Full wwPDB X-ray Structure Validation Report (i)

Feb 6, 2025 – 03:20 pm GMT

PDB ID	:	5JA8
Title	:	Crystal structure of the HigB2 toxin in complex with Nb2
Authors	:	Hadzi, S.; Loris, R.
Deposited on	:	2016-04-12
Resolution	:	2.49 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 (i) 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 (1)) were used in the production of this report:

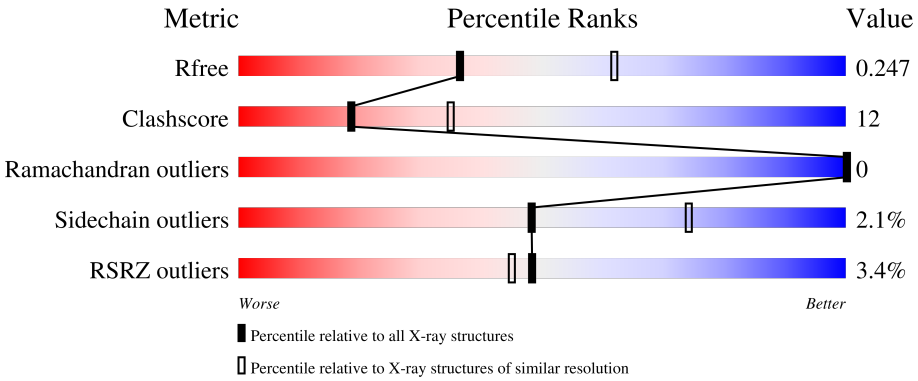
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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 <=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	111	5% 73% 20% • 5%
1	C	111	4% 77% 20% • •
1	E	111	6% 75% 20% • •
1	G	111	5% 70% 23% • 5%
2	B	127	69% 24% • 5%

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Mol	Chain	Length	Quality of chain
2	D	127	2% 77% 23%
2	F	127	2% 79% 20%
2	H	127	3% 71% 24%

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
3	PO4	D	202	-	X	-	-
3	PO4	E	202	-	-	X	-
7	PDO	D	204	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7542 atoms, of which 59 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 Toxin HigB-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	0	0	0
			847	541	145	156	5			
1	C	108	Total	C	N	O	S	0	0	0
			870	554	148	163	5			
1	E	107	Total	C	N	O	S	0	0	0
			861	549	146	161	5			
1	G	105	Total	C	N	O	S	0	0	0
			863	550	149	159	5			

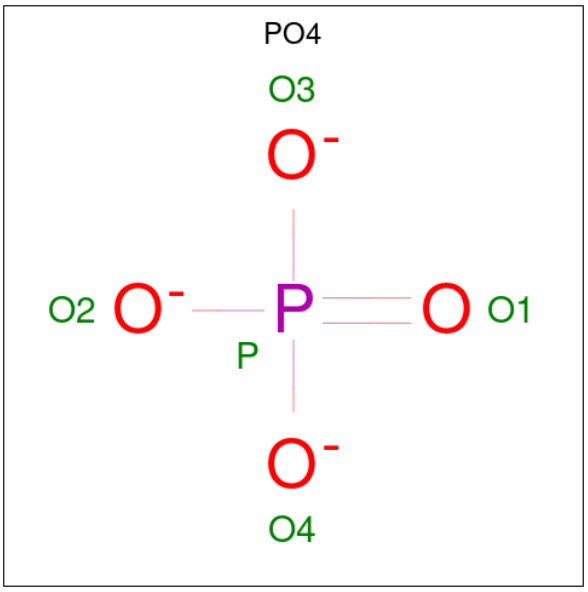
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q9KMA6
C	0	HIS	-	expression tag	UNP Q9KMA6
E	0	HIS	-	expression tag	UNP Q9KMA6
G	0	HIS	-	expression tag	UNP Q9KMA6

- Molecule 2 is a protein called Nanobody 2.

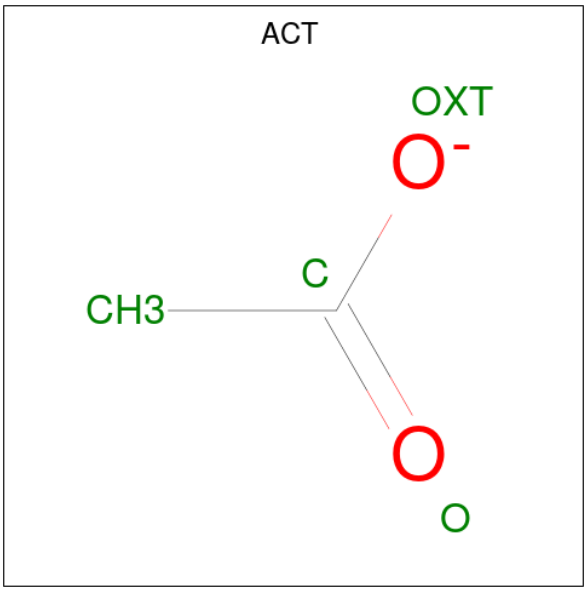
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			920	574	157	184	5			
2	D	127	Total	C	N	O	S	0	0	0
			980	610	175	190	5			
2	F	127	Total	C	N	O	S	0	0	0
			980	610	175	190	5			
2	H	122	Total	C	N	O	S	0	1	0
			934	582	160	187	5			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



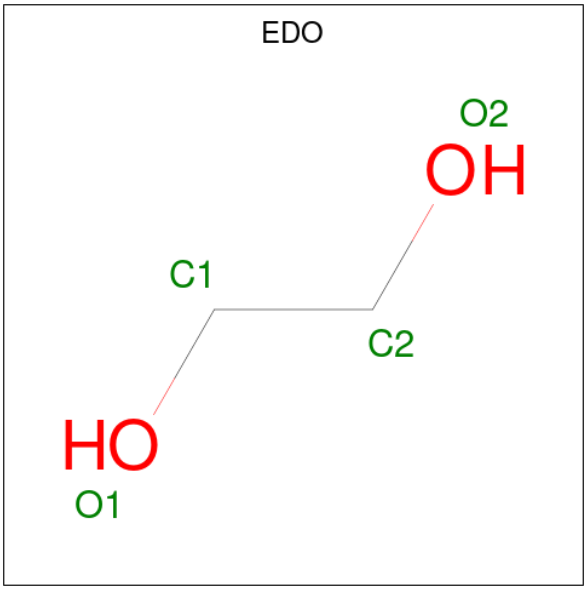
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	G	1	Total O P 5 4 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



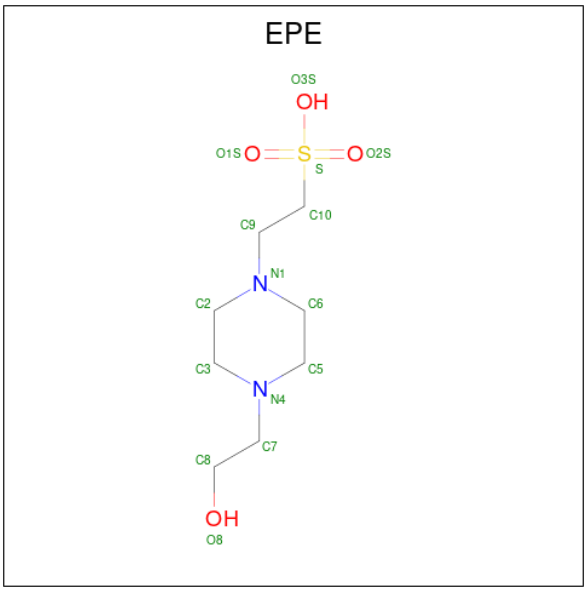
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



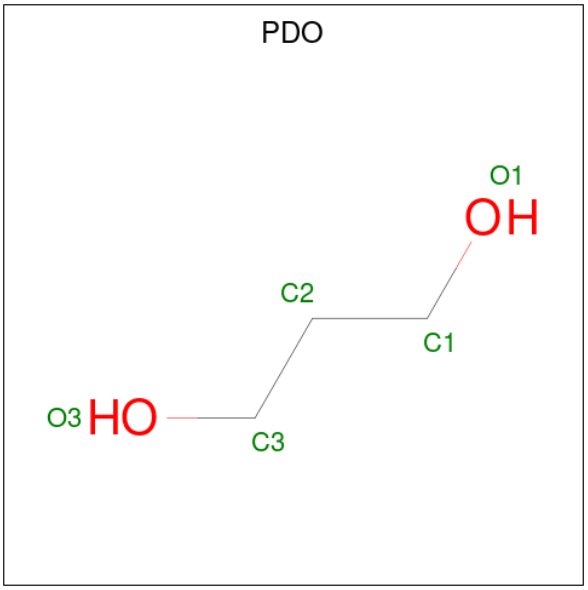
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	D	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
6	F	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

- Molecule 7 is 1,3-PROPANDIOL (three-letter code: PDO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	H	O	0	0
			13	3	8	2		
7	G	1	Total	C	H	O	0	0
			13	3	8	2		

- Molecule 8 is water.

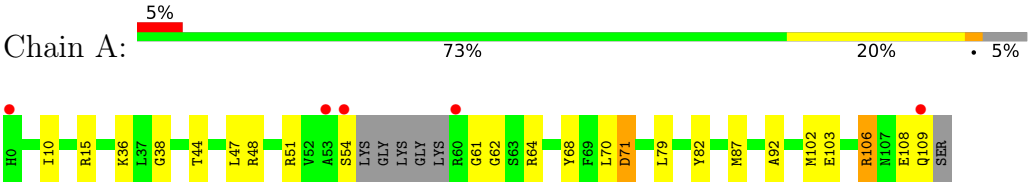
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	17	Total O 17 17	0	0
8	B	23	Total O 23 23	0	0
8	C	16	Total O 16 16	0	0
8	D	14	Total O 14 14	0	0
8	E	15	Total O 15 15	0	0
8	F	20	Total O 20 20	0	0
8	G	10	Total O 10 10	0	0
8	H	15	Total O 15 15	0	0

3 Residue-property plots (i)

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.

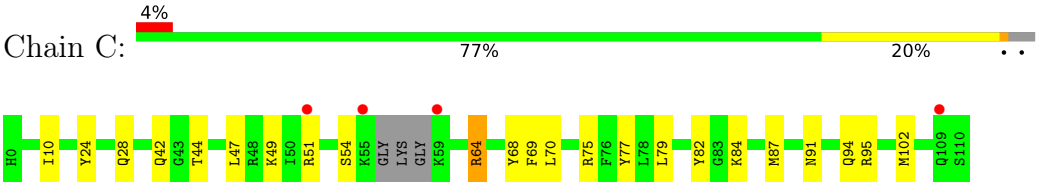
• Molecule 1: Toxin HigB-2

Chain A:



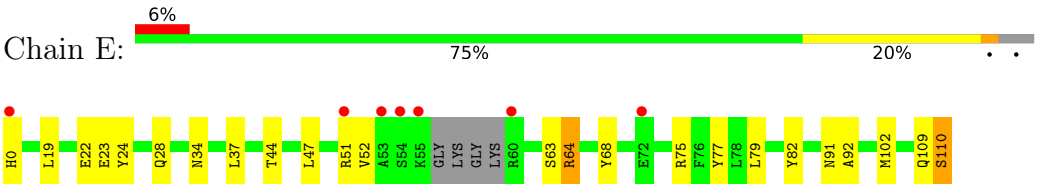
• Molecule 1: Toxin HigB-2

Chain C:



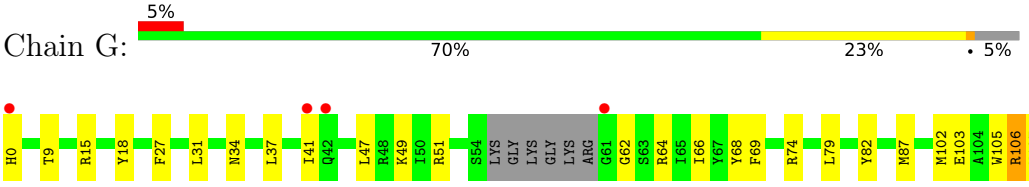
• Molecule 1: Toxin HigB-2

Chain E:



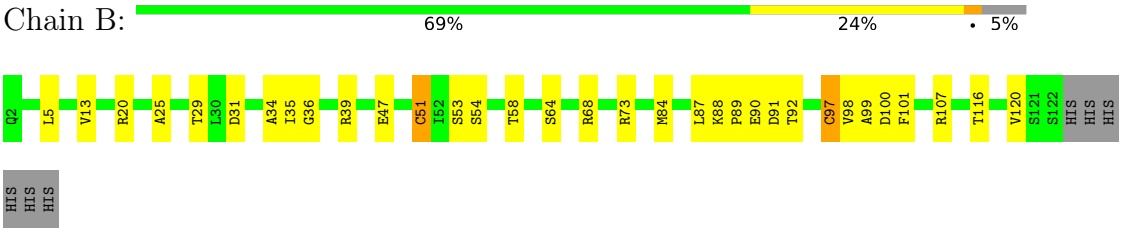
• Molecule 1: Toxin HigB-2

Chain G:



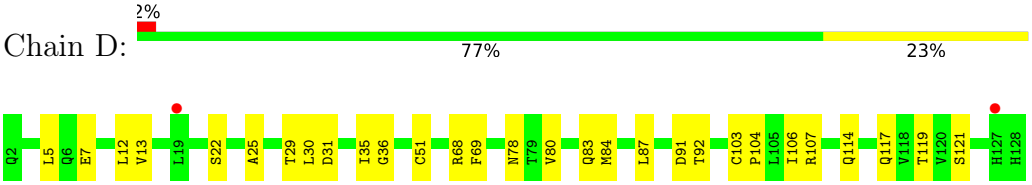
• Molecule 2: Nanobody 2

Chain B:



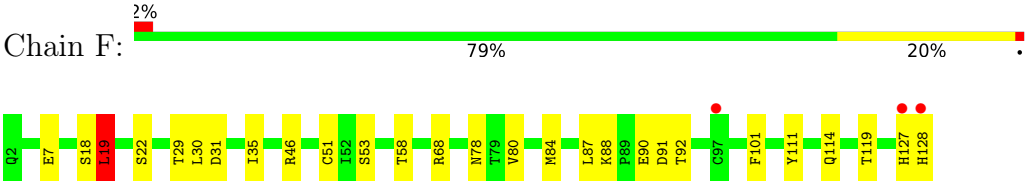
• Molecule 2: Nanobody 2

Chain D:



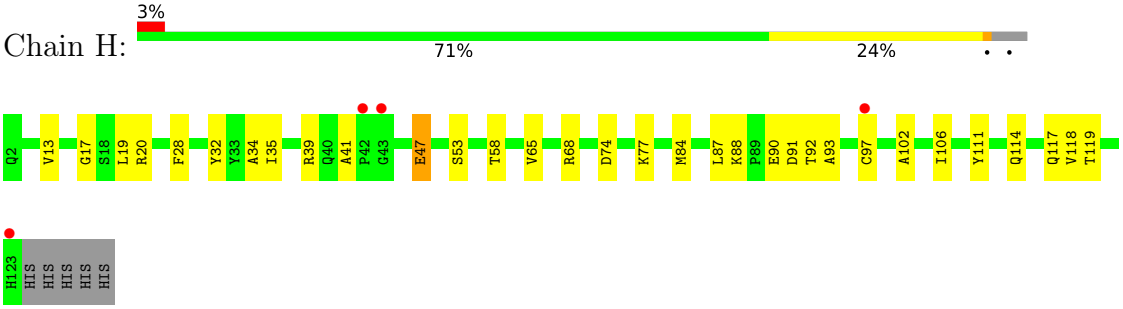
• Molecule 2: Nanobody 2

Chain F:



• Molecule 2: Nanobody 2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.00Å 109.28Å 117.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.48 – 2.49 46.48 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.48-2.49) 99.5 (46.48-2.49)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.201 , 0.248 0.208 , 0.247	Depositor DCC
R_{free} test set	1737 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	43.9	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7542	wwPDB-VP
Average B, all atoms (Å^2)	50.0	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 35.75 % 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 5.5561e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, ACT, PDO, PO4, 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	0.56	1/862 (0.1%)	0.56	0/1157
1	C	0.75	2/884 (0.2%)	0.66	3/1185 (0.3%)
1	E	0.57	0/875	0.55	0/1173
1	G	0.47	0/878	0.51	0/1175
2	B	0.75	1/939 (0.1%)	0.69	3/1273 (0.2%)
2	D	0.39	0/1005	0.53	0/1363
2	F	0.50	2/1005 (0.2%)	0.60	1/1363 (0.1%)
2	H	0.61	2/953 (0.2%)	0.95	9/1292 (0.7%)
All	All	0.59	8/7401 (0.1%)	0.65	16/9981 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	69	PHE	C-N	-14.28	1.01	1.34
2	B	98	VAL	C-N	-13.97	1.01	1.34
2	H	20	ARG	C-N	-12.43	1.05	1.34
2	H	19	LEU	C-N	-9.75	1.11	1.34
2	F	19	LEU	C-N	-9.26	1.12	1.34
1	C	70	LEU	C-N	-8.78	1.13	1.34
1	A	103	GLU	C-N	-8.41	1.14	1.34
2	F	18	SER	C-N	6.07	1.48	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	20	ARG	O-C-N	-14.92	98.83	122.70
2	H	19	LEU	O-C-N	-10.71	105.57	122.70
2	H	20	ARG	CA-C-N	10.49	140.28	117.20
2	B	97	CYS	O-C-N	-10.31	106.20	122.70
2	H	97	CYS	O-C-N	-10.22	106.35	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	20	ARG	C-N-CA	8.07	141.88	121.70
1	C	69	PHE	C-N-CA	7.66	140.85	121.70
2	H	19	LEU	CA-C-N	7.64	134.00	117.20
2	H	19	LEU	C-N-CA	7.47	140.39	121.70
1	C	69	PHE	O-C-N	-7.23	111.13	122.70
2	B	97	CYS	CA-C-N	6.82	132.21	117.20
2	F	19	LEU	O-C-N	-6.65	112.06	122.70
2	H	97	CYS	CA-C-N	6.47	131.44	117.20
2	H	97	CYS	C-N-CA	6.32	137.51	121.70
1	C	70	LEU	O-C-N	5.55	131.58	122.70
2	B	97	CYS	C-N-CA	5.45	135.32	121.70

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	847	0	808	18	0
1	C	870	0	829	17	0
1	E	861	0	826	20	0
1	G	863	0	838	29	0
2	B	920	0	870	27	0
2	D	980	0	913	22	0
2	F	980	0	912	19	0
2	H	934	0	878	23	0
3	A	10	0	0	1	0
3	B	5	0	0	0	0
3	C	10	0	0	1	0
3	D	10	0	0	0	0
3	E	10	0	0	3	0
3	G	5	0	0	1	0
4	A	4	3	3	0	0
5	B	4	6	6	3	0
6	D	15	17	17	2	0
6	F	15	17	17	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	5	8	8	8	0
7	G	5	8	8	0	0
8	A	17	0	0	0	0
8	B	23	0	0	1	0
8	C	16	0	0	1	0
8	D	14	0	0	0	0
8	E	15	0	0	0	0
8	F	20	0	0	1	0
8	G	10	0	0	1	0
8	H	15	0	0	0	0
All	All	7483	59	6933	169	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 12.

All (169) 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:C:95:ARG:NH2	3:C:202:PO4:O1	1.87	1.07
2:B:68:ARG:NH2	2:B:91:ASP:OD2	1.86	1.07
2:F:19:LEU:HD12	2:F:87:LEU:HD11	1.32	1.04
2:F:46:ARG:NH1	8:F:301:HOH:O	1.98	0.96
1:E:92:ALA:N	3:E:202:PO4:O2	1.98	0.95
2:F:68:ARG:NH2	2:F:91:ASP:OD2	2.01	0.93
1:G:18:TYR:OH	8:G:301:HOH:O	1.85	0.93
1:A:92:ALA:N	3:A:202:PO4:O2	2.01	0.93
2:F:19:LEU:CD1	2:F:87:LEU:HD11	2.02	0.90
2:D:68:ARG:NH2	2:D:91:ASP:OD2	2.08	0.87
1:A:79:LEU:HD21	1:A:102:MET:SD	2.16	0.86
1:G:105:TRP:O	1:G:109:GLN:HB2	1.78	0.82
2:B:13:VAL:HG23	2:B:120:VAL:HG12	1.61	0.81
2:B:87:LEU:HB3	2:B:120:VAL:HG11	1.63	0.80
2:B:89:PRO:HA	2:B:120:VAL:HG23	1.63	0.80
1:G:69:PHE:HZ	1:G:74:ARG:HD2	1.45	0.80
1:C:47:LEU:HD23	1:C:68:TYR:HB2	1.65	0.79
1:C:10:ILE:HG21	7:D:204:PDO:H21	1.65	0.79
2:F:127:HIS:O	2:F:128:HIS:ND1	2.15	0.79
1:G:41:ILE:HD11	1:G:49:LYS:HB2	1.65	0.79
2:H:102:ALA:HB3	2:H:106:ILE:HD11	1.67	0.77
2:B:88:LYS:O	2:B:120:VAL:HG21	1.84	0.76
1:C:10:ILE:HD13	7:D:204:PDO:H22	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:19:LEU:HD12	2:F:87:LEU:CD1	2.12	0.74
1:A:47:LEU:HD23	1:A:68:TYR:HB2	1.70	0.74
1:G:79:LEU:HD21	1:G:102:MET:SD	2.28	0.73
1:G:47:LEU:HD23	1:G:68:TYR:HB2	1.69	0.73
1:C:10:ILE:HD13	7:D:204:PDO:C2	2.21	0.69
1:E:64:ARG:NH1	3:E:201:PO4:O4	2.26	0.68
1:E:109:GLN:O	1:E:110:SER:HB2	1.94	0.68
2:B:13:VAL:CG2	2:B:120:VAL:HG12	2.25	0.67
2:F:19:LEU:HD13	2:F:84:MET:HB2	1.76	0.66
2:H:68:ARG:NH2	2:H:91:ASP:OD2	2.27	0.66
2:B:68:ARG:HH22	2:B:91:ASP:CG	2.00	0.65
1:G:109:GLN:HE21	2:H:32:TYR:HE2	1.44	0.65
1:E:47:LEU:HD23	1:E:68:TYR:HB2	1.79	0.64
1:C:79:LEU:HD21	1:C:102:MET:SD	2.38	0.64
2:D:92:THR:HG23	2:D:119:THR:HA	1.80	0.64
1:E:64:ARG:HG3	1:E:82:TYR:CD1	2.33	0.63
2:D:12:LEU:HD11	2:D:121:SER:HB3	1.81	0.63
2:D:107:ARG:HB2	7:D:204:PDO:H32	1.80	0.62
2:H:74:ASP:OD2	2:H:77:LYS:HE2	1.99	0.62
1:G:82:TYR:CE1	1:G:87:MET:HG3	2.35	0.62
2:B:5:LEU:HD23	2:B:25:ALA:HA	1.82	0.62
2:D:13:VAL:HG11	2:D:87:LEU:HD13	1.82	0.61
2:D:107:ARG:CB	7:D:204:PDO:H12	2.31	0.61
1:G:106:ARG:HG2	1:G:107:ASN:N	2.15	0.61
6:F:201:EPE:H32	2:H:111:TYR:CZ	2.36	0.61
1:G:64:ARG:NH2	3:G:201:PO4:O3	2.27	0.60
1:A:36:LYS:HG2	1:A:48:ARG:NH1	2.16	0.60
1:G:47:LEU:HD21	1:G:102:MET:HG3	1.84	0.60
1:A:44:THR:HB	1:A:47:LEU:HD12	1.85	0.59
2:D:35:ILE:HG13	2:D:80:VAL:HG21	1.85	0.59
1:A:70:LEU:HD13	1:A:106:ARG:HE	1.67	0.59
1:G:47:LEU:CD2	1:G:68:TYR:HB2	2.34	0.58
2:D:30:LEU:HG	2:D:78:ASN:OD1	2.05	0.57
2:D:36:GLY:HA2	2:D:51:CYS:HA	1.87	0.57
1:C:10:ILE:CG2	7:D:204:PDO:H21	2.35	0.56
1:A:10:ILE:HD13	5:B:202:EDO:H21	1.87	0.56
1:C:42:GLN:HA	1:C:42:GLN:OE1	2.04	0.56
2:F:53:SER:HB3	2:F:58:THR:HB	1.87	0.56
1:G:51:ARG:HD2	1:G:64:ARG:CZ	2.35	0.56
2:D:107:ARG:HB2	7:D:204:PDO:H12	1.87	0.56
2:H:84:MET:HE2	2:H:87:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:MET:HB3	2:B:87:LEU:HD21	1.89	0.55
2:H:39:ARG:NE	2:H:47:GLU:OE2	2.37	0.55
2:H:34:ALA:C	2:H:35:ILE:HD12	2.27	0.54
1:G:68:TYR:HB3	1:G:102:MET:HE1	1.90	0.54
1:G:51:ARG:CZ	1:G:62:GLY:HA3	2.38	0.53
1:G:66:ILE:HD13	1:G:82:TYR:HE1	1.73	0.53
2:H:13:VAL:HG11	2:H:87:LEU:HD13	1.91	0.53
2:H:88:LYS:HD2	2:H:90:GLU:OE2	2.08	0.53
1:E:51:ARG:CD	1:E:64:ARG:HH21	2.22	0.53
1:A:108:GLU:HG3	1:A:109:GLN:N	2.25	0.52
2:B:99:ALA:O	5:B:202:EDO:O1	2.26	0.52
1:G:82:TYR:CD1	1:G:87:MET:HG3	2.44	0.52
1:C:44:THR:HB	1:C:47:LEU:HD12	1.92	0.51
1:A:47:LEU:CD2	1:A:68:TYR:HB2	2.39	0.51
1:G:66:ILE:CD1	1:G:82:TYR:HE1	2.23	0.51
1:E:75:ARG:HD2	1:E:77:TYR:CE1	2.46	0.51
1:A:71:ASP:N	1:A:71:ASP:OD1	2.42	0.51
2:B:84:MET:HE2	2:B:87:LEU:HD21	1.93	0.51
1:E:51:ARG:HD2	1:E:64:ARG:HH21	1.76	0.50
2:H:68:ARG:NE	2:H:88:LYS:HE3	2.26	0.50
1:E:44:THR:HB	1:E:47:LEU:HD12	1.93	0.50
1:C:49:LYS:HE2	1:C:82:TYR:OH	2.11	0.50
1:G:66:ILE:O	1:G:79:LEU:HB2	2.11	0.50
2:B:54:SER:HA	2:B:73:ARG:NH1	2.26	0.50
2:H:92:THR:HG23	2:H:119:THR:HA	1.94	0.50
2:B:34:ALA:C	2:B:35:ILE:HD12	2.32	0.49
2:F:88:LYS:HB2	2:F:90:GLU:HG2	1.94	0.49
2:B:54:SER:HA	2:B:73:ARG:CZ	2.43	0.49
1:C:64:ARG:NH1	1:C:84:LYS:HG2	2.28	0.49
1:A:82:TYR:CE2	1:A:87:MET:HG3	2.48	0.48
2:F:30:LEU:HG	2:F:78:ASN:OD1	2.13	0.48
2:B:39:ARG:NE	2:B:47:GLU:OE2	2.41	0.48
2:H:84:MET:HE2	2:H:87:LEU:CD2	2.43	0.48
1:A:82:TYR:CD2	1:A:87:MET:HG3	2.49	0.48
2:D:29:THR:HG23	2:D:31:ASP:OD1	2.14	0.48
1:E:47:LEU:HD21	1:E:102:MET:HG3	1.96	0.48
1:E:64:ARG:HG3	1:E:82:TYR:CE1	2.48	0.48
2:D:117:GLN:N	6:D:201:EPE:O3S	2.34	0.47
1:G:15:ARG:HD2	1:G:15:ARG:C	2.35	0.47
1:C:54:SER:N	8:C:302:HOH:O	2.47	0.47
2:F:68:ARG:HH22	2:F:91:ASP:CG	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ALA:O	2:B:35:ILE:HD12	2.15	0.47
1:C:87:MET:SD	2:D:106:ILE:HG22	2.55	0.47
2:B:29:THR:HG23	2:B:31:ASP:OD1	2.14	0.47
2:B:92:THR:OG1	2:B:120:VAL:HG22	2.15	0.47
2:D:84:MET:HE2	2:D:87:LEU:HD21	1.97	0.47
2:B:53:SER:HB3	2:B:58:THR:HB	1.97	0.46
2:H:84:MET:HB3	2:H:87:LEU:HD21	1.96	0.46
2:D:107:ARG:NH1	7:D:204:PDO:O3	2.33	0.46
1:E:91:ASN:HB2	3:E:202:PO4:O2	2.16	0.46
2:H:41:ALA:HB2	2:H:93:ALA:HB2	1.97	0.46
2:D:68:ARG:HH22	2:D:91:ASP:CG	2.17	0.46
1:A:38:GLY:O	1:A:48:ARG:HD3	2.15	0.46
1:G:9:THR:HG21	2:H:28:PHE:CD2	2.51	0.46
2:D:114:GLN:HB3	6:D:201:EPE:H32	1.98	0.45
2:F:111:TYR:CD2	2:H:114[A]:GLN:HG3	2.51	0.45
1:G:51:ARG:HD2	1:G:64:ARG:NH2	2.31	0.45
1:A:47:LEU:HD21	1:A:102:MET:HG3	1.99	0.45
1:A:51:ARG:CZ	1:A:62:GLY:HA3	2.47	0.45
2:F:29:THR:HG23	2:F:31:ASP:OD1	2.16	0.45
1:G:27:PHE:CZ	1:G:31:LEU:HD11	2.52	0.45
1:G:68:TYR:HB3	1:G:102:MET:CE	2.46	0.45
2:H:53:SER:HB3	2:H:58:THR:HB	1.99	0.44
2:B:107:ARG:HB2	5:B:202:EDO:H22	2.00	0.44
1:E:79:LEU:HD12	2:F:101:PHE:CE1	2.52	0.44
2:D:5:LEU:HD23	2:D:25:ALA:HA	2.00	0.44
1:A:54:SER:HB3	1:A:61:GLY:O	2.17	0.44
2:D:7:GLU:HA	2:D:22:SER:O	2.18	0.44
1:G:34:ASN:O	1:G:37:LEU:HB2	2.18	0.44
1:G:103:GLU:OE2	1:G:107:ASN:OD1	2.35	0.43
2:D:25:ALA:HB2	2:D:30:LEU:HD23	2.00	0.43
1:C:91:ASN:OD1	1:C:94:GLN:HG3	2.18	0.43
2:F:7:GLU:HA	2:F:22:SER:O	2.19	0.43
2:B:100:ASP:OD1	2:B:101:PHE:N	2.46	0.43
1:E:0:HIS:HA	1:G:0:HIS:HB3	2.01	0.43
2:H:88:LYS:CD	2:H:90:GLU:OE2	2.67	0.43
2:B:64:SER:O	2:B:68:ARG:NH1	2.52	0.42
2:B:36:GLY:HA2	2:B:51:CYS:HA	2.01	0.42
1:E:64:ARG:HG2	1:E:82:TYR:O	2.18	0.42
2:F:84:MET:HE2	2:F:87:LEU:HD21	2.01	0.42
2:H:65:VAL:HA	2:H:68:ARG:HH11	1.85	0.42
2:H:117:GLN:OE1	2:H:118:VAL:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:MET:HB2	1:C:87:MET:HE2	1.94	0.42
2:D:69:PHE:HA	2:D:83:GLN:O	2.20	0.41
1:E:19:LEU:HD22	1:E:23:GLU:HB3	2.02	0.41
2:H:102:ALA:HB3	2:H:106:ILE:CD1	2.44	0.41
1:E:34:ASN:O	1:E:37:LEU:HB2	2.19	0.41
2:B:89:PRO:HA	2:B:120:VAL:CG2	2.43	0.41
1:C:75:ARG:HD2	1:C:77:TYR:CE1	2.56	0.41
2:F:35:ILE:HG13	2:F:80:VAL:HG21	2.02	0.41
1:E:52:VAL:O	1:E:63:SER:N	2.51	0.41
2:B:120:VAL:HG23	2:B:120:VAL:O	2.20	0.41
2:F:92:THR:HG23	2:F:119:THR:HA	2.03	0.41
2:B:84:MET:CE	2:B:87:LEU:HD21	2.50	0.41
1:G:49:LYS:HE2	1:G:82:TYR:OH	2.19	0.41
1:E:24:TYR:O	1:E:28:GLN:HG3	2.20	0.41
2:F:114:GLN:O	6:F:201:EPE:H52	2.21	0.40
1:G:66:ILE:HG22	1:G:79:LEU:HB2	2.03	0.40
1:A:15:ARG:HD2	1:A:15:ARG:C	2.41	0.40
1:A:68:TYR:CE2	1:A:106:ARG:NH2	2.89	0.40
2:B:20:ARG:HD3	8:B:302:HOH:O	2.22	0.40
1:C:24:TYR:O	1:C:28:GLN:HG3	2.21	0.40
1:E:64:ARG:HG2	1:E:64:ARG:H	1.54	0.40
2:D:103:CYS:HA	2:D:104:PRO:C	2.41	0.40
2:H:13:VAL:CG2	2:H:17:GLY:HA3	2.52	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	101/111 (91%)	100 (99%)	1 (1%)	0	100	100
1	C	104/111 (94%)	103 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	103/111 (93%)	102 (99%)	1 (1%)	0	100	100
1	G	101/111 (91%)	100 (99%)	1 (1%)	0	100	100
2	B	119/127 (94%)	118 (99%)	1 (1%)	0	100	100
2	D	125/127 (98%)	123 (98%)	2 (2%)	0	100	100
2	F	125/127 (98%)	123 (98%)	2 (2%)	0	100	100
2	H	121/127 (95%)	120 (99%)	1 (1%)	0	100	100
All	All	899/952 (94%)	889 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	85/97 (88%)	82 (96%)	3 (4%)	31	57
1	C	88/97 (91%)	86 (98%)	2 (2%)	45	72
1	E	87/97 (90%)	84 (97%)	3 (3%)	32	58
1	G	89/97 (92%)	88 (99%)	1 (1%)	70	87
2	B	98/104 (94%)	94 (96%)	4 (4%)	26	50
2	D	104/104 (100%)	104 (100%)	0	100	100
2	F	104/104 (100%)	102 (98%)	2 (2%)	52	77
2	H	99/104 (95%)	98 (99%)	1 (1%)	73	88
All	All	754/804 (94%)	738 (98%)	16 (2%)	48	74

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	71	ASP
1	A	106	ARG
2	B	51	CYS

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Mol	Chain	Res	Type
2	B	90	GLU
2	B	97	CYS
2	B	116	THR
1	C	51	ARG
1	C	64	ARG
1	E	22	GLU
1	E	64	ARG
1	E	110	SER
2	F	19	LEU
2	F	51	CYS
1	G	106	ARG
2	H	47	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	60	ASN
2	F	127	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

16 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	$\#\|Z\| > 2$
3	PO4	A	202	-	4,4,4	1.41	0	6,6,6	0.91	0
3	PO4	C	202	-	4,4,4	1.59	0	6,6,6	0.88	0
3	PO4	C	201	-	4,4,4	0.92	0	6,6,6	0.40	0
3	PO4	G	201	-	4,4,4	0.95	0	6,6,6	0.45	0
3	PO4	E	202	-	4,4,4	1.82	1 (25%)	6,6,6	0.78	0
7	PDO	G	202	-	4,4,4	0.17	0	3,3,3	0.29	0
7	PDO	D	204	-	4,4,4	0.23	0	3,3,3	0.24	0
3	PO4	A	201	-	4,4,4	1.74	2 (50%)	6,6,6	0.62	0
3	PO4	B	201	-	4,4,4	1.62	0	6,6,6	0.49	0
3	PO4	E	201	-	4,4,4	0.91	0	6,6,6	0.37	0
3	PO4	D	203	-	4,4,4	0.94	0	6,6,6	0.64	0
6	EPE	D	201	-	15,15,15	2.40	1 (6%)	18,20,20	1.93	6 (33%)
4	ACT	A	203	-	3,3,3	0.74	0	3,3,3	1.39	0
3	PO4	D	202	-	4,4,4	3.00	4 (100%)	6,6,6	1.01	0
6	EPE	F	201	-	15,15,15	2.51	1 (6%)	18,20,20	2.05	7 (38%)
5	EDO	B	202	-	3,3,3	0.48	0	2,2,2	0.16	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
7	PDO	G	202	-	-	1/2/2/2	-
7	PDO	D	204	-	-	2/2/2/2	-
6	EPE	D	201	-	-	4/9/19/19	0/1/1/1
6	EPE	F	201	-	-	0/9/19/19	0/1/1/1
5	EDO	B	202	-	-	1/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	201	EPE	C10-S	-9.60	1.63	1.77
6	D	201	EPE	C10-S	-9.21	1.64	1.77
3	D	202	PO4	P-O2	-3.28	1.44	1.54
3	D	202	PO4	P-O3	-3.27	1.44	1.54
3	D	202	PO4	P-O4	-3.06	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	202	PO4	P-O4	-2.45	1.47	1.54
3	D	202	PO4	P-O1	-2.27	1.45	1.50
3	A	201	PO4	P-O3	-2.10	1.48	1.54
3	A	201	PO4	P-O2	-2.01	1.48	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	201	EPE	O1S-S-C10	4.63	112.49	106.92
6	F	201	EPE	C6-N1-C2	4.24	118.38	108.83
6	F	201	EPE	O1S-S-C10	3.39	111.00	106.92
6	F	201	EPE	C6-C5-N4	3.35	117.51	110.64
6	D	201	EPE	C9-N1-C2	-3.29	102.83	111.23
6	F	201	EPE	C5-N4-C3	3.05	115.70	108.83
6	D	201	EPE	C7-N4-C5	-2.70	104.33	111.23
6	D	201	EPE	O3S-S-C10	2.64	110.03	105.77
6	D	201	EPE	O2S-S-C10	2.41	109.82	106.92
6	F	201	EPE	O3S-S-C10	2.41	109.67	105.77
6	F	201	EPE	C3-C2-N1	2.40	115.58	110.64
6	F	201	EPE	O3S-S-O2S	-2.32	105.59	111.27
6	D	201	EPE	C6-N1-C2	2.16	113.68	108.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	201	EPE	C9-C10-S-O2S
6	D	201	EPE	C9-C10-S-O3S
7	D	204	PDO	O1-C1-C2-C3
7	D	204	PDO	C1-C2-C3-O3
7	G	202	PDO	C1-C2-C3-O3
6	D	201	EPE	N4-C7-C8-O8
5	B	202	EDO	O1-C1-C2-O2
6	D	201	EPE	C9-C10-S-O1S

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	PO4	1	0
3	C	202	PO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	201	PO4	1	0
3	E	202	PO4	2	0
7	D	204	PDO	8	0
3	E	201	PO4	1	0
6	D	201	EPE	2	0
6	F	201	EPE	2	0
5	B	202	EDO	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2
2	H	2
1	A	1
2	F	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	103:GLU	C	104:ALA	N	1.14
1	C	70:LEU	C	71:ASP	N	1.13
1	F	19:LEU	C	20:ARG	N	1.12
1	H	19:LEU	C	20:ARG	N	1.11
1	H	20:ARG	C	21:LEU	N	1.05
1	B	98:VAL	C	99:ALA	N	1.01
1	C	69:PHE	C	70:LEU	N	1.01

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, 95^{th} 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	105/111 (94%)	0.04	5 (4%)	36	34	25, 44, 88, 116	0
1	C	108/111 (97%)	0.09	4 (3%)	45	42	27, 48, 87, 116	0
1	E	107/111 (96%)	0.12	7 (6%)	26	24	27, 43, 87, 123	0
1	G	105/111 (94%)	0.45	6 (5%)	30	28	36, 62, 101, 138	0
2	B	121/127 (95%)	-0.26	0	100	100	24, 42, 61, 80	0
2	D	127/127 (100%)	-0.14	2 (1%)	70	67	25, 44, 70, 95	0
2	F	127/127 (100%)	-0.24	3 (2%)	59	56	23, 36, 59, 155	0
2	H	122/127 (96%)	0.25	4 (3%)	49	46	18, 57, 79, 127	1 (0%)
All	All	922/952 (96%)	0.03	31 (3%)	48	45	18, 46, 86, 155	1 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	SER	4.4
2	F	128	HIS	3.8
1	E	54	SER	3.7
2	H	123	HIS	3.7
1	A	109	GLN	3.7
1	C	55	LYS	3.6
2	F	127	HIS	3.6
1	E	60	ARG	3.5
1	G	108	GLU	3.5
1	A	60	ARG	3.0
2	D	127	HIS	3.0
1	G	0	HIS	2.9
1	C	109	GLN	2.8
1	E	55	LYS	2.6
1	E	0	HIS	2.5
2	H	42	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	110	SER	2.4
2	D	19	LEU	2.3
1	G	42	GLN	2.3
1	G	61	GLY	2.3
1	C	59	LYS	2.3
2	H	43	GLY	2.2
1	E	72	GLU	2.2
1	C	51	ARG	2.2
1	A	0	HIS	2.2
1	G	41	ILE	2.1
1	A	53	ALA	2.1
2	F	97	CYS	2.1
2	H	97	CYS	2.1
1	E	53	ALA	2.1
1	E	51	ARG	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 monosaccharides 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, 95^{th} 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
7	PDO	G	202	5/5	0.59	0.20	69,83,88,89	0
4	ACT	A	203	4/4	0.63	0.20	57,61,69,69	0
3	PO4	D	203	5/5	0.71	0.19	113,114,114,115	0
3	PO4	A	202	5/5	0.72	0.11	113,113,114,114	0
3	PO4	C	202	5/5	0.75	0.11	118,119,119,120	0
3	PO4	E	202	5/5	0.75	0.12	104,105,106,106	0
6	EPE	D	201	15/15	0.77	0.14	57,77,104,104	0
3	PO4	A	201	5/5	0.78	0.15	85,86,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	E	201	5/5	0.79	0.11	79,82,84,84	0
3	PO4	C	201	5/5	0.81	0.10	86,87,88,89	0
3	PO4	B	201	5/5	0.86	0.34	30,30,30,30	0
6	EPE	F	201	15/15	0.87	0.14	76,91,98,101	0
7	PDO	D	204	5/5	0.90	0.26	43,52,60,60	0
5	EDO	B	202	4/4	0.90	0.21	50,61,66,73	0
3	PO4	G	201	5/5	0.92	0.12	69,70,71,72	0
3	PO4	D	202	5/5	0.95	0.09	67,69,70,72	0

6.5 Other polymers (i)

There are no such residues in this entry.