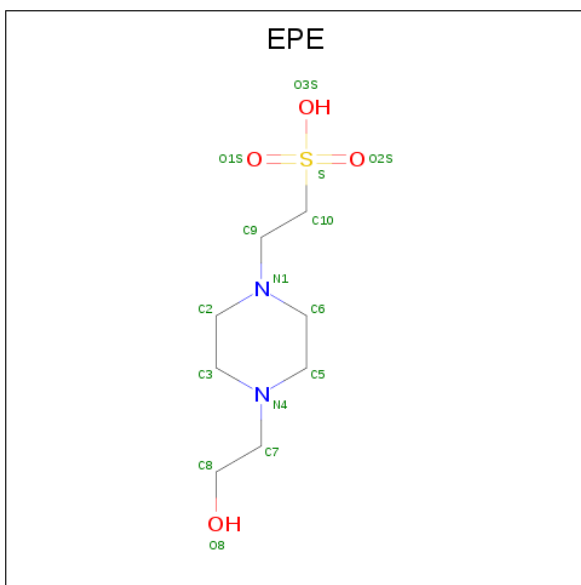
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	E	1	6	3	3	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 10 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



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

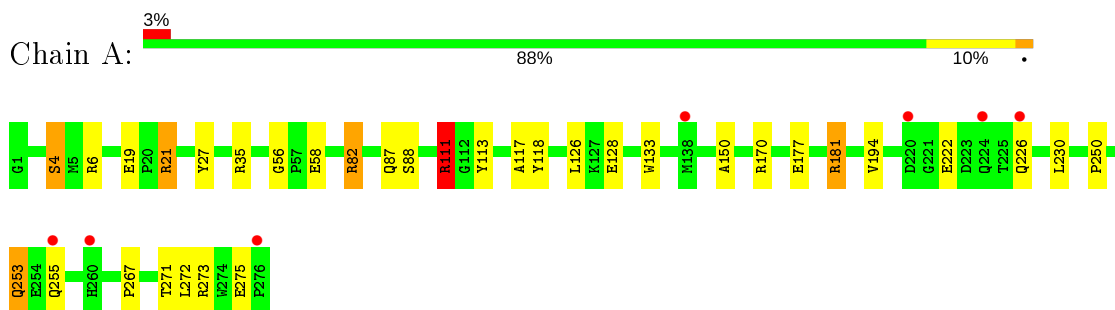
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	141	Total	O	0	0
			141	141		
11	B	54	Total	O	0	0
			54	54		
11	C	9	Total	O	0	0
			9	9		
11	D	68	Total	O	0	0
			68	68		
11	E	108	Total	O	0	0
			108	108		

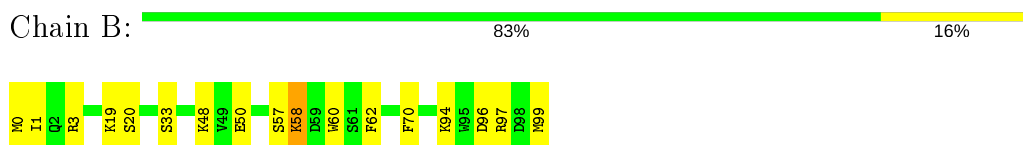
3 Residue-property plots [i](#)

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.

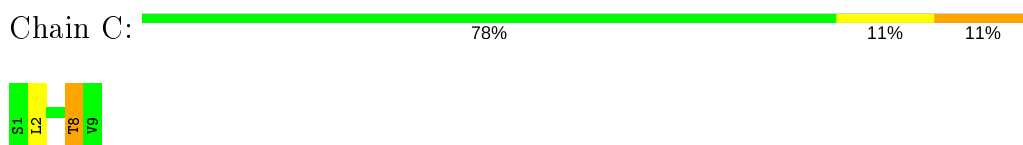
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



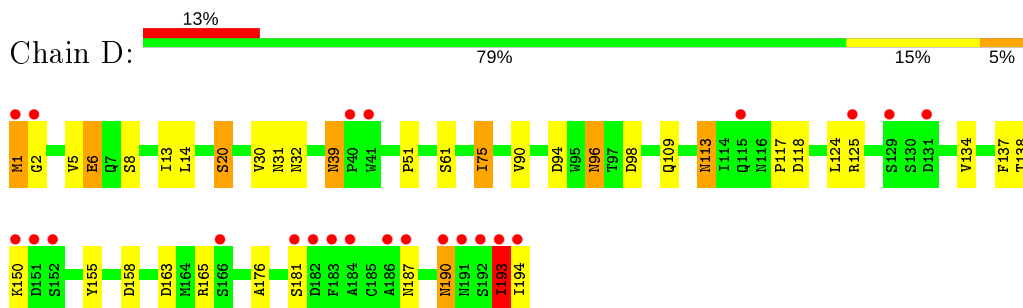
- Molecule 2: Beta-2-microglobulin



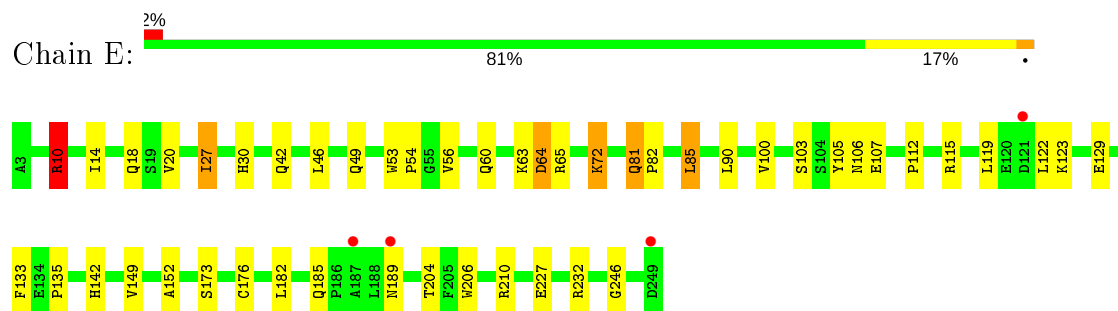
- Molecule 3: SER-LEU-SER-LYS-ILE-LEU-ASP-THR-VAL



- Molecule 4: T cell receptor alpha variable 22,Human nkt tcr alpha chain



- Molecule 5: T cell receptor beta variable 11-2,Human nkt tcr beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.21Å 99.33Å 111.44Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	52.21 – 2.30 52.21 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (52.21-2.30) 99.7 (52.21-2.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.214 , 0.265 0.219 , 0.271	Depositor DCC
R_{free} test set	2435 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtrriage
Anisotropy	0.206	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7152	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: PEG, GOL, EPE, 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	0.80	1/2329 (0.0%)	1.01	6/3161 (0.2%)
2	B	0.85	0/860	1.00	2/1162 (0.2%)
3	C	1.01	0/67	1.38	1/88 (1.1%)
4	D	0.83	1/1569 (0.1%)	0.98	0/2133
5	E	0.76	0/2039	0.99	2/2778 (0.1%)
All	All	0.81	2/6864 (0.0%)	1.00	11/9322 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
4	D	0	2
5	E	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	6	GLU	CD-OE2	8.39	1.34	1.25
1	A	19	GLU	CD-OE2	6.33	1.32	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	21	ARG	NE-CZ-NH2	-7.49	116.56	120.30
5	E	10	ARG	NE-CZ-NH1	-6.06	117.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	ARG	NE-CZ-NH1	5.87	123.23	120.30
2	B	97	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	181	ARG	CG-CD-NE	5.82	124.02	111.80
1	A	111	ARG	CG-CD-NE	5.81	124.01	111.80
2	B	3	ARG	NE-CZ-NH2	-5.51	117.55	120.30
5	E	10	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	82	ARG	NE-CZ-NH2	-5.24	117.68	120.30
3	C	8	THR	N-CA-CB	-5.22	100.38	110.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	TYR	Peptide
1	A	4	SER	Peptide
4	D	117	PRO	Peptide
4	D	2	GLY	Peptide
5	E	246	GLY	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2263	0	2108	16	0
2	B	837	0	803	11	0
3	C	68	0	78	0	0
4	D	1535	0	1446	21	0
5	E	1981	0	1905	22	0
6	A	7	0	10	2	0
7	A	8	0	12	0	0
8	A	12	0	16	4	0
8	E	6	0	8	0	0
9	A	20	0	0	0	0
9	B	10	0	0	0	0
9	D	5	0	0	0	0
9	E	5	0	0	0	0
10	B	15	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	141	0	0	1	0
11	B	54	0	0	0	0
11	C	9	0	0	1	0
11	D	68	0	0	0	0
11	E	108	0	0	1	0
All	All	7152	0	6404	62	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 5.

All (62) 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)
4:D:98:ASP:H	5:E:49:GLN:HE22	1.23	0.85
4:D:134:VAL:HG21	5:E:149:VAL:HG11	1.69	0.74
2:B:58:LYS:H	2:B:58:LYS:CE	2.08	0.66
4:D:96:ASN:H	4:D:96:ASN:HD22	1.45	0.65
4:D:124:LEU:HD22	5:E:149:VAL:HG12	1.77	0.65
5:E:27:ILE:HG12	5:E:30:HIS:CE1	2.31	0.65
1:A:150:ALA:HB1	11:C:103:HOH:O	1.98	0.62
5:E:133:PHE:HB2	5:E:149:VAL:HG13	1.82	0.62
4:D:39:ASN:HD22	4:D:39:ASN:C	2.04	0.61
5:E:64:ASP:OD1	5:E:65:ARG:HG3	2.01	0.61
4:D:30:VAL:HG11	4:D:90:VAL:HB	1.84	0.60
4:D:20:SER:HB2	4:D:75:ILE:HG23	1.85	0.59
5:E:81:GLN:HB3	5:E:82:PRO:HD3	1.83	0.59
5:E:133:PHE:HB2	5:E:149:VAL:CG1	2.34	0.57
4:D:124:LEU:CD2	5:E:149:VAL:HG12	2.35	0.56
4:D:138:THR:O	4:D:138:THR:OG1	2.12	0.56
4:D:1:MET:SD	4:D:94:ASP:OD2	2.65	0.54
4:D:163:ASP:O	5:E:173:SER:O	2.26	0.54
4:D:187:ASN:O	4:D:190:ASN:HB2	2.07	0.53
2:B:57:SER:HA	2:B:58:LYS:HE3	1.90	0.52
4:D:148:GLN:HA	4:D:148:GLN:HE21	1.75	0.51
1:A:88:SER:N	8:A:304:GOL:H11	2.26	0.51
1:A:111:ARG:NH2	1:A:128:GLU:OE1	2.44	0.50
2:B:57:SER:CA	2:B:58:LYS:HE3	2.42	0.50
4:D:13:ILE:HD12	4:D:109:GLN:HB3	1.93	0.50
5:E:105:TYR:OH	5:E:107:GLU:OE1	2.27	0.50
4:D:96:ASN:HD22	4:D:96:ASN:N	2.11	0.49
1:A:126:LEU:HD13	1:A:133:TRP:CH2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD13	1:A:133:TRP:CZ3	2.48	0.48
4:D:118:ASP:OD2	5:E:142:HIS:NE2	2.46	0.48
5:E:14:ILE:HG13	5:E:18:GLN:HE21	1.78	0.48
2:B:58:LYS:CD	2:B:58:LYS:H	2.25	0.48
5:E:135:PRO:HD2	5:E:206:TRP:CZ2	2.50	0.47
4:D:124:LEU:HD22	5:E:149:VAL:CG1	2.44	0.47
1:A:88:SER:HB3	8:A:304:GOL:C1	2.44	0.47
4:D:155:TYR:O	4:D:176:ALA:HA	2.15	0.47
4:D:113:ASN:HD22	4:D:113:ASN:C	2.18	0.47
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.50	0.47
1:A:88:SER:H	8:A:304:GOL:H11	1.79	0.46
2:B:57:SER:CB	2:B:58:LYS:HE3	2.45	0.46
2:B:57:SER:HB3	2:B:58:LYS:HE3	1.97	0.46
5:E:129:GLU:O	5:E:152:ALA:HA	2.15	0.46
5:E:53:TRP:N	5:E:54:PRO:HD2	2.32	0.45
5:E:100:VAL:HG13	11:E:463:HOH:O	2.16	0.45
1:A:56:GLY:HA3	6:A:301:PEG:H21	2.00	0.44
4:D:31:ASN:O	4:D:51:PRO:HB3	2.18	0.43
5:E:27:ILE:CG1	5:E:30:HIS:CE1	3.01	0.43
1:A:58[B]:GLU:HB2	6:A:301:PEG:C1	2.49	0.43
1:A:87:GLN:NE2	1:A:118:TYR:OH	2.41	0.43
1:A:255:GLN:O	1:A:273:ARG:HD3	2.18	0.43
5:E:123:LYS:O	5:E:232:ARG:NH2	2.52	0.43
1:A:250:PRO:HG2	1:A:253:GLN:HB2	2.00	0.42
2:B:1:ILE:HA	2:B:1:ILE:HD12	1.88	0.42
1:A:226:GLN:HB2	11:A:538:HOH:O	2.19	0.41
5:E:10:ARG:NH1	5:E:112:PRO:HG2	2.36	0.41
1:A:111:ARG:HD3	1:A:113:TYR:OH	2.21	0.41
2:B:58:LYS:HE3	2:B:58:LYS:H	1.82	0.41
4:D:137:PHE:CE1	4:D:193:ILE:HG13	2.56	0.40
5:E:85:LEU:HD12	5:E:85:LEU:HA	1.95	0.40
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.56	0.40
1:A:88:SER:HB3	8:A:304:GOL:H12	2.03	0.40
2:B:96:ASP:OD2	2:B:99:MET:HE2	2.21	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	275/276 (100%)	266 (97%)	9 (3%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	D	194/194 (100%)	181 (93%)	11 (6%)	2 (1%)	15	17
5	E	246/247 (100%)	230 (94%)	15 (6%)	1 (0%)	34	42
All	All	820/826 (99%)	781 (95%)	36 (4%)	3 (0%)	34	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	193	ILE
5	E	72	LYS
4	D	181	SER

5.3.2 Protein sidechains [i](#)

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	233/232 (100%)	217 (93%)	16 (7%)	15	20
2	B	95/95 (100%)	87 (92%)	8 (8%)	11	13
3	C	9/9 (100%)	7 (78%)	2 (22%)	1	1
4	D	176/174 (101%)	156 (89%)	20 (11%)	5	6
5	E	216/215 (100%)	190 (88%)	26 (12%)	5	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	729/725 (101%)	657 (90%)	72 (10%)	8 9

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	21	ARG
1	A	35	ARG
1	A	82	ARG
1	A	111	ARG
1	A	170	ARG
1	A	177	GLU
1	A	181	ARG
1	A	194	VAL
1	A	222	GLU
1	A	230	LEU
1	A	253	GLN
1	A	267	PRO
1	A	271	THR
1	A	272	LEU
1	A	275	GLU
2	B	0	MET
2	B	19	LYS
2	B	20	SER
2	B	48	LYS
2	B	50	GLU
2	B	58	LYS
2	B	70	PHE
2	B	94	LYS
3	C	2	LEU
3	C	8	THR
4	D	1	MET
4	D	5	VAL
4	D	6	GLU
4	D	8	SER
4	D	14	LEU
4	D	20	SER
4	D	32	ASN
4	D	39	ASN
4	D	61	SER
4	D	75	ILE
4	D	96	ASN

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Mol	Chain	Res	Type
4	D	113	ASN
4	D	125	ARG
4	D	148	GLN
4	D	150	LYS
4	D	158	ASP
4	D	165	ARG
4	D	190	ASN
4	D	193	ILE
4	D	194	ILE
5	E	10	ARG
5	E	20	VAL
5	E	27	ILE
5	E	42	GLN
5	E	46	LEU
5	E	56	VAL
5	E	60[A]	GLN
5	E	60[B]	GLN
5	E	63	LYS
5	E	64	ASP
5	E	72	LYS
5	E	81	GLN
5	E	85	LEU
5	E	90	LEU
5	E	103	SER
5	E	106	ASN
5	E	115	ARG
5	E	119	LEU
5	E	122	LEU
5	E	176	CYS
5	E	182	LEU
5	E	185	GLN
5	E	189	ASN
5	E	204	THR
5	E	210	ARG
5	E	227	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	86	ASN
1	A	87	GLN

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Mol	Chain	Res	Type
1	A	155	GLN
1	A	174	ASN
1	A	253	GLN
4	D	4	GLN
4	D	32	ASN
4	D	38	GLN
4	D	39	ASN
4	D	96	ASN
4	D	113	ASN
4	D	148	GLN
5	E	18	GLN
5	E	38	GLN
5	E	49	GLN
5	E	106	ASN
5	E	144	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](#)

15 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
8	GOL	A	305	-	5,5,5	0.19	0	5,5,5	0.46	0
7	EDO	A	302	-	3,3,3	0.04	0	2,2,2	0.13	0
9	SO4	A	307	-	4,4,4	0.36	0	6,6,6	0.07	0
9	SO4	A	308	-	4,4,4	0.38	0	6,6,6	0.07	0
9	SO4	D	201	-	4,4,4	0.36	0	6,6,6	0.08	0
6	PEG	A	301	-	6,6,6	0.23	0	5,5,5	0.23	0
9	SO4	B	303	-	4,4,4	0.37	0	6,6,6	0.07	0
9	SO4	A	306	-	4,4,4	0.36	0	6,6,6	0.06	0
9	SO4	E	302	-	4,4,4	0.37	0	6,6,6	0.05	0
8	GOL	A	304	-	5,5,5	0.21	0	5,5,5	0.64	0
9	SO4	B	302	-	4,4,4	0.36	0	6,6,6	0.10	0
7	EDO	A	303	-	3,3,3	0.15	0	2,2,2	0.25	0
9	SO4	A	309	-	4,4,4	0.35	0	6,6,6	0.05	0
8	GOL	E	301	-	5,5,5	0.14	0	5,5,5	0.45	0
10	EPE	B	301	-	15,15,15	2.09	1 (6%)	18,20,20	1.54	3 (16%)

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
8	GOL	A	305	-	-	0/4/4/4	-
7	EDO	A	302	-	-	1/1/1/1	-
6	PEG	A	301	-	-	2/4/4/4	-
8	GOL	A	304	-	-	2/4/4/4	-
7	EDO	A	303	-	-	0/1/1/1	-
8	GOL	E	301	-	-	4/4/4/4	-
10	EPE	B	301	-	-	4/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	301	EPE	C10-S	-7.63	1.66	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	301	EPE	O2S-S-C10	3.35	110.95	106.92
10	B	301	EPE	O3S-S-C10	3.08	110.75	105.77
10	B	301	EPE	C5-C6-N1	-2.79	104.92	110.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	304	GOL	O1-C1-C2-C3
8	E	301	GOL	C1-C2-C3-O3
10	B	301	EPE	S-C10-C9-N1
10	B	301	EPE	N4-C7-C8-O8
8	E	301	GOL	O1-C1-C2-O2
6	A	301	PEG	O2-C3-C4-O4
8	E	301	GOL	O1-C1-C2-C3
8	A	304	GOL	O1-C1-C2-O2
7	A	302	EDO	O1-C1-C2-O2
10	B	301	EPE	C10-C9-N1-C2
10	B	301	EPE	C10-C9-N1-C6
6	A	301	PEG	C4-C3-O2-C2
8	E	301	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	301	PEG	2	0
8	A	304	GOL	4	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%)	0.05	7 (2%) 57 64	21, 34, 81, 99	0
2	B	100/100 (100%)	-0.24	0 100 100	23, 32, 57, 74	0
3	C	9/9 (100%)	0.16	0 100 100	22, 22, 28, 28	0
4	D	194/194 (100%)	0.61	25 (12%) 3 5	19, 47, 93, 119	0
5	E	247/247 (100%)	0.08	4 (1%) 72 77	22, 44, 66, 98	0
All	All	826/826 (100%)	0.16	36 (4%) 34 41	19, 40, 81, 119	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	151	ASP	9.0
4	D	193	ILE	6.5
4	D	194	ILE	5.6
4	D	191	ASN	5.6
4	D	150	LYS	5.5
4	D	129	SER	4.9
4	D	184	ALA	4.4
1	A	276	PRO	4.0
4	D	187	ASN	4.0
4	D	125	ARG	3.8
4	D	181	SER	3.6
4	D	190	ASN	3.5
5	E	189	ASN	3.4
4	D	131	ASP	3.3
1	A	226	GLN	3.2
4	D	166	SER	3.0
4	D	192	SER	3.0
4	D	152	SER	2.9
4	D	41	TRP	2.8
1	A	255	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
5	E	249	ASP	2.6
4	D	182	ASP	2.5
4	D	40	PRO	2.4
4	D	145	ASN	2.4
4	D	149	SER	2.3
4	D	115	GLN	2.2
5	E	187	ALA	2.2
4	D	1	MET	2.2
1	A	224	GLN	2.2
5	E	121	ASP	2.1
4	D	186	ALA	2.1
4	D	2	GLY	2.1
4	D	183	PHE	2.1
1	A	260	HIS	2.1
1	A	220	ASP	2.1
1	A	138	MET	2.1

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
6	PEG	A	301	7/7	0.60	0.36	61,73,77,77	0
9	SO4	A	308	5/5	0.65	0.60	148,150,154,155	0
10	EPE	B	301	15/15	0.67	0.25	72,88,110,115	0
7	EDO	A	303	4/4	0.68	0.27	55,59,59,61	0
9	SO4	E	302	5/5	0.72	0.51	142,144,146,149	0
8	GOL	A	305	6/6	0.75	0.34	58,61,62,63	0
9	SO4	B	303	5/5	0.75	0.51	132,133,137,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	SO4	A	309	5/5	0.82	0.34	104,111,115,121	0
8	GOL	E	301	6/6	0.82	0.33	63,65,70,71	0
8	GOL	A	304	6/6	0.82	0.30	44,49,50,51	0
9	SO4	B	302	5/5	0.89	0.32	79,91,96,102	0
9	SO4	A	307	5/5	0.90	0.28	94,97,101,101	0
7	EDO	A	302	4/4	0.92	0.19	31,33,35,39	0
9	SO4	A	306	5/5	0.92	0.22	91,96,100,104	0
9	SO4	D	201	5/5	0.97	0.17	66,67,72,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.