



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2020 – 12:32 PM BST

PDB ID : 6J0J
Title : Crystal structure of Proliferating Cell Nuclear Antigen from Leishmania donovani with an unexplained density near residues Pro229,Pr0267 and Ala285
Authors : Iqbal, N.; Sharma, S.; Singh, T.P.
Deposited on : 2018-12-24
Resolution : 3.10 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 : 2.13
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) : 2.13

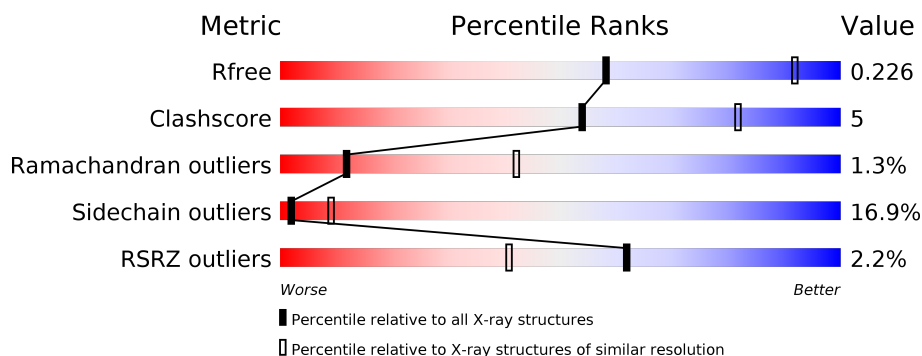
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	302	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 65%, yellow 65%, yellow 89%, orange 89%, orange 93%, grey 93%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 65% 14% • 18% </div> </div>
1	B	302	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 63%, yellow 63%, yellow 80%, orange 80%, orange 87%, grey 87%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 63% 17% •• 18% </div> </div>
1	C	302	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, green 2%, green 60%, yellow 60%, yellow 80%, orange 80%, orange 88%, grey 88%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 60% 20% • 18% </div> </div>
1	D	302	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 59%, yellow 59%, yellow 80%, orange 80%, orange 87%, grey 87%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 59% 21% •• 17% </div> </div>
1	E	302	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 62%, yellow 62%, yellow 81%, orange 81%, orange 86%, grey 86%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 62% 19% • 15% </div> </div>
1	F	302	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, green 4%, green 57%, yellow 57%, yellow 78%, orange 78%, orange 86%, grey 86%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 4% 57% 21% •• 18% </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11713 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	251	Total	C	N	O	S	0	0	0
			1941	1222	320	384	15			
1	E	258	Total	C	N	O	S	0	0	0
			1967	1238	327	387	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			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	HIS	-	expression tag	UNP B5TV91
A	-8	SER	-	expression tag	UNP B5TV91
A	-7	GLY	-	expression tag	UNP B5TV91
A	-6	ARG	-	expression tag	UNP B5TV91
A	-5	PRO	-	expression tag	UNP B5TV91
A	-4	VAL	-	expression tag	UNP B5TV91
A	-3	LEU	-	expression tag	UNP B5TV91
A	-2	GLY	-	expression tag	UNP B5TV91
A	-1	SER	-	expression tag	UNP B5TV91
A	0	SER	-	expression tag	UNP B5TV91
D	-9	HIS	-	expression tag	UNP B5TV91
D	-8	SER	-	expression tag	UNP B5TV91
D	-7	GLY	-	expression tag	UNP B5TV91
D	-6	ARG	-	expression tag	UNP B5TV91
D	-5	PRO	-	expression tag	UNP B5TV91
D	-4	VAL	-	expression tag	UNP B5TV91
D	-3	LEU	-	expression tag	UNP B5TV91

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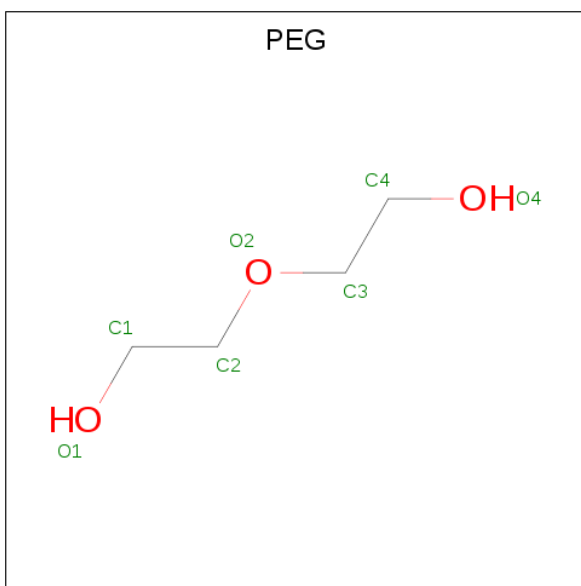
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP B5TV91
D	-1	SER	-	expression tag	UNP B5TV91
D	0	SER	-	expression tag	UNP B5TV91
E	-9	HIS	-	expression tag	UNP B5TV91
E	-8	SER	-	expression tag	UNP B5TV91
E	-7	GLY	-	expression tag	UNP B5TV91
E	-6	ARG	-	expression tag	UNP B5TV91
E	-5	PRO	-	expression tag	UNP B5TV91
E	-4	VAL	-	expression tag	UNP B5TV91
E	-3	LEU	-	expression tag	UNP B5TV91
E	-2	GLY	-	expression tag	UNP B5TV91
E	-1	SER	-	expression tag	UNP B5TV91
E	0	SER	-	expression tag	UNP B5TV91
B	-9	HIS	-	expression tag	UNP B5TV91
B	-8	SER	-	expression tag	UNP B5TV91
B	-7	GLY	-	expression tag	UNP B5TV91
B	-6	ARG	-	expression tag	UNP B5TV91
B	-5	PRO	-	expression tag	UNP B5TV91
B	-4	VAL	-	expression tag	UNP B5TV91
B	-3	LEU	-	expression tag	UNP B5TV91
B	-2	GLY	-	expression tag	UNP B5TV91
B	-1	SER	-	expression tag	UNP B5TV91
B	0	SER	-	expression tag	UNP B5TV91
C	-9	HIS	-	expression tag	UNP B5TV91
C	-8	SER	-	expression tag	UNP B5TV91
C	-7	GLY	-	expression tag	UNP B5TV91
C	-6	ARG	-	expression tag	UNP B5TV91
C	-5	PRO	-	expression tag	UNP B5TV91
C	-4	VAL	-	expression tag	UNP B5TV91
C	-3	LEU	-	expression tag	UNP B5TV91
C	-2	GLY	-	expression tag	UNP B5TV91
C	-1	SER	-	expression tag	UNP B5TV91
C	0	SER	-	expression tag	UNP B5TV91
F	-9	HIS	-	expression tag	UNP B5TV91
F	-8	SER	-	expression tag	UNP B5TV91
F	-7	GLY	-	expression tag	UNP B5TV91
F	-6	ARG	-	expression tag	UNP B5TV91
F	-5	PRO	-	expression tag	UNP B5TV91
F	-4	VAL	-	expression tag	UNP B5TV91
F	-3	LEU	-	expression tag	UNP B5TV91
F	-2	GLY	-	expression tag	UNP B5TV91
F	-1	SER	-	expression tag	UNP B5TV91

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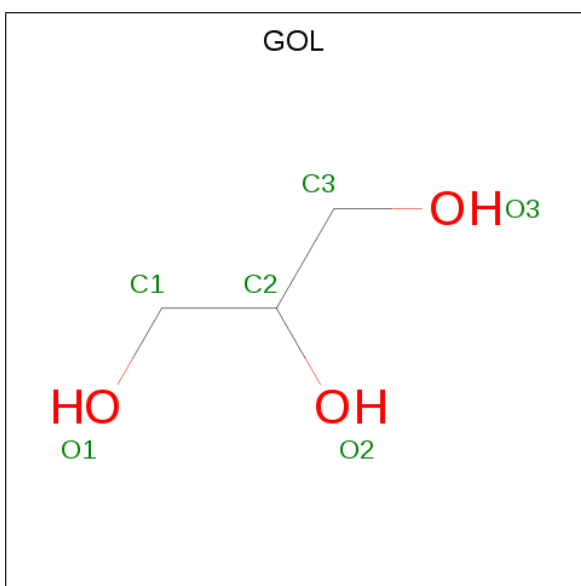
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	expression tag	UNP B5TV91

- 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	0	0
			7	4	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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


- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total	O	0	0
			28	28		
4	D	32	Total	O	0	0
			32	32		
4	E	21	Total	O	0	0
			21	21		
4	B	11	Total	O	0	0
			11	11		
4	C	9	Total	O	0	0
			9	9		
4	F	15	Total	O	0	0
			15	15		

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.

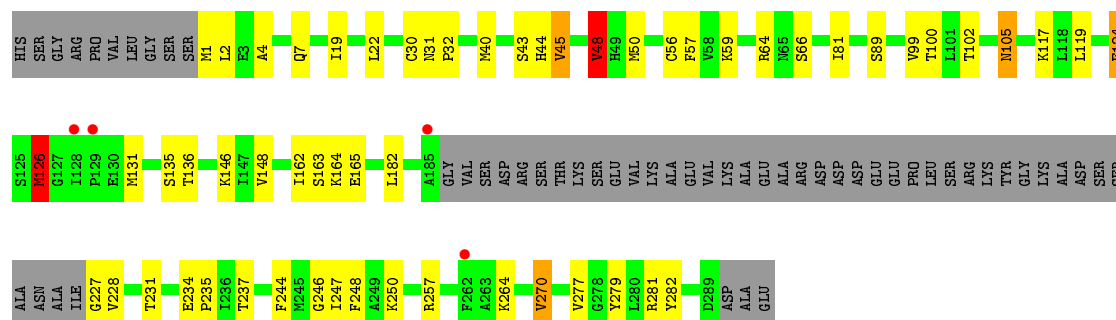
- Chain A:
-
- 65% 14% 1%
- Residues (Left): HIS, SER, GLY, ARG, PRO, VAL, LEU, GLY, SER, SER, M1, L2, Q7, S40, C18, I19, L22, Q38, D41, V45, A46, A47, V48, R49, Y50, L51, L52, R53, D54, R64, I67, S76, R77, V78, L79, R80, R81, S87, L90, R91, R92, D93, D97, T102, S103.
- Residues (Right): K108, T109, L116, E124, S125, M126, M131, R134, V137, M140, R149, K164, E165, G166, V167, A185, VAL, SER, ASP, ARG, SER, THR, LYS, SER, GLU, VAL, LYS, ALA, GLU, VAL, LYS, ALA, GLU, ALA, LYS, ARG, ASP, ASP, GLU, PRO, LEU, SER, ARG, LYS, THR, LYS, ALA, ASP.

- Chain D:

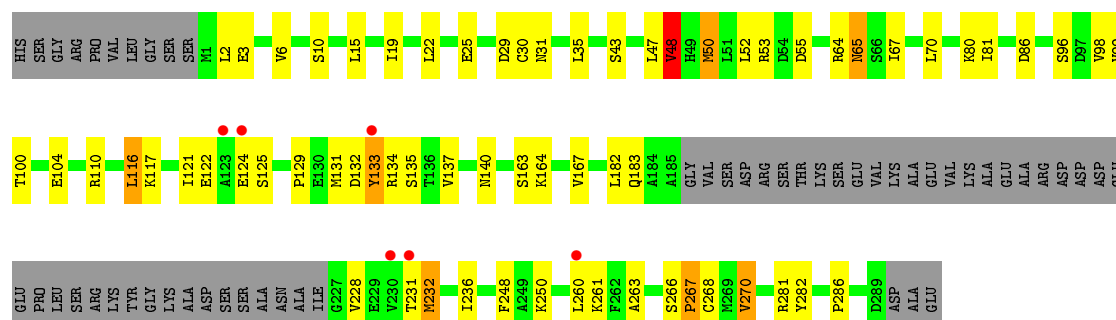
- Chain E: 



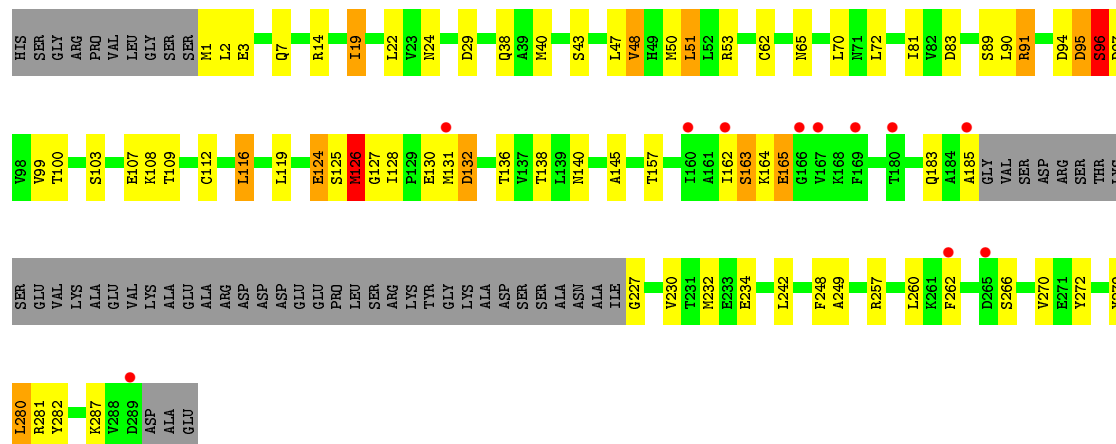
• Molecule 1: Proliferating cell nuclear antigen



• Molecule 1: Proliferating cell nuclear antigen



• Molecule 1: Proliferating cell nuclear antigen



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.46Å 150.91Å 170.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.02 – 3.10 75.45 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (113.02-3.10) 99.5 (75.45-3.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0135, REFMAC	Depositor
R, R_{free}	0.174 , 0.223 0.180 , 0.226	Depositor DCC
R_{free} test set	1575 reflections (2.47%)	wwPDB-VP
Wilson B-factor (Å ²)	91.5	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11713	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.86	0/1947	1.05	3/2627 (0.1%)
1	B	0.75	0/1947	0.95	1/2627 (0.0%)
1	C	0.74	0/1947	0.97	2/2627 (0.1%)
1	D	0.84	0/1969	1.06	3/2657 (0.1%)
1	E	0.87	0/1995	1.06	6/2693 (0.2%)
1	F	0.78	0/1947	1.11	8/2627 (0.3%)
All	All	0.81	0/11752	1.03	23/15858 (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	1
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	2
All	All	0	8

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	96	SER	N-CA-C	18.46	160.84	111.00
1	F	96	SER	N-CA-CB	-15.61	87.09	110.50
1	D	48	VAL	CB-CA-C	-7.88	96.43	111.40
1	B	48	VAL	CB-CA-C	-7.79	96.60	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	48	VAL	CB-CA-C	-7.03	98.05	111.40
1	A	48	VAL	CB-CA-C	-6.81	98.46	111.40
1	E	-5	PRO	N-CA-CB	6.80	111.47	103.30
1	A	53	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	E	126	MET	CG-SD-CE	6.39	110.43	100.20
1	D	64	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	E	91	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	F	126	MET	CG-SD-CE	5.75	109.40	100.20
1	F	51	LEU	CA-CB-CG	5.57	128.12	115.30
1	E	14	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	F	53	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	F	97	ASP	CB-CG-OD1	5.31	123.08	118.30
1	F	83	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	48	VAL	CB-CA-C	-5.21	101.50	111.40
1	C	53	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	50	MET	CB-CG-SD	-5.10	97.09	112.40
1	F	14	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	D	54	ASP	CB-CG-OD1	5.05	122.85	118.30
1	E	47	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	93	ASP	Peptide
1	B	105	ASN	Peptide
1	C	125	SER	Peptide
1	D	1	MET	Peptide
1	D	119	LEU	Peptide
1	E	95	ASP	Peptide
1	F	227	GLY	Peptide
1	F	230	VAL	Peptide

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	1919	0	1914	12	0
1	B	1919	0	1914	18	0
1	C	1919	0	1914	19	0
1	D	1941	0	1929	24	0
1	E	1967	0	1935	22	0
1	F	1919	0	1914	29	0
2	A	7	0	10	0	0
3	E	6	0	8	0	0
4	A	28	0	0	0	0
4	B	11	0	0	0	0
4	C	9	0	0	0	0
4	D	32	0	0	0	0
4	E	21	0	0	0	0
4	F	15	0	0	0	0
All	All	11713	0	11538	123	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 (123) 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:B:124:GLU:HB2	1:B:126:MET:SD	2.39	0.63
1:E:0:SER:CB	1:E:91:ARG:HH12	2.11	0.63
1:E:22:LEU:HD12	1:E:48:VAL:HG22	1.80	0.62
1:E:269:MET:HE1	1:E:281:ARG:HD2	1.80	0.62
1:F:70:LEU:HD21	1:F:99:VAL:HG11	1.82	0.61
1:A:126:MET:HA	1:A:126:MET:HE3	1.83	0.60
1:D:48:VAL:HG13	1:D:282:TYR:CD1	2.35	0.60
1:C:70:LEU:HD21	1:C:99:VAL:HG11	1.84	0.59
1:B:22:LEU:HD23	1:B:48:VAL:HG22	1.84	0.59
1:D:269:MET:HE3	1:D:271:GLU:HB2	1.85	0.58
1:F:19:ILE:HD11	1:F:72:LEU:HD11	1.85	0.58
1:D:48:VAL:HG13	1:D:282:TYR:CE1	2.39	0.58
1:D:56:CYS:HB2	1:D:277:VAL:HG13	1.86	0.58
1:F:2:LEU:HD23	1:F:3:GLU:N	2.18	0.58
1:B:48:VAL:HG13	1:B:282:TYR:CE1	2.41	0.56
1:F:116:LEU:HD23	1:F:116:LEU:N	2.20	0.56
1:F:280:LEU:HD21	1:F:282:TYR:CE2	2.41	0.56
1:C:263:ALA:HB3	1:C:266:SER:HB3	1.87	0.55
1:A:1:MET:HB3	1:A:93:ASP:HA	1.90	0.54
1:B:165:GLU:OE1	1:B:165:GLU:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:ARG:HD2	1:E:253:THR:HB	1.89	0.54
1:E:139:LEU:HD23	1:E:139:LEU:N	2.24	0.53
1:D:39:ALA:O	1:D:47:LEU:HD22	2.08	0.53
1:C:116:LEU:HD12	1:C:116:LEU:N	2.24	0.52
1:D:35:LEU:O	1:D:51:LEU:HD12	2.08	0.52
1:C:2:LEU:HD23	1:C:3:GLU:N	2.24	0.52
1:C:248:PHE:CD1	1:C:282:TYR:CG	2.98	0.52
1:A:22:LEU:HD12	1:A:48:VAL:CG2	2.40	0.52
1:B:43:SER:OG	1:B:45:VAL:HG23	2.10	0.51
1:A:22:LEU:HD12	1:A:48:VAL:HG22	1.93	0.51
1:C:133:TYR:HB3	1:C:261:LYS:HB3	1.91	0.51
1:D:49:HIS:HB2	1:D:128:ILE:HD11	1.94	0.50
1:E:-2:GLY:O	1:E:-1:SER:CB	2.59	0.50
1:D:72:LEU:O	1:D:76:SER:HB2	2.12	0.49
1:F:183:GLN:HG2	1:F:185:ALA:HB2	1.95	0.49
1:C:96:SER:O	1:C:98:VAL:N	2.43	0.49
1:F:162:ILE:HD11	1:F:262:PHE:CE2	2.47	0.49
1:C:86:ASP:OD2	1:C:110:ARG:NH2	2.46	0.48
1:B:31:ASN:HB3	1:B:32:PRO:HD2	1.95	0.48
1:E:-9:HIS:O	1:E:-7:GLY:N	2.46	0.48
1:E:68:LEU:HD13	1:E:99:VAL:HG23	1.95	0.48
1:B:43:SER:OG	1:B:45:VAL:CG2	2.62	0.48
1:D:275:ASP:OD1	1:D:276:ASN:N	2.46	0.48
1:D:92:HIS:HD2	1:D:98:VAL:O	1.96	0.48
1:F:138:THR:HG22	1:F:257:ARG:HH21	1.79	0.48
1:B:40:MET:SD	1:B:44:HIS:HA	2.54	0.47
1:C:163:SER:HA	1:C:232:MET:HE3	1.96	0.47
1:D:125:SER:O	1:D:126:MET:C	2.51	0.47
1:F:248:PHE:CD1	1:F:282:TYR:CG	3.02	0.47
1:A:46:ALA:HA	1:A:283:TYR:O	2.15	0.47
1:C:31:ASN:OD1	1:C:65:ASN:ND2	2.48	0.47
1:D:105:ASN:HB2	1:D:106:PRO:HD2	1.96	0.47
1:B:4:ALA:HB1	1:B:57:PHE:CE2	2.50	0.47
1:D:130:GLU:OE1	1:D:130:GLU:N	2.46	0.47
1:B:148:VAL:HG21	1:B:246:GLY:HA2	1.97	0.47
1:A:78:VAL:O	1:A:81:ILE:HG12	2.14	0.46
1:F:145:ALA:HB2	1:F:249:ALA:HB1	1.96	0.46
1:F:249:ALA:HA	1:F:272:TYR:OH	2.16	0.46
1:F:95:ASP:CG	1:F:96:SER:H	2.18	0.46
1:E:19:ILE:CD1	1:E:37:VAL:HG11	2.46	0.46
1:C:132:ASP:CG	1:C:133:TYR:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:SER:OG	1:F:165:GLU:OE1	2.34	0.46
1:D:131:MET:HG2	1:D:133:TYR:CE1	2.51	0.45
1:F:125:SER:O	1:F:127:GLY:N	2.49	0.45
1:F:100:THR:O	1:F:100:THR:HG22	2.17	0.45
1:F:280:LEU:HD21	1:F:282:TYR:CZ	2.51	0.45
1:D:105:ASN:HB2	1:D:106:PRO:CD	2.46	0.45
1:E:134:ARG:HA	1:E:134:ARG:HE	1.81	0.45
1:B:279:TYR:CZ	1:B:281:ARG:NH2	2.85	0.45
1:E:2:LEU:HD12	1:E:3:GLU:N	2.33	0.44
1:E:182:LEU:HB3	1:E:228:VAL:HG21	1.99	0.44
1:F:116:LEU:N	1:F:116:LEU:CD2	2.80	0.44
1:D:46:ALA:HA	1:D:283:TYR:O	2.18	0.44
1:C:267:PRO:HA	1:C:286:PRO:HD3	2.00	0.43
1:F:99:VAL:HG22	1:F:100:THR:N	2.33	0.43
1:F:90:LEU:HD23	1:F:91:ARG:N	2.33	0.43
1:E:180:THR:HG23	1:F:112:CYS:SG	2.58	0.43
1:C:96:SER:C	1:C:98:VAL:H	2.21	0.43
1:D:56:CYS:HB2	1:D:277:VAL:CG1	2.47	0.43
1:A:87:SER:O	1:A:103:SER:HA	2.18	0.42
1:D:249:ALA:HA	1:D:272:TYR:OH	2.19	0.42
1:D:22:LEU:HD23	1:D:48:VAL:HG22	2.00	0.42
1:E:94:ASP:OD1	1:E:95:ASP:N	2.52	0.42
1:B:248:PHE:CD1	1:B:282:TYR:CG	3.06	0.42
1:C:15:LEU:HD13	1:C:50:MET:HE3	2.00	0.42
1:B:182:LEU:HB3	1:B:228:VAL:HG21	2.00	0.42
1:B:244:PHE:HA	1:B:247:ILE:HD12	2.02	0.42
1:B:270:VAL:HG22	1:B:282:TYR:HB2	2.01	0.42
1:C:48:VAL:HG13	1:C:282:TYR:CE1	2.54	0.42
1:D:153:VAL:HG22	1:D:154:PHE:CD2	2.55	0.42
1:F:163:SER:O	1:F:164:LYS:C	2.58	0.42
1:B:56:CYS:HB2	1:B:277:VAL:CG2	2.50	0.42
1:C:182:LEU:HB3	1:C:228:VAL:HG21	2.02	0.41
1:C:260:LEU:HD23	1:C:270:VAL:HB	2.02	0.41
1:F:38:GLN:HA	1:F:48:VAL:O	2.20	0.41
1:D:122:GLU:OE1	1:D:122:GLU:N	2.52	0.41
1:E:144:PHE:O	1:E:148:VAL:HG13	2.20	0.41
1:F:242:LEU:HA	1:F:242:LEU:HD23	1.95	0.41
1:B:124:GLU:CB	1:B:126:MET:SD	3.07	0.41
1:E:260:LEU:N	1:E:260:LEU:HD23	2.36	0.41
1:E:75:LEU:HA	1:E:116:LEU:HD21	2.01	0.41
1:D:103:SER:HB3	1:D:112:CYS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:LEU:HD23	1:E:70:LEU:HA	1.91	0.41
1:F:2:LEU:HD23	1:F:3:GLU:H	1.84	0.41
1:A:1:MET:HB2	1:A:2:LEU:H	1.70	0.41
1:E:15:LEU:HD22	1:E:50:MET:CE	2.51	0.41
1:D:74:SER:O	1:D:75:LEU:C	2.59	0.41
1:F:260:LEU:HD23	1:F:270:VAL:HB	2.01	0.41
1:A:288:VAL:O	1:A:289:ASP:HB2	2.20	0.41
1:B:227:GLY:O	1:B:257:ARG:NH2	2.54	0.41
1:D:150:ASP:O	1:D:153:VAL:HG13	2.21	0.41
1:F:131:MET:O	1:F:132:ASP:CB	2.68	0.41
1:A:18:CYS:HB3	1:A:282:TYR:OH	2.21	0.41
1:C:30:CYS:SG	1:C:35:LEU:HD22	2.61	0.41
1:E:69:GLY:HA3	1:E:119:LEU:O	2.21	0.41
1:A:230:VAL:HG12	1:A:231:THR:N	2.35	0.40
1:C:50:MET:HE1	1:C:52:LEU:HG	2.04	0.40
1:E:22:LEU:HD12	1:E:48:VAL:CG2	2.51	0.40
1:F:131:MET:O	1:F:132:ASP:HB3	2.21	0.40
1:F:279:TYR:CZ	1:F:281:ARG:NH2	2.89	0.40
1:E:53:ARG:HB3	1:E:55:ASP:OD1	2.22	0.40
1:F:124:GLU:OE2	1:F:127:GLY:HA2	2.21	0.40
1:A:19:ILE:HD13	1:A:19:ILE:HG21	1.85	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	244/302 (81%)	224 (92%)	20 (8%)	0	100	100
1	B	244/302 (81%)	216 (88%)	25 (10%)	3 (1%)	13	44
1	C	244/302 (81%)	206 (84%)	35 (14%)	3 (1%)	13	44
1	D	247/302 (82%)	218 (88%)	27 (11%)	2 (1%)	19	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	254/302 (84%)	223 (88%)	26 (10%)	5 (2%)	7	31
1	F	244/302 (81%)	207 (85%)	31 (13%)	6 (2%)	5	27
All	All	1477/1812 (82%)	1294 (88%)	164 (11%)	19 (1%)	12	42

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	277	VAL
1	E	-8	SER
1	F	96	SER
1	F	128	ILE
1	E	-7	GLY
1	B	126	MET
1	C	133	TYR
1	D	265	ASP
1	E	-2	GLY
1	F	95	ASP
1	F	126	MET
1	F	132	ASP
1	E	131	MET
1	B	235	PRO
1	F	130	GLU
1	E	-1	SER
1	C	129	PRO
1	C	267	PRO
1	B	105	ASN

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	216/259 (83%)	178 (82%)	38 (18%)	2	8
1	B	216/259 (83%)	183 (85%)	33 (15%)	2	12
1	C	216/259 (83%)	178 (82%)	38 (18%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	218/259 (84%)	181 (83%)	37 (17%)	2	9
1	E	216/259 (83%)	180 (83%)	36 (17%)	2	9
1	F	216/259 (83%)	179 (83%)	37 (17%)	2	9
All	All	1298/1554 (84%)	1079 (83%)	219 (17%)	2	9

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LEU
1	A	7	GLN
1	A	10	SER
1	A	19	ILE
1	A	22	LEU
1	A	38	GLN
1	A	41	ASP
1	A	45	VAL
1	A	50	MET
1	A	51	LEU
1	A	54	ASP
1	A	64	ARG
1	A	67	ILE
1	A	76	SER
1	A	80	LYS
1	A	81	ILE
1	A	90	LEU
1	A	91	ARG
1	A	97	ASP
1	A	102	THR
1	A	103	SER
1	A	108	LYS
1	A	109	THR
1	A	116	LEU
1	A	124	GLU
1	A	125	SER
1	A	126	MET
1	A	131	MET
1	A	134	ARG
1	A	137	VAL
1	A	140	ASN
1	A	149	ARG

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Mol	Chain	Res	Type
1	A	164	LYS
1	A	165	GLU
1	A	167	VAL
1	A	264	LYS
1	A	270	VAL
1	D	1	MET
1	D	10	SER
1	D	19	ILE
1	D	25	GLU
1	D	30	CYS
1	D	40	MET
1	D	41	ASP
1	D	45	VAL
1	D	48	VAL
1	D	53	ARG
1	D	56	CYS
1	D	59	LYS
1	D	61	GLN
1	D	64	ARG
1	D	68	LEU
1	D	76	SER
1	D	80	LYS
1	D	94	ASP
1	D	97	ASP
1	D	105	ASN
1	D	108	LYS
1	D	111	LYS
1	D	116	LEU
1	D	132	ASP
1	D	134	ARG
1	D	136	THR
1	D	137	VAL
1	D	148	VAL
1	D	153	VAL
1	D	164	LYS
1	D	171	SER
1	D	183	GLN
1	D	232	MET
1	D	250	LYS
1	D	256	GLU
1	D	270	VAL
1	D	277	VAL

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Mol	Chain	Res	Type
1	E	10	SER
1	E	19	ILE
1	E	22	LEU
1	E	29	ASP
1	E	36	SER
1	E	38	GLN
1	E	40	MET
1	E	41	ASP
1	E	45	VAL
1	E	50	MET
1	E	51	LEU
1	E	64	ARG
1	E	84	SER
1	E	91	ARG
1	E	97	ASP
1	E	99	VAL
1	E	100	THR
1	E	108	LYS
1	E	124	GLU
1	E	125	SER
1	E	130	GLU
1	E	134	ARG
1	E	137	VAL
1	E	139	LEU
1	E	140	ASN
1	E	146	LYS
1	E	152	GLN
1	E	170	SER
1	E	172	SER
1	E	232	MET
1	E	260	LEU
1	E	268	CYS
1	E	270	VAL
1	E	277	VAL
1	E	287	LYS
1	E	288	VAL
1	B	1	MET
1	B	2	LEU
1	B	7	GLN
1	B	19	ILE
1	B	30	CYS
1	B	45	VAL

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Mol	Chain	Res	Type
1	B	48	VAL
1	B	50	MET
1	B	59	LYS
1	B	64	ARG
1	B	66	SER
1	B	81	ILE
1	B	89	SER
1	B	99	VAL
1	B	100	THR
1	B	102	THR
1	B	117	LYS
1	B	119	LEU
1	B	124	GLU
1	B	126	MET
1	B	131	MET
1	B	135	SER
1	B	136	THR
1	B	146	LYS
1	B	162	ILE
1	B	163	SER
1	B	164	LYS
1	B	231	THR
1	B	234	GLU
1	B	237	THR
1	B	250	LYS
1	B	264	LYS
1	B	270	VAL
1	C	6	VAL
1	C	10	SER
1	C	19	ILE
1	C	22	LEU
1	C	25	GLU
1	C	29	ASP
1	C	43	SER
1	C	47	LEU
1	C	48	VAL
1	C	50	MET
1	C	55	ASP
1	C	64	ARG
1	C	65	ASN
1	C	67	ILE
1	C	80	LYS

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Mol	Chain	Res	Type
1	C	81	ILE
1	C	100	THR
1	C	104	GLU
1	C	116	LEU
1	C	117	LYS
1	C	121	ILE
1	C	122	GLU
1	C	124	GLU
1	C	131	MET
1	C	134	ARG
1	C	135	SER
1	C	137	VAL
1	C	140	ASN
1	C	164	LYS
1	C	167	VAL
1	C	183	GLN
1	C	231	THR
1	C	232	MET
1	C	236	ILE
1	C	250	LYS
1	C	268	CYS
1	C	270	VAL
1	C	281	ARG
1	F	1	MET
1	F	7	GLN
1	F	19	ILE
1	F	22	LEU
1	F	24	ASN
1	F	29	ASP
1	F	40	MET
1	F	43	SER
1	F	47	LEU
1	F	48	VAL
1	F	50	MET
1	F	51	LEU
1	F	62	CYS
1	F	65	ASN
1	F	81	ILE
1	F	89	SER
1	F	91	ARG
1	F	94	ASP
1	F	96	SER

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Mol	Chain	Res	Type
1	F	103	SER
1	F	107	GLU
1	F	108	LYS
1	F	109	THR
1	F	116	LEU
1	F	119	LEU
1	F	124	GLU
1	F	126	MET
1	F	136	THR
1	F	140	ASN
1	F	157	THR
1	F	163	SER
1	F	165	GLU
1	F	232	MET
1	F	234	GLU
1	F	266	SER
1	F	280	LEU
1	F	287	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	38	GLN
1	A	177	GLN
1	A	183	GLN
1	D	5	GLN
1	D	44	HIS
1	D	92	HIS
1	D	105	ASN
1	D	140	ASN
1	E	7	GLN
1	E	49	HIS
1	B	61	GLN
1	B	105	ASN
1	B	115	GLN
1	C	20	ASN
1	C	44	HIS
1	C	115	GLN
1	F	31	ASN
1	F	44	HIS
1	F	49	HIS

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Mol	Chain	Res	Type
1	F	61	GLN
1	F	115	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	GOL	E	301	-	5,5,5	0.95	0	5,5,5	1.39	1 (20%)
2	PEG	A	301	-	6,6,6	0.67	0	5,5,5	0.58	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
3	GOL	E	301	-	-	1/4/4/4	-
2	PEG	A	301	-	-	1/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	E	301	GOL	O1-C1-C2	2.56	122.48	110.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	301	GOL	C1-C2-C3-O3
2	A	301	PEG	C4-C3-O2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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	248/302 (82%)	0.10	4 (1%) 72 51	50, 82, 140, 188	0
1	B	248/302 (82%)	0.08	4 (1%) 72 51	63, 98, 145, 171	0
1	C	248/302 (82%)	0.21	6 (2%) 59 37	67, 99, 158, 187	0
1	D	251/302 (83%)	0.03	4 (1%) 72 51	54, 91, 141, 177	0
1	E	258/302 (85%)	0.14	4 (1%) 72 51	58, 87, 145, 167	0
1	F	248/302 (82%)	0.22	11 (4%) 34 17	69, 105, 164, 188	0
All	All	1501/1812 (82%)	0.13	33 (2%) 62 41	50, 95, 151, 188	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	ASP	6.9
1	D	185	ALA	5.4
1	A	185	ALA	5.1
1	D	128	ILE	3.9
1	F	265	ASP	3.7
1	C	124	GLU	3.7
1	B	129	PRO	3.6
1	F	289	ASP	3.5
1	E	289	ASP	3.1
1	D	127	GLY	2.9
1	E	288	VAL	2.8
1	F	262	PHE	2.7
1	C	123	ALA	2.7
1	D	129	PRO	2.6
1	C	260	LEU	2.6
1	E	132	ASP	2.6
1	B	128	ILE	2.4
1	A	231	THR	2.4
1	F	166	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	230	VAL	2.3
1	F	169	PHE	2.3
1	F	185	ALA	2.2
1	F	162	ILE	2.2
1	F	180	THR	2.2
1	B	185	ALA	2.1
1	F	160	ILE	2.1
1	C	231	THR	2.1
1	F	167	VAL	2.1
1	E	231	THR	2.1
1	C	133	TYR	2.1
1	F	131	MET	2.1
1	B	262	PHE	2.0
1	A	232	MET	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, 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(\AA^2)	Q<0.9
3	GOL	E	301	6/6	0.80	0.36	91,115,120,122	0
2	PEG	A	301	7/7	0.86	0.31	105,118,135,137	0

6.5 Other polymers [i](#)

There are no such residues in this entry.