Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2016 – 11:34 AM EST

PDB ID	:	5H0T
Title	:	Crystal structure of proliferating cell nuclear antigen from Leishmania donovani at 2.73 Angstrom resolution
Authors	:	Singh, P.K.; Yadav, S.P.; Sharma, P.S.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2016-10-06
Resolution	:	2.73 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

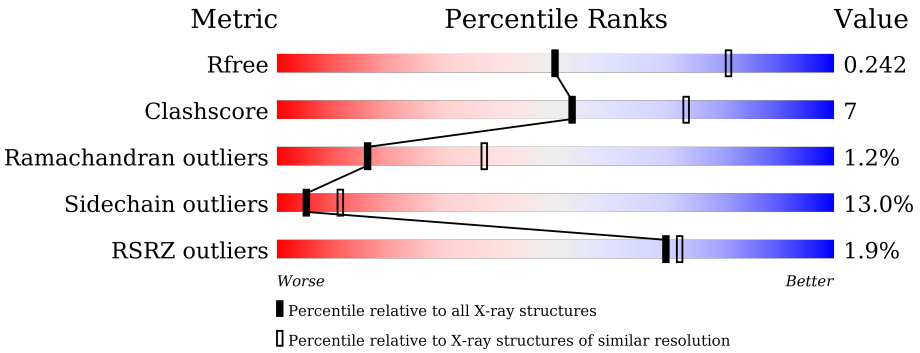
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 2.73 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}	91344	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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 <=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	292	.% 65% 14% 5% 15%
1	B	292	2% 66% 16% • 15%
1	C	292	.% 61% 18% • • 15%
1	D	292	.% 63% 17% • • 15%
1	E	292	3% 64% 14% • • 15%
1	F	292	2% 63% 17% • • 15%

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
2	PEG	A	301	-	-	-	X

2 Entry composition

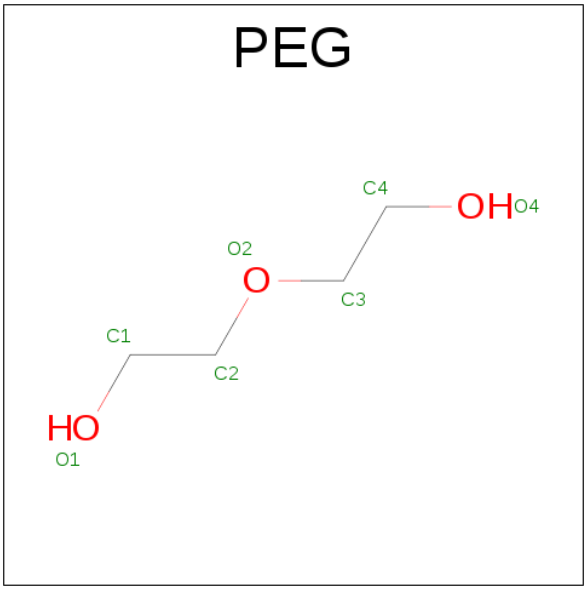
There are 3 unique types of molecules in this entry. The entry contains 11778 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	D	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	E	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	B	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	C	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	F	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

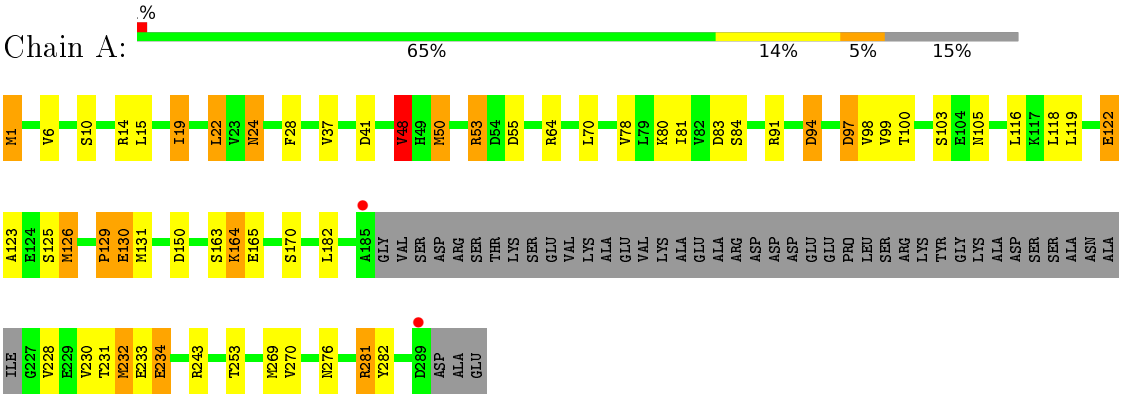
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	55	Total O 55 55	0	0
3	D	59	Total O 59 59	0	0
3	E	53	Total O 53 53	0	0
3	B	26	Total O 26 26	0	0
3	C	30	Total O 30 30	0	0
3	F	27	Total O 27 27	0	0

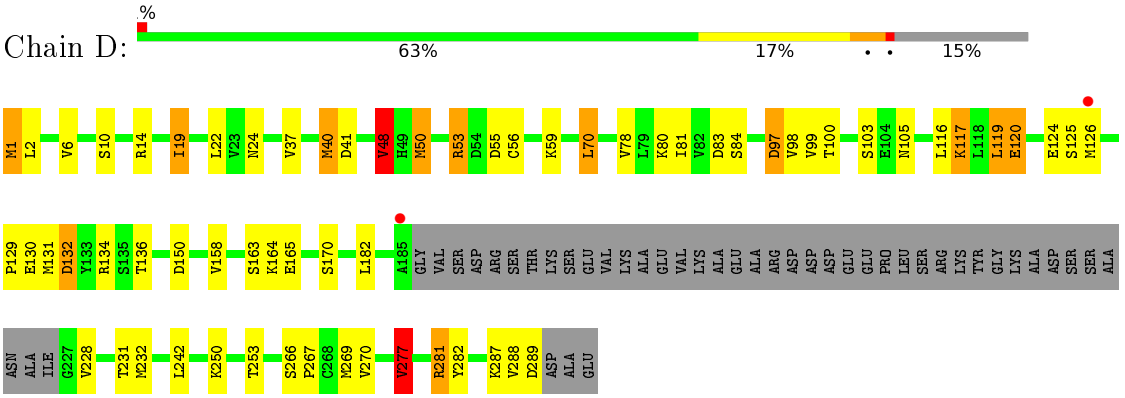
3 Residue-property plots (i)

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

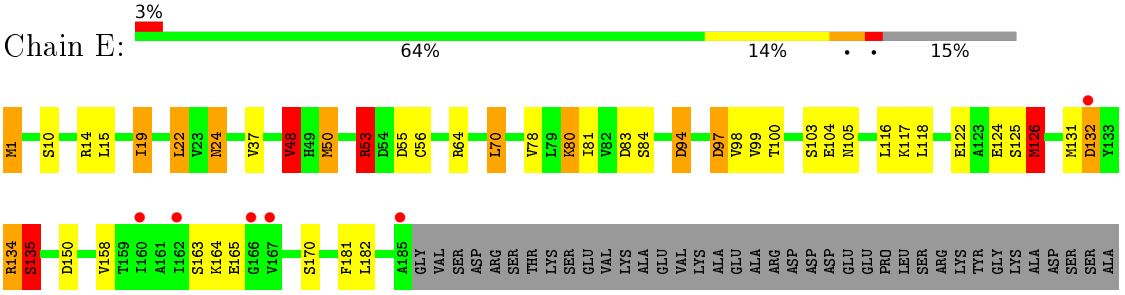
- Molecule 1: Proliferating cell nuclear antigen

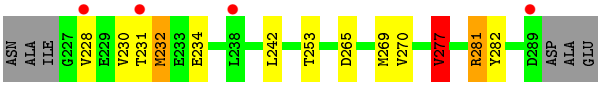


- Molecule 1: Proliferating cell nuclear antigen



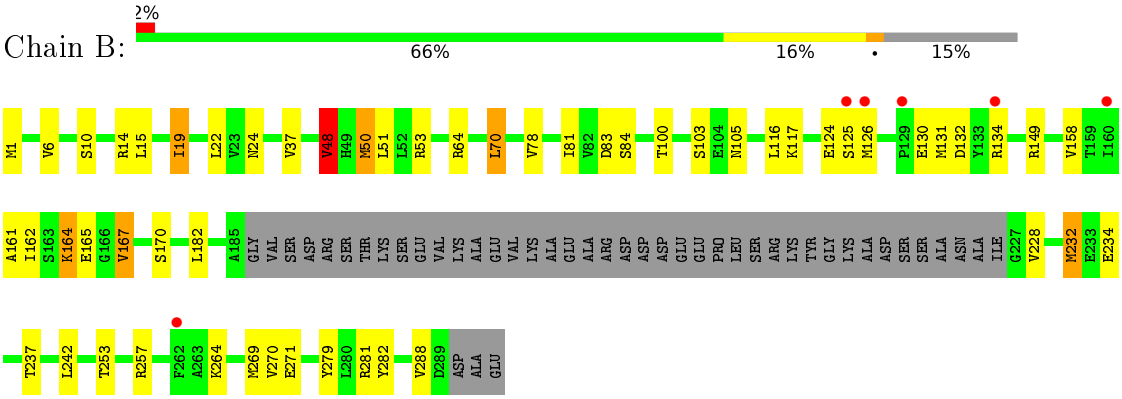
- Molecule 1: Proliferating cell nuclear antigen





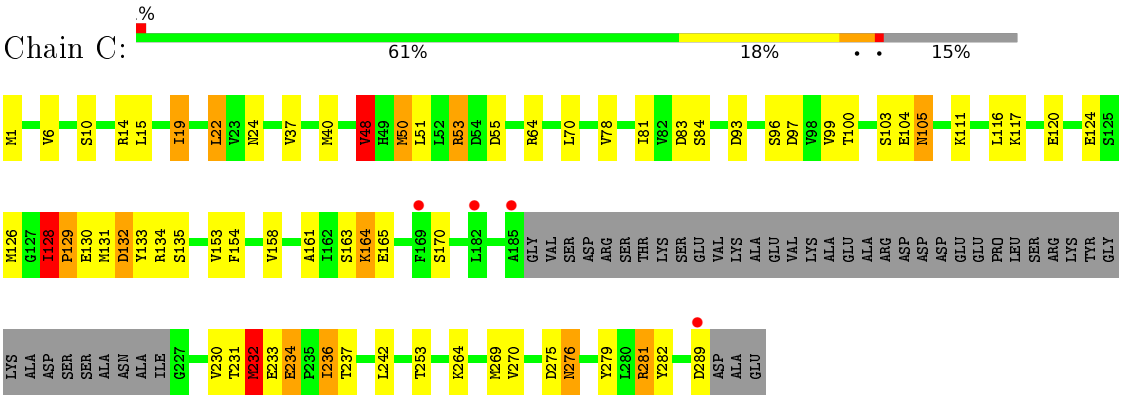
• Molecule 1: Proliferating cell nuclear antigen

Chain B:



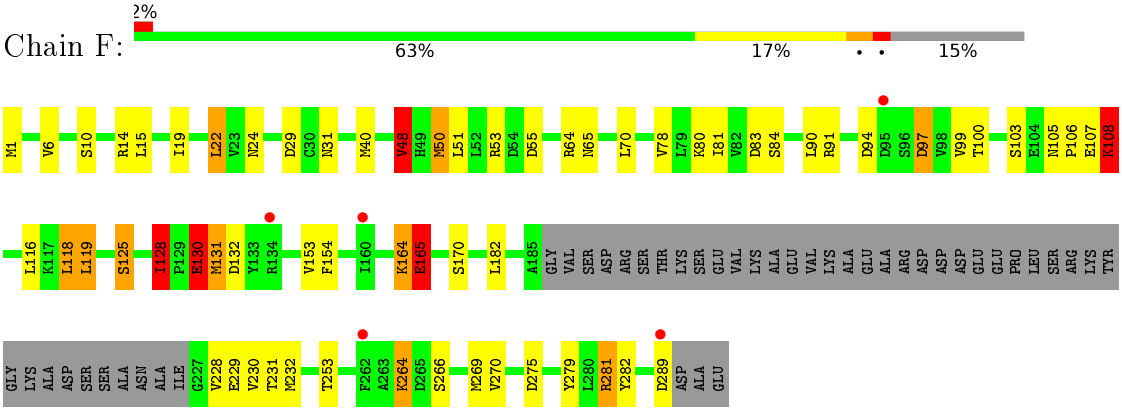
• Molecule 1: Proliferating cell nuclear antigen

Chain C:



• Molecule 1: Proliferating cell nuclear antigen

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	133.80Å 149.57Å 169.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.08 – 2.73 43.13 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.3 (112.08-2.73) 99.3 (43.13-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.197 , 0.239 0.202 , 0.242	Depositor DCC
R_{free} test set	927 reflections (1.04%)	DCC
Wilson B-factor (Å^2)	80.7	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11778	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG

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	0.93	1/1947 (0.1%)	1.17	12/2627 (0.5%)
1	B	0.86	0/1947	1.16	10/2627 (0.4%)
1	C	0.91	0/1947	1.11	5/2627 (0.2%)
1	D	0.90	1/1947 (0.1%)	1.18	18/2627 (0.7%)
1	E	0.89	0/1947	1.14	11/2627 (0.4%)
1	F	0.85	0/1947	1.14	16/2627 (0.6%)
All	All	0.89	2/11682 (0.0%)	1.15	72/15762 (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	2
1	B	0	2
1	C	0	2
1	D	0	1
1	F	0	3
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	N-CA	5.74	1.57	1.46
1	D	287	LYS	C-O	-5.05	1.13	1.23

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	70	LEU	CB-CG-CD1	16.92	139.76	111.00
1	A	1	MET	CG-SD-CE	10.28	116.65	100.20
1	E	277	VAL	CG1-CB-CG2	9.75	126.50	110.90
1	D	277	VAL	CG1-CB-CG2	9.71	126.44	110.90
1	B	70	LEU	CB-CG-CD2	-9.09	95.55	111.00
1	F	48	VAL	CB-CA-C	-8.65	94.97	111.40
1	C	48	VAL	CB-CA-C	-8.64	94.99	111.40
1	D	48	VAL	CB-CA-C	-8.56	95.14	111.40
1	B	48	VAL	CB-CA-C	-8.49	95.27	111.40
1	E	48	VAL	CB-CA-C	-8.35	95.54	111.40
1	A	48	VAL	CB-CA-C	-8.20	95.82	111.40
1	F	40	MET	CG-SD-CE	8.05	113.08	100.20
1	B	257	ARG	CG-CD-NE	-7.91	95.18	111.80
1	F	119	LEU	O-C-N	-7.63	110.49	122.70
1	E	135	SER	N-CA-CB	7.63	121.94	110.50
1	F	130	GLU	N-CA-C	7.50	131.25	111.00
1	B	53	ARG	CA-CB-CG	-7.12	97.73	113.40
1	D	119	LEU	O-C-N	-7.04	111.43	122.70
1	D	117	LYS	CA-CB-CG	6.64	128.02	113.40
1	F	164	LYS	N-CA-C	-6.54	93.34	111.00
1	C	105	ASN	CB-CA-C	-6.51	97.37	110.40
1	D	50	MET	CG-SD-CE	6.50	110.60	100.20
1	F	128	ILE	C-N-CD	-6.42	106.47	120.60
1	E	1	MET	CA-CB-CG	6.32	124.04	113.30
1	A	105	ASN	CB-CA-C	-6.19	98.03	110.40
1	A	97	ASP	CB-CG-OD1	6.14	123.83	118.30
1	E	97	ASP	CB-CG-OD1	6.14	123.83	118.30
1	B	105	ASN	CB-CA-C	-6.09	98.22	110.40
1	D	126	MET	CG-SD-CE	6.06	109.89	100.20
1	D	40	MET	CG-SD-CE	-6.03	90.56	100.20
1	F	105	ASN	CB-CA-C	6.02	122.44	110.40
1	F	119	LEU	CA-C-N	6.00	130.39	117.20
1	D	105	ASN	CB-CA-C	-5.99	98.43	110.40
1	F	289	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	164	LYS	CA-CB-CG	5.87	126.32	113.40
1	A	129	PRO	N-CA-C	-5.76	97.11	112.10
1	A	130	GLU	OE1-CD-OE2	-5.75	116.41	123.30
1	E	150	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	83	ASP	CB-CG-OD1	5.67	123.40	118.30
1	F	91	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	E	53	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	B	1	MET	CG-SD-CE	5.65	109.23	100.20
1	D	97	ASP	CB-CG-OD1	5.64	123.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	105	ASN	CB-CA-C	5.64	121.68	110.40
1	C	232	MET	CG-SD-CE	5.63	109.21	100.20
1	A	126	MET	CA-CB-CG	5.62	122.85	113.30
1	C	83	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	275	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	91	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	F	264	LYS	CD-CE-NZ	5.57	124.51	111.70
1	D	1	MET	CG-SD-CE	5.49	108.99	100.20
1	D	83	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	289	ASP	CB-CG-OD1	5.45	123.20	118.30
1	E	83	ASP	CB-CG-OD1	5.42	123.18	118.30
1	D	2	LEU	CB-CG-CD1	5.42	120.21	111.00
1	E	70	LEU	CB-CG-CD2	5.41	120.19	111.00
1	B	83	ASP	CB-CG-OD1	5.40	123.16	118.30
1	D	150	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	F	97	ASP	CB-CG-OD1	5.37	123.14	118.30
1	F	83	ASP	CB-CG-OD1	5.37	123.13	118.30
1	F	108	LYS	CD-CE-NZ	5.31	123.92	111.70
1	F	275	ASP	N-CA-C	5.31	125.33	111.00
1	D	119	LEU	CA-C-N	5.28	128.82	117.20
1	E	80	LYS	CB-CG-CD	5.22	125.17	111.60
1	F	108	LYS	CB-CG-CD	5.22	125.17	111.60
1	D	70	LEU	CB-CG-CD2	5.21	119.86	111.00
1	B	257	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	164	LYS	CA-CB-CG	5.18	124.81	113.40
1	D	287	LYS	CD-CE-NZ	5.15	123.55	111.70
1	A	91	ARG	CD-NE-CZ	5.06	130.68	123.60
1	A	150	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	D	120	GLU	CA-CB-CG	5.02	124.44	113.40

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	GLU	Peptide
1	A	276	ASN	Sidechain
1	B	130	GLU	Peptide
1	B	288	VAL	Peptide
1	C	128	ILE	Peptide
1	C	132	ASP	Peptide
1	D	119	LEU	Peptide
1	F	119	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	F	125	SER	Peptide
1	F	165	GLU	Mainchain

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	1919	0	1914	27	0
1	B	1919	0	1914	19	0
1	C	1919	0	1914	36	0
1	D	1919	0	1914	23	0
1	E	1919	0	1914	27	0
1	F	1919	0	1914	20	0
2	A	7	0	10	0	0
2	E	7	0	10	1	0
3	A	55	0	0	3	0
3	B	26	0	0	1	0
3	C	30	0	0	2	0
3	D	59	0	0	2	0
3	E	53	0	0	0	0
3	F	27	0	0	1	0
All	All	11778	0	11504	151	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 7.

All (151) 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:233:GLU:O	1:C:234:GLU:HB2	1.75	0.85
1:C:232:MET:CG	1:C:234:GLU:O	2.35	0.74
1:C:232:MET:HG3	1:C:234:GLU:O	1.91	0.70
1:C:93:ASP:HB2	1:C:96:SER:OG	1.92	0.67
1:B:124:GLU:HB2	1:B:126:MET:SD	2.35	0.65
1:C:232:MET:HG2	1:C:234:GLU:O	1.99	0.62
1:A:1:MET:CE	1:A:94:ASP:HA	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:LEU:HD12	1:F:48:VAL:HG22	1.83	0.60
1:E:22:LEU:HD12	1:E:48:VAL:HG22	1.83	0.60
1:E:56:CYS:HB2	1:E:277:VAL:HG13	1.84	0.60
1:A:24:ASN:HB3	3:A:427:HOH:O	2.03	0.59
1:F:229:GLU:HG2	3:F:325:HOH:O	2.03	0.59
1:C:22:LEU:HD12	1:C:48:VAL:HG22	1.86	0.58
1:E:182:LEU:HD12	1:E:182:LEU:N	2.18	0.58
1:D:56:CYS:HB2	1:D:277:VAL:HG13	1.85	0.57
1:A:53:ARG:HB3	1:A:55:ASP:OD1	2.05	0.57
1:D:56:CYS:CB	1:D:277:VAL:HG13	2.35	0.57
1:D:48:VAL:HG13	1:D:282:TYR:CE1	2.40	0.57
1:A:233:GLU:C	1:A:234:GLU:HG3	2.23	0.57
1:B:48:VAL:HG13	1:B:282:TYR:CE1	2.40	0.56
1:C:135:SER:OG	1:C:236:ILE:HD11	2.05	0.56
1:A:22:LEU:HD12	1:A:48:VAL:HG22	1.87	0.56
1:E:56:CYS:CB	1:E:277:VAL:HG13	2.36	0.56
1:C:163:SER:C	1:C:232:MET:HE3	2.26	0.56
1:E:53:ARG:HB3	1:E:55:ASP:OD1	2.06	0.56
1:C:48:VAL:HG13	1:C:282:TYR:CE1	2.41	0.55
1:C:15:LEU:HD13	1:C:50:MET:CE	2.36	0.55
1:D:53:ARG:HG3	3:D:307:HOH:O	2.06	0.55
1:E:24:ASN:OD1	2:E:301:PEG:H41	2.06	0.55
1:A:269:MET:HE3	1:A:281:ARG:HD2	1.88	0.55
1:E:269:MET:HE3	1:E:281:ARG:HD2	1.89	0.55
1:F:51:LEU:HD23	1:F:279:TYR:CE1	2.42	0.55
1:C:130:GLU:N	1:C:130:GLU:OE1	2.39	0.55
1:F:48:VAL:HG13	1:F:282:TYR:CE1	2.42	0.55
1:F:164:LYS:O	1:F:165:GLU:OE1	2.25	0.54
1:A:48:VAL:HG13	1:A:282:TYR:CE1	2.42	0.54
3:A:413:HOH:O	1:E:122:GLU:HB2	2.08	0.54
1:A:1:MET:HE2	1:A:94:ASP:HA	1.89	0.54
1:B:51:LEU:HD23	1:B:279:TYR:CE1	2.42	0.54
1:D:129:PRO:HB2	1:D:131:MET:CE	2.38	0.54
1:E:48:VAL:HG13	1:E:282:TYR:CE1	2.43	0.54
1:C:53:ARG:HB3	1:C:55:ASP:OD1	2.08	0.54
1:A:243:ARG:HD3	3:A:421:HOH:O	2.08	0.53
1:D:53:ARG:HB3	1:D:55:ASP:OD1	2.08	0.53
1:C:269:MET:HE3	1:C:281:ARG:HD2	1.91	0.53
1:E:124:GLU:OE1	1:E:126:MET:O	2.25	0.53
1:F:106:PRO:O	1:F:108:LYS:HD2	2.07	0.53
1:C:51:LEU:HD23	1:C:279:TYR:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:PRO:HB2	1:D:131:MET:HE2	1.92	0.52
1:A:163:SER:C	1:A:232:MET:CE	2.78	0.51
1:B:15:LEU:HD13	1:B:50:MET:CE	2.39	0.51
1:F:31:ASN:ND2	1:F:65:ASN:HD22	2.08	0.51
1:A:24:ASN:OD1	1:E:122:GLU:OE2	2.28	0.51
1:A:118:LEU:C	1:A:119:LEU:HD12	2.31	0.51
1:E:14:ARG:HD2	1:E:253:THR:HB	1.92	0.51
1:E:163:SER:C	1:E:232:MET:HE3	2.32	0.51
1:C:135:SER:OG	1:C:236:ILE:CD1	2.58	0.51
1:F:15:LEU:HD13	1:F:50:MET:CE	2.41	0.51
1:D:14:ARG:HD2	1:D:253:THR:HB	1.92	0.50
1:E:163:SER:C	1:E:232:MET:CE	2.80	0.50
1:A:163:SER:C	1:A:232:MET:HE3	2.32	0.49
1:B:22:LEU:HD23	1:B:48:VAL:HG22	1.95	0.49
1:F:269:MET:HE3	1:F:281:ARG:HD2	1.93	0.49
1:A:14:ARG:HD2	1:A:253:THR:HB	1.94	0.49
1:C:40:MET:HG3	1:C:124:GLU:OE2	2.12	0.49
1:C:163:SER:C	1:C:232:MET:CE	2.80	0.49
1:B:51:LEU:HD23	1:B:279:TYR:HE1	1.78	0.49
1:C:14:ARG:HD2	1:C:253:THR:HB	1.95	0.49
1:C:19:ILE:HD12	1:C:37:VAL:HG11	1.94	0.49
1:F:14:ARG:HD2	1:F:253:THR:HB	1.94	0.49
1:B:14:ARG:HD2	1:B:253:THR:HB	1.94	0.48
1:A:78:VAL:O	1:A:81:ILE:HG12	2.13	0.48
1:B:78:VAL:O	1:B:81:ILE:HG12	2.14	0.48
1:D:269:MET:HE3	1:D:281:ARG:HD2	1.94	0.48
1:C:78:VAL:O	1:C:81:ILE:HG12	2.13	0.48
1:C:97:ASP:OD1	1:C:97:ASP:O	2.31	0.48
1:E:78:VAL:O	1:E:81:ILE:HG12	2.14	0.48
1:F:78:VAL:O	1:F:81:ILE:HG12	2.14	0.48
1:F:70:LEU:HD21	1:F:99:VAL:HG11	1.96	0.48
1:D:78:VAL:O	1:D:81:ILE:HG12	2.13	0.48
1:C:161:ALA:CB	1:C:237:THR:HG22	2.44	0.47
1:E:1:MET:SD	1:E:94:ASP:HA	2.54	0.47
1:D:130:GLU:OE1	1:D:130:GLU:N	2.47	0.47
1:F:106:PRO:O	1:F:108:LYS:HE2	2.15	0.47
1:A:1:MET:HE3	1:A:94:ASP:HA	1.96	0.46
1:A:123:ALA:HB1	1:A:125:SER:OG	2.16	0.46
1:B:19:ILE:HD12	1:B:37:VAL:HG11	1.97	0.46
1:C:153:VAL:HG22	1:C:154:PHE:CE1	2.51	0.46
1:C:24:ASN:ND2	3:C:303:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:MET:O	1:E:132:ASP:HB2	2.16	0.46
1:A:126:MET:HE3	1:A:126:MET:HA	1.97	0.46
1:C:15:LEU:HD13	1:C:50:MET:HE2	1.96	0.46
1:E:19:ILE:HD12	1:E:37:VAL:HG11	1.97	0.46
1:E:134:ARG:O	1:E:135:SER:OG	2.26	0.46
1:D:136:THR:HG22	3:D:317:HOH:O	2.16	0.45
1:C:70:LEU:HD21	1:C:99:VAL:HG11	1.98	0.45
1:F:153:VAL:HG22	1:F:154:PHE:CE1	2.52	0.45
1:F:118:LEU:N	1:F:118:LEU:HD23	2.32	0.45
1:A:70:LEU:HD21	1:A:99:VAL:HG11	1.98	0.45
1:C:165:GLU:N	1:C:165:GLU:OE1	2.44	0.45
1:B:162:ILE:HG12	1:B:167:VAL:HG12	1.98	0.45
1:D:182:LEU:HB3	1:D:228:VAL:HG21	1.98	0.45
1:E:15:LEU:HD13	1:E:50:MET:CE	2.47	0.44
1:A:15:LEU:HD13	1:A:50:MET:CE	2.47	0.44
1:D:19:ILE:HD12	1:D:37:VAL:HG11	1.98	0.44
1:B:269:MET:HE3	1:B:271:GLU:HB2	1.99	0.44
1:B:158:VAL:HB	1:B:242:LEU:HD21	1.99	0.44
1:C:132:ASP:O	1:C:133:TYR:CG	2.71	0.44
1:B:182:LEU:HB3	1:B:228:VAL:HG21	1.98	0.44
1:C:161:ALA:HB1	1:C:237:THR:HG22	2.00	0.44
1:D:131:MET:O	1:D:132:ASP:CB	2.65	0.44
1:E:165:GLU:OE1	1:E:165:GLU:N	2.50	0.44
1:D:40:MET:HG3	1:D:124:GLU:OE2	2.18	0.44
1:D:56:CYS:SG	1:D:277:VAL:HG13	2.58	0.44
1:F:15:LEU:HD13	1:F:50:MET:HE2	2.00	0.44
1:C:164:LYS:N	1:C:232:MET:HE1	2.33	0.44
1:B:165:GLU:OE1	1:B:165:GLU:N	2.44	0.43
1:D:131:MET:HE1	1:D:267:PRO:HG2	2.00	0.43
1:F:51:LEU:HD23	1:F:279:TYR:HE1	1.81	0.43
1:E:182:LEU:HB3	1:E:228:VAL:HG21	1.99	0.43
1:A:130:GLU:HA	1:A:130:GLU:OE2	2.19	0.43
1:B:161:ALA:CB	1:B:237:THR:HG22	2.49	0.43
1:C:51:LEU:HD23	1:C:279:TYR:HE1	1.81	0.43
1:C:158:VAL:HB	1:C:242:LEU:HD21	2.01	0.43
1:C:276:ASN:OD1	1:C:276:ASN:N	2.50	0.43
1:F:182:LEU:HB3	1:F:228:VAL:HG21	2.01	0.42
1:B:15:LEU:HD13	1:B:50:MET:HE2	2.00	0.42
1:C:128:ILE:HG22	1:C:129:PRO:HD2	2.01	0.42
1:E:181:PHE:C	1:E:182:LEU:HD12	2.39	0.42
1:E:182:LEU:N	1:E:182:LEU:CD1	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:VAL:O	1:F:231:THR:HG23	2.19	0.42
1:D:165:GLU:N	1:D:165:GLU:OE1	2.44	0.42
1:E:158:VAL:HB	1:E:242:LEU:HD21	2.01	0.42
1:C:120:GLU:HG3	3:C:327:HOH:O	2.18	0.42
1:A:28:PHE:CE1	1:A:70:LEU:HD12	2.55	0.42
1:E:230:VAL:O	1:E:231:THR:HG23	2.19	0.42
1:F:90:LEU:C	1:F:90:LEU:HD23	2.40	0.42
1:A:230:VAL:O	1:A:231:THR:HG23	2.19	0.41
1:D:158:VAL:HB	1:D:242:LEU:HD21	2.02	0.41
1:D:70:LEU:HD21	1:D:99:VAL:HG11	2.03	0.41
1:D:22:LEU:CD2	1:D:48:VAL:HG22	2.50	0.41
1:C:230:VAL:O	1:C:231:THR:HG23	2.20	0.41
1:A:119:LEU:CD1	1:A:119:LEU:N	2.84	0.41
1:D:22:LEU:HD23	1:D:48:VAL:HG22	2.03	0.41
1:B:22:LEU:CD2	1:B:48:VAL:HG22	2.51	0.41
1:B:149:ARG:HD2	3:B:324:HOH:O	2.21	0.41
1:A:19:ILE:HD12	1:A:37:VAL:HG11	2.03	0.40
1:B:232:MET:HG2	1:B:234:GLU:H	1.86	0.40
1:E:70:LEU:HD21	1:E:99:VAL:HG11	2.03	0.40
1:A:119:LEU:N	1:A:119:LEU:HD12	2.36	0.40
1:A:182:LEU:HB3	1:A:228:VAL:HG21	2.03	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	244/292 (84%)	229 (94%)	13 (5%)	2 (1%)	24 50
1	B	244/292 (84%)	230 (94%)	13 (5%)	1 (0%)	39 68
1	C	244/292 (84%)	228 (93%)	12 (5%)	4 (2%)	12 28
1	D	244/292 (84%)	228 (93%)	12 (5%)	4 (2%)	12 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	244/292 (84%)	227 (93%)	14 (6%)	3 (1%)	16 37
1	F	244/292 (84%)	225 (92%)	15 (6%)	4 (2%)	12 28
All	All	1464/1752 (84%)	1367 (93%)	79 (5%)	18 (1%)	16 37

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	135	SER
1	C	129	PRO
1	C	234	GLU
1	F	130	GLU
1	C	128	ILE
1	F	131	MET
1	A	129	PRO
1	D	288	VAL
1	E	126	MET
1	F	84	SER
1	A	84	SER
1	D	84	SER
1	D	125	SER
1	E	84	SER
1	B	84	SER
1	C	84	SER
1	F	128	ILE
1	D	132	ASP

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	216/251 (86%)	190 (88%)	26 (12%)	6 13
1	B	216/251 (86%)	193 (89%)	23 (11%)	8 18
1	C	216/251 (86%)	188 (87%)	28 (13%)	5 11
1	D	216/251 (86%)	187 (87%)	29 (13%)	5 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	216/251 (86%)	186 (86%)	30 (14%)	4 9
1	F	216/251 (86%)	183 (85%)	33 (15%)	3 7
All	All	1296/1506 (86%)	1127 (87%)	169 (13%)	5 11

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	10	SER
1	A	19	ILE
1	A	22	LEU
1	A	24	ASN
1	A	41	ASP
1	A	48	VAL
1	A	50	MET
1	A	53	ARG
1	A	64	ARG
1	A	80	LYS
1	A	94	ASP
1	A	97	ASP
1	A	98	VAL
1	A	100	THR
1	A	103	SER
1	A	116	LEU
1	A	122	GLU
1	A	131	MET
1	A	164	LYS
1	A	165	GLU
1	A	170	SER
1	A	232	MET
1	A	234	GLU
1	A	270	VAL
1	A	281	ARG
1	D	1	MET
1	D	6	VAL
1	D	10	SER
1	D	19	ILE
1	D	24	ASN
1	D	41	ASP
1	D	48	VAL
1	D	50	MET

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Mol	Chain	Res	Type
1	D	53	ARG
1	D	59	LYS
1	D	80	LYS
1	D	97	ASP
1	D	98	VAL
1	D	100	THR
1	D	103	SER
1	D	116	LEU
1	D	117	LYS
1	D	120	GLU
1	D	134	ARG
1	D	163	SER
1	D	164	LYS
1	D	170	SER
1	D	231	THR
1	D	232	MET
1	D	250	LYS
1	D	266	SER
1	D	270	VAL
1	D	277	VAL
1	D	281	ARG
1	E	10	SER
1	E	19	ILE
1	E	22	LEU
1	E	24	ASN
1	E	48	VAL
1	E	50	MET
1	E	53	ARG
1	E	64	ARG
1	E	80	LYS
1	E	94	ASP
1	E	97	ASP
1	E	98	VAL
1	E	100	THR
1	E	103	SER
1	E	104	GLU
1	E	116	LEU
1	E	117	LYS
1	E	118	LEU
1	E	125	SER
1	E	126	MET
1	E	132	ASP

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Mol	Chain	Res	Type
1	E	134	ARG
1	E	164	LYS
1	E	170	SER
1	E	232	MET
1	E	234	GLU
1	E	265	ASP
1	E	270	VAL
1	E	277	VAL
1	E	281	ARG
1	B	6	VAL
1	B	10	SER
1	B	19	ILE
1	B	24	ASN
1	B	48	VAL
1	B	50	MET
1	B	64	ARG
1	B	70	LEU
1	B	100	THR
1	B	103	SER
1	B	116	LEU
1	B	117	LYS
1	B	125	SER
1	B	131	MET
1	B	132	ASP
1	B	134	ARG
1	B	164	LYS
1	B	167	VAL
1	B	170	SER
1	B	232	MET
1	B	264	LYS
1	B	270	VAL
1	B	281	ARG
1	C	1	MET
1	C	6	VAL
1	C	10	SER
1	C	19	ILE
1	C	22	LEU
1	C	48	VAL
1	C	50	MET
1	C	53	ARG
1	C	64	ARG
1	C	100	THR

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Mol	Chain	Res	Type
1	C	103	SER
1	C	104	GLU
1	C	105	ASN
1	C	111	LYS
1	C	116	LEU
1	C	117	LYS
1	C	126	MET
1	C	131	MET
1	C	134	ARG
1	C	164	LYS
1	C	170	SER
1	C	232	MET
1	C	236	ILE
1	C	264	LYS
1	C	270	VAL
1	C	276	ASN
1	C	281	ARG
1	C	289	ASP
1	F	1	MET
1	F	6	VAL
1	F	10	SER
1	F	19	ILE
1	F	22	LEU
1	F	24	ASN
1	F	29	ASP
1	F	48	VAL
1	F	50	MET
1	F	53	ARG
1	F	55	ASP
1	F	64	ARG
1	F	80	LYS
1	F	94	ASP
1	F	97	ASP
1	F	100	THR
1	F	103	SER
1	F	107	GLU
1	F	108	LYS
1	F	116	LEU
1	F	118	LEU
1	F	125	SER
1	F	128	ILE
1	F	130	GLU

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Mol	Chain	Res	Type
1	F	131	MET
1	F	132	ASP
1	F	165	GLU
1	F	170	SER
1	F	232	MET
1	F	264	LYS
1	F	266	SER
1	F	270	VAL
1	F	281	ARG

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	49	HIS
1	A	115	GLN
1	D	38	GLN
1	D	49	HIS
1	D	92	HIS
1	D	115	GLN
1	E	38	GLN
1	E	49	HIS
1	E	92	HIS
1	E	115	GLN
1	B	38	GLN
1	B	49	HIS
1	B	115	GLN
1	C	38	GLN
1	C	49	HIS
1	C	65	ASN
1	C	115	GLN
1	F	31	ASN
1	F	44	HIS
1	F	49	HIS
1	F	92	HIS
1	F	115	GLN
1	F	276	ASN

5.3.3 RNA

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)

2 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	$\#\|Z\| > 2$
2	PEG	A	301	-	6,6,6	0.58	0	5,5,5	0.40	0
2	PEG	E	301	-	6,6,6	0.83	0	5,5,5	0.88	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
2	PEG	A	301	-	-	0/4/4/4	0/0/0/0
2	PEG	E	301	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	PEG	1	0

5.7 Other polymers

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, 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	248/292 (84%)	0.22	2 (0%)	87 88	50, 75, 127, 177	0
1	B	248/292 (84%)	0.27	6 (2%)	62 64	59, 91, 140, 171	0
1	C	248/292 (84%)	0.29	4 (1%)	74 77	63, 92, 152, 187	0
1	D	248/292 (84%)	0.26	2 (0%)	87 88	51, 83, 139, 182	0
1	E	248/292 (84%)	0.30	10 (4%)	42 43	55, 82, 138, 160	0
1	F	248/292 (84%)	0.34	5 (2%)	68 71	64, 99, 157, 195	0
All	All	1488/1752 (84%)	0.28	29 (1%)	70 72	50, 88, 145, 195	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	ASP	8.0
1	D	185	ALA	4.2
1	E	289	ASP	4.1
1	E	185	ALA	4.0
1	C	169	PHE	4.0
1	C	289	ASP	3.8
1	E	167	VAL	3.5
1	E	228	VAL	3.5
1	C	182	LEU	3.4
1	E	166	GLY	3.4
1	E	162	ILE	3.3
1	F	262	PHE	3.1
1	F	95	ASP	3.0
1	A	185	ALA	3.0
1	E	160	ILE	2.9
1	B	125	SER	2.8
1	C	185	ALA	2.6
1	B	134	ARG	2.6
1	F	160	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	289	ASP	2.5
1	B	126	MET	2.5
1	E	132	ASP	2.4
1	D	126	MET	2.4
1	B	160	ILE	2.3
1	E	231	THR	2.2
1	B	262	PHE	2.2
1	F	134	ARG	2.2
1	E	238	LEU	2.1
1	B	129	PRO	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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	PEG	A	301	7/7	0.84	0.31	5.60	93,113,124,140	0
2	PEG	E	301	7/7	0.86	0.17	-0.30	88,99,105,111	0

6.5 Other polymers (i)

There are no such residues in this entry.