



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2024 – 12:06 PM EDT

PDB ID : 9DRD
Title : Crystal structure of ADP-ribose diphosphatase from *Klebsiella pneumoniae* (Apo, monoclinic P form 2)
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2024-09-25
Resolution : 1.65 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

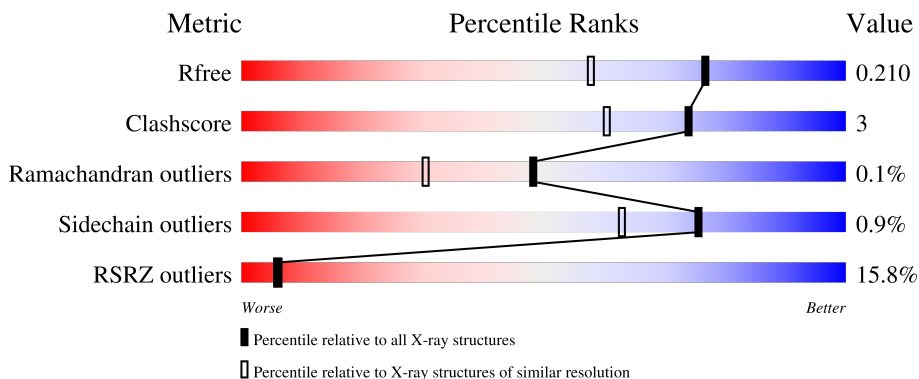
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2328 (1.66-1.66)
Clashscore	180529	2515 (1.66-1.66)
Ramachandran outliers	177936	2475 (1.66-1.66)
Sidechain outliers	177891	2475 (1.66-1.66)
RSRZ outliers	164620	2328 (1.66-1.66)

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 $\leq 5\%$. 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	218	
1	B	218	
1	C	218	
1	D	218	
1	E	218	

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Mol	Chain	Length	Quality of chain
1	F	218	
1	G	218	
1	H	218	

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	C	301	-	-	X	-

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 13511 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 ADP-ribose pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	199	Total 1599	C 1009	N 285	O 301	S 4	0	2	0
1	B	204	Total 1624	C 1028	N 284	O 309	S 3	0	4	0
1	C	196	Total 1544	C 976	N 268	O 297	S 3	0	1	0
1	D	206	Total 1621	C 1023	N 283	O 312	S 3	0	1	0
1	E	194	Total 1551	C 983	N 273	O 292	S 3	0	3	0
1	F	198	Total 1571	C 994	N 277	O 297	S 3	0	1	0
1	G	196	Total 1540	C 976	N 265	O 296	S 3	0	1	0
1	H	198	Total 1580	C 999	N 277	O 301	S 3	0	2	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP A0A0H3GVQ7
A	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
A	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
A	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
A	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
A	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
A	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
A	0	HIS	-	expression tag	UNP A0A0H3GVQ7
B	-7	MET	-	expression tag	UNP A0A0H3GVQ7
B	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
B	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
B	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
B	-3	HIS	-	expression tag	UNP A0A0H3GVQ7

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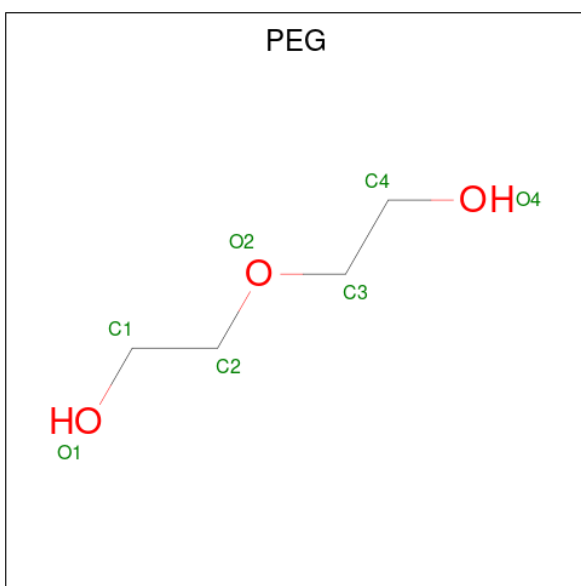
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
B	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
B	0	HIS	-	expression tag	UNP A0A0H3GVQ7
C	-7	MET	-	expression tag	UNP A0A0H3GVQ7
C	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
C	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
C	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
C	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
C	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
C	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
C	0	HIS	-	expression tag	UNP A0A0H3GVQ7
D	-7	MET	-	expression tag	UNP A0A0H3GVQ7
D	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
D	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
D	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
D	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
D	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
D	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
D	0	HIS	-	expression tag	UNP A0A0H3GVQ7
E	-7	MET	-	expression tag	UNP A0A0H3GVQ7
E	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
E	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
E	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
E	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
E	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
E	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
E	0	HIS	-	expression tag	UNP A0A0H3GVQ7
F	-7	MET	-	expression tag	UNP A0A0H3GVQ7
F	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
F	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
F	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
F	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
F	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
F	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
F	0	HIS	-	expression tag	UNP A0A0H3GVQ7
G	-7	MET	-	expression tag	UNP A0A0H3GVQ7
G	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
G	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
G	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
G	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
G	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
G	-1	HIS	-	expression tag	UNP A0A0H3GVQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP A0A0H3GVQ7
H	-7	MET	-	expression tag	UNP A0A0H3GVQ7
H	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
H	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
H	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
H	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
H	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
H	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
H	0	HIS	-	expression tag	UNP A0A0H3GVQ7

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 7 4 3	0	0
2	C	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	F	1	Total C O 7 4 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	117	Total O 117 117	0	0

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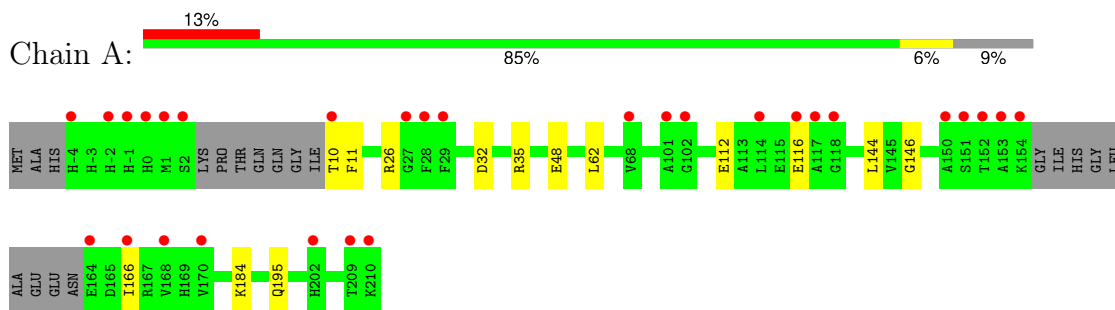
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	138	Total 138	O 138	0	0
3	C	100	Total 100	O 100	0	0
3	D	121	Total 121	O 121	0	0
3	E	93	Total 93	O 93	0	0
3	F	110	Total 110	O 110	0	0
3	G	77	Total 77	O 77	0	0
3	H	97	Total 97	O 97	0	0

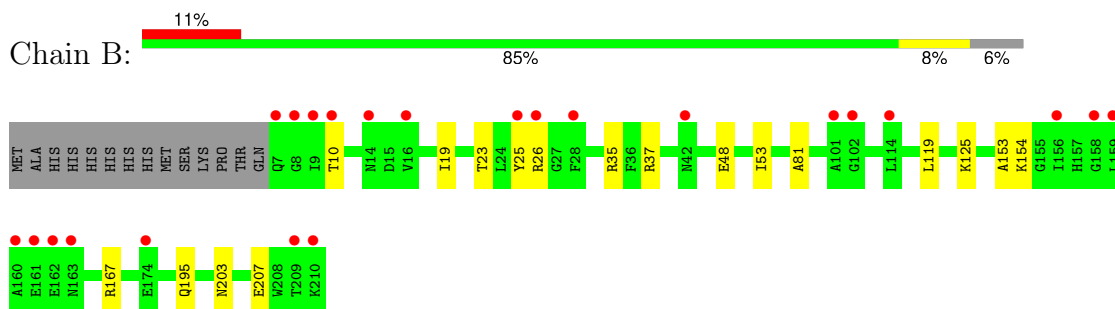
3 Residue-property plots [i](#)

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.

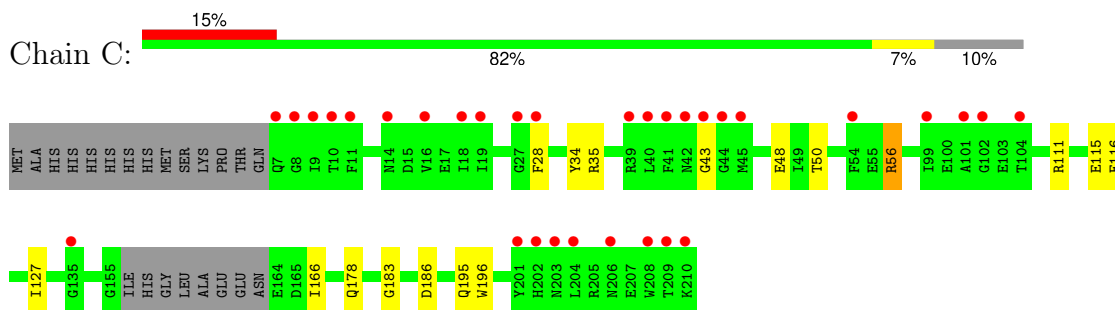
- Molecule 1: ADP-ribose pyrophosphatase



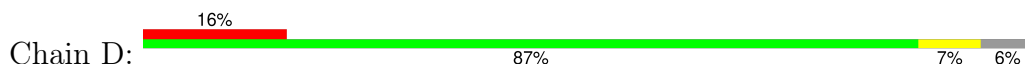
- Molecule 1: ADP-ribose pyrophosphatase

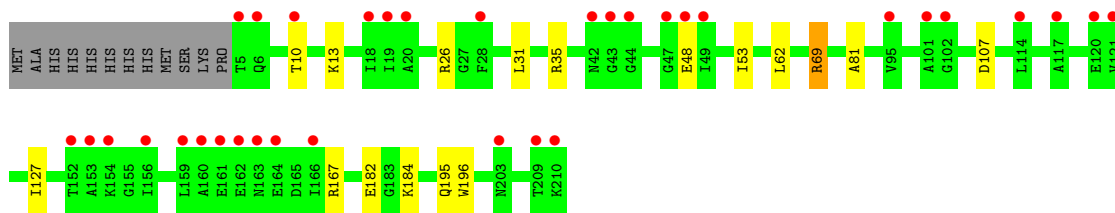


- Molecule 1: ADP-ribose pyrophosphatase

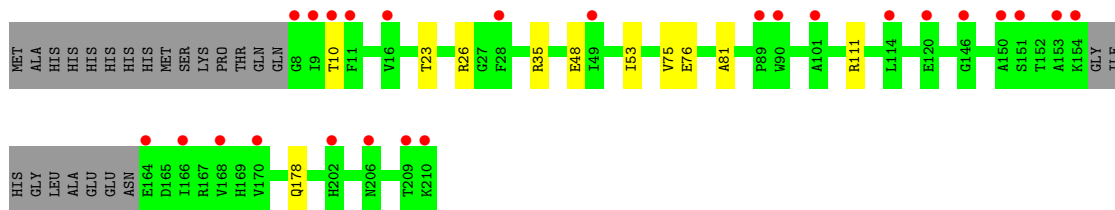
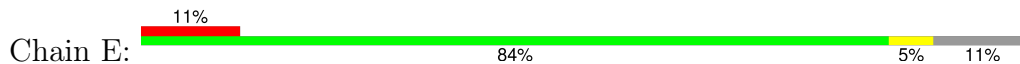


- Molecule 1: ADP-ribose pyrophosphatase

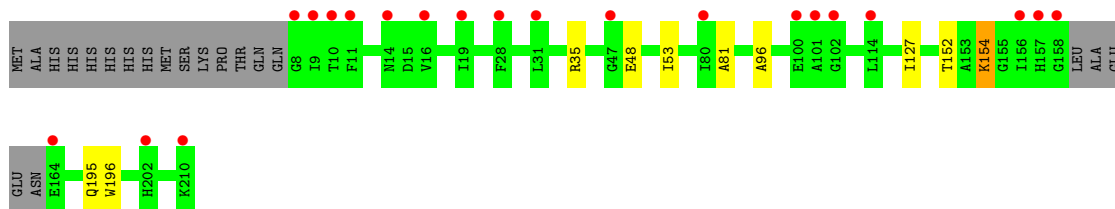
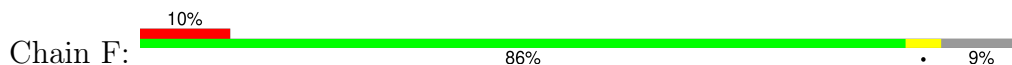




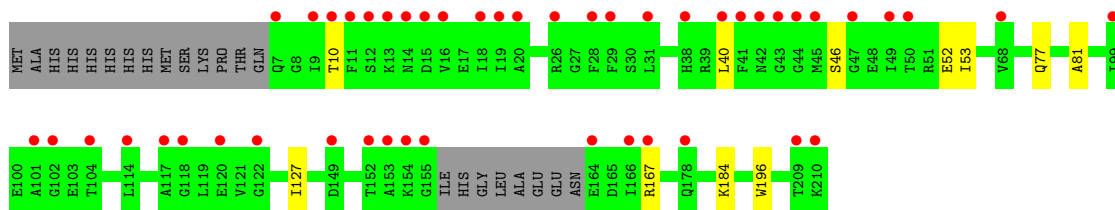
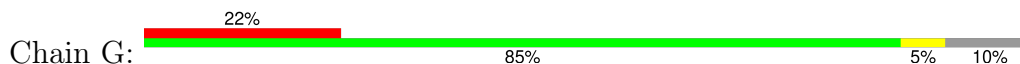
- Molecule 1: ADP-ribose pyrophosphatase



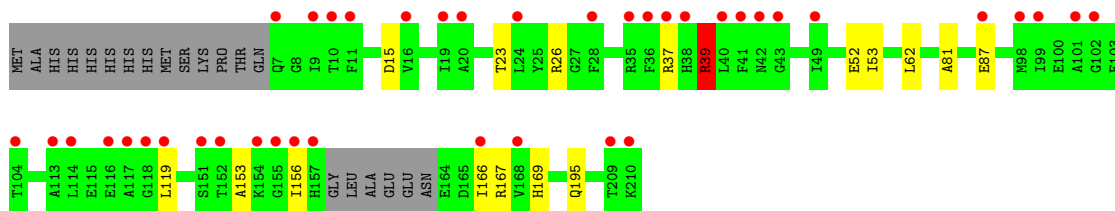
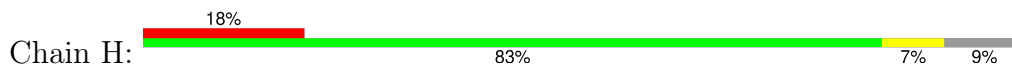
- Molecule 1: ADP-ribose pyrophosphatase



- Molecule 1: ADP-ribose pyrophosphatase



- Molecule 1: ADP-ribose pyrophosphatase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.74Å 79.72Å 115.71Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	49.22 – 1.65 49.22 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.22-1.65) 99.8 (49.22-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.65Å)	Xtrriage
Refinement program	PHENIX (dev_5267: ???)	Depositor
R, R_{free}	0.174 , 0.203 0.183 , 0.210	Depositor DCC
R_{free} test set	10347 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtrriage
Anisotropy	0.599	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13511	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.45 % 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 3.6479e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.41	0/1638	0.66	0/2217
1	B	0.42	0/1667	0.67	0/2259
1	C	0.37	0/1576	0.62	0/2135
1	D	0.40	0/1655	0.66	0/2245
1	E	0.38	0/1589	0.65	0/2152
1	F	0.39	0/1604	0.66	0/2171
1	G	0.36	0/1572	0.62	0/2131
1	H	0.38	0/1616	0.64	0/2188
All	All	0.39	0/12917	0.65	0/17498

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	D	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	69	ARG	Sidechain
1	H	39	ARG	Sidechain

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	1599	0	1545	9	0
1	B	1624	0	1590	14	0
1	C	1544	0	1486	11	0
1	D	1621	0	1567	20	0
1	E	1551	0	1519	13	0
1	F	1571	0	1537	7	0
1	G	1540	0	1487	9	0
1	H	1580	0	1536	9	0
2	C	14	0	20	4	0
2	D	7	0	10	0	0
2	F	7	0	10	0	0
3	A	117	0	0	0	0
3	B	138	0	0	2	0
3	C	100	0	0	5	0
3	D	121	0	0	4	0
3	E	93	0	0	3	0
3	F	110	0	0	1	0
3	G	77	0	0	2	0
3	H	97	0	0	0	0
All	All	13511	0	12307	74	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 3.

All (74) 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:F:81:ALA:HB2	1:H:53:ILE:HD12	1.62	0.82
1:D:69:ARG:NH2	1:E:26:ARG:HH22	1.78	0.80
1:E:178:GLN:NE2	3:E:301:HOH:O	2.20	0.73
1:B:81:ALA:HB2	1:D:53:ILE:HD12	1.72	0.70
1:D:69:ARG:NH2	1:E:26:ARG:NH2	2.38	0.70
1:B:53:ILE:HD12	1:D:81:ALA:HB2	1.74	0.68
1:B:35:ARG:NH1	1:B:48:GLU:OE2	2.21	0.67
1:B:195[B]:GLN:OE1	1:D:195[B]:GLN:OE1	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:LEU:HD21	1:G:46:SER:HB3	1.80	0.62
1:E:81:ALA:HB2	1:G:53:ILE:HD12	1.82	0.62
1:A:116:GLU:HG3	1:A:166:ILE:HD13	1.82	0.61
1:F:53:ILE:HD12	1:H:81:ALA:HB2	1.83	0.61
1:H:119:LEU:HD21	1:H:153:ALA:HB2	1.81	0.60
1:D:35:ARG:NH1	3:D:405:HOH:O	2.33	0.60
1:A:10:THR:HG22	1:A:11:PHE:N	2.15	0.60
1:G:52:GLU:O	1:G:53:ILE:HD13	2.01	0.60
1:F:35:ARG:NH1	1:F:48:GLU:OE2	2.30	0.57
1:D:182:GLU:OE1	1:D:184:LYS:HE2	2.05	0.57
1:D:69:ARG:NH1	3:D:406:HOH:O	2.38	0.56
1:C:116:GLU:HG2	1:C:166:ILE:HD13	1.89	0.55
1:B:203:ASN:ND2	3:B:305:HOH:O	2.37	0.54
1:E:23:THR:HG23	1:E:26:ARG:NH1	2.22	0.54
1:B:25:TYR:CD1	1:D:31:LEU:HD22	2.43	0.54
1:E:111:ARG:NH2	3:E:302:HOH:O	2.41	0.53
1:E:10:THR:CB	1:G:167:ARG:HH22	2.22	0.52
3:B:324:HOH:O	1:D:13:LYS:HE3	2.09	0.52
1:B:119:LEU:HD21	1:B:153:ALA:HB2	1.91	0.51
1:B:23:THR:HG23	1:B:26:ARG:NH1	2.26	0.50
1:C:186:ASP:OD2	2:C:301:PEG:H32	2.09	0.50
2:C:301:PEG:H11	3:C:470:HOH:O	2.11	0.50
1:C:178:GLN:HG3	3:C:493:HOH:O	2.11	0.50
1:B:167:ARG:CZ	1:D:10:THR:OG1	2.60	0.50
1:G:184:LYS:HG3	3:G:335:HOH:O	2.11	0.50
1:E:53:ILE:HD12	1:G:81:ALA:HB2	1.93	0.49
2:C:301:PEG:C1	3:C:470:HOH:O	2.59	0.49
1:B:19:ILE:HD11	1:B:37:ARG:HG3	1.94	0.49
1:C:56:ARG:HD2	3:C:467:HOH:O	2.13	0.49
1:D:107:ASP:OD2	3:D:401:HOH:O	2.20	0.49
1:H:52:GLU:O	1:H:53:ILE:HD13	2.12	0.48
1:A:112:GLU:O	1:A:116:GLU:HB2	2.12	0.48
1:A:195[B]:GLN:OE1	1:C:195[B]:GLN:OE1	2.30	0.48
1:A:10:THR:HB	3:C:412:HOH:O	2.13	0.48
1:C:111:ARG:O	1:C:115:GLU:HG3	2.13	0.48
1:D:69:ARG:HH21	1:E:26:ARG:HH22	1.60	0.48
1:D:69:ARG:HH21	1:E:26:ARG:NH2	2.10	0.48
1:E:35:ARG:NH1	1:E:48:GLU:OE2	2.38	0.47
1:A:35:ARG:NH1	1:A:48:GLU:OE2	2.36	0.47
1:F:127:ILE:HG23	1:F:196:TRP:CG	2.50	0.47
1:H:167:ARG:HD2	1:H:169:HIS:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:GLY:O	2:C:301:PEG:C3	2.63	0.46
1:B:25:TYR:CE1	1:D:31:LEU:HD22	2.50	0.46
1:H:15:ASP:HB3	1:H:39:ARG:HG3	1.99	0.45
1:E:76:GLU:OE1	1:G:10:THR:HG23	2.17	0.45
1:F:96:ALA:O	3:F:401:HOH:O	2.21	0.44
1:F:195[B]:GLN:OE1	1:H:195[B]:GLN:OE1	2.35	0.43
1:C:127:ILE:HG23	1:C:196:TRP:CG	2.54	0.43
1:C:35:ARG:HD3	1:C:48:GLU:OE2	2.18	0.43
1:C:116:GLU:CG	1:C:166:ILE:HD13	2.48	0.42
1:A:26:ARG:NH1	1:A:32:ASP:OD1	2.50	0.42
1:D:195[A]:GLN:NE2	3:D:404:HOH:O	2.28	0.42
1:H:156:ILE:HA	1:H:166:ILE:O	2.20	0.42
1:B:25:TYR:CE1	1:D:31:LEU:CD2	3.03	0.42
1:D:35:ARG:HD3	1:D:48:GLU:OE2	2.20	0.42
1:F:152:THR:O	1:F:154:LYS:HE2	2.20	0.42
1:A:62:LEU:HD11	1:A:146:GLY:HA3	2.02	0.41
1:G:77:GLN:HG2	3:G:304:HOH:O	2.19	0.41
1:B:125:LYS:NZ	1:B:207:GLU:OE1	2.42	0.41
1:E:75:VAL:HG23	3:E:311:HOH:O	2.20	0.41
1:B:10:THR:OG1	1:D:167:ARG:NH1	2.55	0.40
1:G:127:ILE:HG23	1:G:196:TRP:CG	2.56	0.40
1:A:184:LYS:NZ	1:A:184:LYS:HB2	2.36	0.40
1:D:127:ILE:HG23	1:D:196:TRP:CG	2.56	0.40
1:H:23:THR:HG21	1:H:26:ARG:HB2	2.03	0.40
1:C:34:TYR:O	1:C:50:THR:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	195/218 (89%)	189 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	206/218 (94%)	199 (97%)	7 (3%)	0	100	100
1	C	193/218 (88%)	184 (95%)	8 (4%)	1 (0%)	25	11
1	D	205/218 (94%)	199 (97%)	6 (3%)	0	100	100
1	E	193/218 (88%)	186 (96%)	7 (4%)	0	100	100
1	F	195/218 (89%)	189 (97%)	6 (3%)	0	100	100
1	G	193/218 (88%)	185 (96%)	8 (4%)	0	100	100
1	H	196/218 (90%)	188 (96%)	8 (4%)	0	100	100
All	All	1576/1744 (90%)	1519 (96%)	56 (4%)	1 (0%)	48	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	43	GLY

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	167/183 (91%)	166 (99%)	1 (1%)	84	75
1	B	169/183 (92%)	168 (99%)	1 (1%)	84	75
1	C	158/183 (86%)	156 (99%)	2 (1%)	65	47
1	D	167/183 (91%)	165 (99%)	2 (1%)	67	50
1	E	161/183 (88%)	161 (100%)	0	100	100
1	F	163/183 (89%)	162 (99%)	1 (1%)	84	75
1	G	158/183 (86%)	158 (100%)	0	100	100
1	H	164/183 (90%)	160 (98%)	4 (2%)	44	21
All	All	1307/1464 (89%)	1296 (99%)	11 (1%)	75	68

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	LEU
1	B	154	LYS
1	C	28	PHE
1	C	56	ARG
1	D	26	ARG
1	D	62	LEU
1	F	154	LYS
1	H	37	ARG
1	H	39	ARG
1	H	62	LEU
1	H	87	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	202	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	C	301	-	6,6,6	0.23	0	5,5,5	0.37	0
2	PEG	D	301	-	6,6,6	0.23	0	5,5,5	0.50	0
2	PEG	F	301	-	6,6,6	0.26	0	5,5,5	0.16	0
2	PEG	C	302	-	6,6,6	0.25	0	5,5,5	0.22	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	C	301	-	-	2/4/4/4	-
2	PEG	D	301	-	-	0/4/4/4	-
2	PEG	F	301	-	-	2/4/4/4	-
2	PEG	C	302	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	302	PEG	O1-C1-C2-O2
2	C	302	PEG	O2-C3-C4-O4
2	F	301	PEG	O1-C1-C2-O2
2	C	302	PEG	C4-C3-O2-C2
2	C	301	PEG	C4-C3-O2-C2
2	F	301	PEG	C4-C3-O2-C2
2	C	301	PEG	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	PEG	4	0

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	199/218 (91%)	0.95	29 (14%) 7 7	13, 34, 57, 88	2 (1%)
1	B	204/218 (93%)	0.61	23 (11%) 11 12	11, 27, 53, 86	4 (1%)
1	C	196/218 (89%)	0.92	32 (16%) 5 5	13, 33, 66, 80	1 (0%)
1	D	206/218 (94%)	0.91	34 (16%) 5 5	12, 33, 59, 97	1 (0%)
1	E	194/218 (88%)	1.01	25 (12%) 9 9	14, 34, 58, 80	3 (1%)
1	F	198/218 (90%)	0.66	21 (10%) 13 14	12, 30, 47, 72	1 (0%)
1	G	196/218 (89%)	1.19	47 (23%) 2 2	14, 37, 68, 79	1 (0%)
1	H	198/218 (90%)	1.07	40 (20%) 3 4	12, 37, 63, 82	2 (1%)
All	All	1591/1744 (91%)	0.92	251 (15%) 6 6	11, 33, 62, 97	15 (0%)

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-4	HIS	6.6
1	E	154	LYS	6.6
1	C	7	GLN	5.8
1	E	10	THR	5.6
1	H	156	ILE	5.3
1	H	10	THR	5.2
1	D	5	THR	5.0
1	D	159	LEU	5.0
1	B	160	ALA	4.9
1	G	16	VAL	4.8
1	G	10	THR	4.7
1	C	19	ILE	4.6
1	G	101	ALA	4.6
1	G	43	GLY	4.6
1	B	159	LEU	4.5
1	H	155	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	16	VAL	4.5
1	A	0	HIS	4.4
1	H	157	HIS	4.4
1	E	150	ALA	4.2
1	B	7	GLN	4.1
1	H	43	GLY	4.1
1	G	42	ASN	4.1
1	A	10	THR	4.0
1	B	101	ALA	3.9
1	H	209	THR	3.9
1	G	155	GLY	3.9
1	B	8	GLY	3.8
1	G	14	ASN	3.8
1	H	119	LEU	3.8
1	F	210	LYS	3.8
1	F	10	THR	3.7
1	A	29	PHE	3.7
1	B	9	ILE	3.7
1	G	18	ILE	3.6
1	C	101	ALA	3.6
1	C	28	PHE	3.6
1	G	44	GLY	3.6
1	C	209	THR	3.6
1	E	151	SER	3.6
1	C	43	GLY	3.6
1	G	11	PHE	3.5
1	F	19	ILE	3.5
1	H	16	VAL	3.5
1	C	10	THR	3.5
1	G	19	ILE	3.5
1	G	40	LEU	3.5
1	D	28	PHE	3.4
1	H	41	PHE	3.4
1	E	153	ALA	3.4
1	A	154	LYS	3.4
1	D	43	GLY	3.4
1	F	14	ASN	3.4
1	D	152	THR	3.4
1	F	101	ALA	3.4
1	G	102	GLY	3.4
1	G	12	SER	3.3
1	H	42	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	114	LEU	3.3
1	B	163	ASN	3.3
1	D	160	ALA	3.3
1	A	168	VAL	3.3
1	H	19	ILE	3.3
1	C	41	PHE	3.3
1	E	168	VAL	3.2
1	G	9	ILE	3.2
1	C	42	ASN	3.2
1	C	202	HIS	3.2
1	D	210	LYS	3.2
1	D	156	ILE	3.2
1	D	161	GLU	3.2
1	H	101	ALA	3.2
1	D	19	ILE	3.1
1	A	28	PHE	3.1
1	G	28	PHE	3.1
1	A	166	ILE	3.1
1	A	101	ALA	3.1
1	F	9	ILE	3.1
1	E	28	PHE	3.1
1	H	210	LYS	3.1
1	C	9	ILE	3.0
1	B	42	ASN	3.0
1	D	102	GLY	3.0
1	H	102	GLY	3.0
1	A	114	LEU	3.0
1	C	39	ARG	3.0
1	H	151	SER	3.0
1	G	45	MET	3.0
1	G	47	GLY	3.0
1	G	15	ASP	3.0
1	G	154	LYS	3.0
1	G	209	THR	2.9
1	B	210	LYS	2.9
1	E	164	GLU	2.9
1	D	101	ALA	2.9
1	D	209	THR	2.9
1	A	102	GLY	2.9
1	B	162	GLU	2.9
1	E	114	LEU	2.8
1	E	101	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	28	PHE	2.8
1	A	-2	HIS	2.8
1	A	68	VAL	2.8
1	B	16	VAL	2.8
1	D	203	ASN	2.8
1	G	13	LYS	2.8
1	H	168	VAL	2.8
1	A	118	GLY	2.8
1	G	99	ILE	2.7
1	C	11	PHE	2.7
1	G	114	LEU	2.7
1	B	156	ILE	2.7
1	E	49	ILE	2.7
1	G	152	THR	2.7
1	A	153	ALA	2.7
1	D	154	LYS	2.7
1	C	102	GLY	2.7
1	F	158	GLY	2.7
1	H	36	PHE	2.7
1	G	104	THR	2.7
1	G	49	ILE	2.7
1	B	161	GLU	2.7
1	F	164	GLU	2.7
1	E	206	ASN	2.7
1	D	114	LEU	2.6
1	H	9	ILE	2.6
1	F	11	PHE	2.6
1	C	40	LEU	2.6
1	C	206	ASN	2.6
1	E	9	ILE	2.6
1	G	149	ASP	2.6
1	G	7	GLN	2.6
1	B	26	ARG	2.6
1	C	99	ILE	2.6
1	H	99	ILE	2.6
1	D	6	GLN	2.6
1	B	10	THR	2.6
1	B	102	GLY	2.6
1	G	118	GLY	2.6
1	G	31	LEU	2.5
1	A	152	THR	2.5
1	A	164	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	54	PHE	2.5
1	D	18	ILE	2.5
1	E	166	ILE	2.5
1	D	120	GLU	2.5
1	A	150	ALA	2.5
1	B	28	PHE	2.5
1	H	40	LEU	2.5
1	G	164	GLU	2.5
1	E	90	TRP	2.5
1	H	104	THR	2.5
1	A	170	VAL	2.5
1	F	16	VAL	2.5
1	A	117	ALA	2.5
1	D	163	ASN	2.5
1	C	204	LEU	2.4
1	A	209	THR	2.4
1	D	10	THR	2.4
1	E	210	LYS	2.4
1	F	31	LEU	2.4
1	F	114	LEU	2.4
1	C	44	GLY	2.4
1	C	208	TRP	2.4
1	C	8	GLY	2.4
1	G	166	ILE	2.4
1	H	154	LYS	2.4
1	G	26	ARG	2.4
1	H	7	GLN	2.4
1	E	16	VAL	2.4
1	D	44	GLY	2.4
1	E	146	GLY	2.4
1	F	156	ILE	2.3
1	H	49	ILE	2.3
1	B	14	ASN	2.3
1	G	38	HIS	2.3
1	H	116	GLU	2.3
1	C	45	MET	2.3
1	C	203	ASN	2.3
1	B	158	GLY	2.3
1	G	210	LYS	2.3
1	G	29	PHE	2.3
1	D	20	ALA	2.3
1	G	20	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	117	ALA	2.3
1	E	202	HIS	2.3
1	F	157	HIS	2.3
1	G	68	VAL	2.3
1	D	166	ILE	2.2
1	C	27	GLY	2.2
1	F	102	GLY	2.2
1	G	153	ALA	2.2
1	C	104	THR	2.2
1	D	162	GLU	2.2
1	A	27	GLY	2.2
1	E	11	PHE	2.2
1	F	28	PHE	2.2
1	F	80	ILE	2.2
1	A	1	MET	2.2
1	B	25	TYR	2.2
1	D	42	ASN	2.2
1	H	24	LEU	2.2
1	C	135	GLY	2.2
1	F	47	GLY	2.2
1	D	49	ILE	2.2
1	D	153	ALA	2.2
1	H	20	ALA	2.2
1	A	2	SER	2.2
1	A	210	LYS	2.2
1	A	116	GLU	2.2
1	B	174	GLU	2.2
1	F	100	GLU	2.2
1	D	121	VAL	2.2
1	F	8	GLY	2.2
1	H	118	GLY	2.2
1	H	117	ALA	2.1
1	C	18	ILE	2.1
1	G	178	GLN	2.1
1	C	14	ASN	2.1
1	E	209	THR	2.1
1	H	11	PHE	2.1
1	H	152	THR	2.1
1	H	98	MET	2.1
1	A	-1	HIS	2.1
1	E	89	PRO	2.1
1	G	122	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	35	ARG	2.1
1	H	37	ARG	2.1
1	D	48	GLU	2.1
1	F	202	HIS	2.1
1	G	41	PHE	2.1
1	C	210	LYS	2.1
1	E	8	GLY	2.1
1	A	151	SER	2.1
1	B	114	LEU	2.1
1	C	201	TYR	2.1
1	D	95	VAL	2.1
1	E	170	VAL	2.1
1	D	117	ALA	2.0
1	A	202	HIS	2.0
1	B	209	THR	2.0
1	G	50	THR	2.0
1	H	38	HIS	2.0
1	G	120	GLU	2.0
1	H	166	ILE	2.0
1	D	47	GLY	2.0
1	G	167	ARG	2.0
1	D	164	GLU	2.0
1	E	120	GLU	2.0
1	H	87	GLU	2.0
1	H	113	ALA	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
2	PEG	C	301	7/7	0.75	0.16	26,35,45,59	0
2	PEG	C	302	7/7	0.76	0.18	50,52,55,57	0
2	PEG	F	301	7/7	0.82	0.16	42,51,54,59	0
2	PEG	D	301	7/7	0.83	0.13	44,49,55,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.