



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:09 am GMT

PDB ID : 4NA4
Title : Crystal structure of mouse poly(ADP-ribose) glycohydrolase (PARG) catalytic domain with ADP-HPD
Authors : Wang, Z.; Cheng, Z.; Xu, W.
Deposited on : 2013-10-21
Resolution : 2.50 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

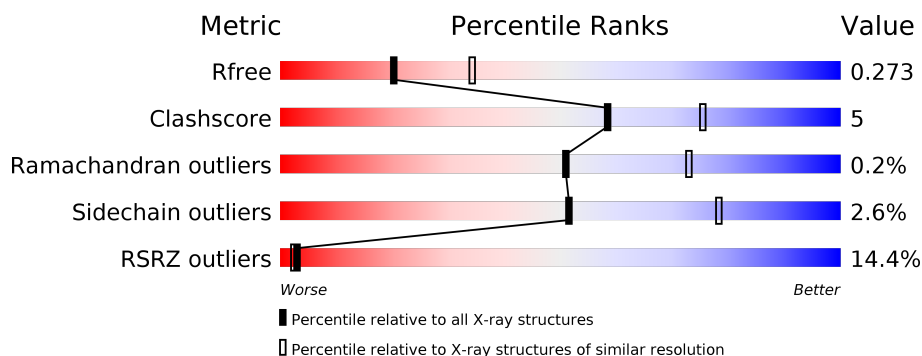
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	522	<div> <div>13%</div> <div>87%</div> <div>9%</div> <div>..</div> </div>
1	B	522	<div> <div>19%</div> <div>80%</div> <div>14%</div> <div>5%</div> </div>
1	C	522	<div> <div>9%</div> <div>84%</div> <div>11%</div> <div>..</div> </div>

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 12421 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.

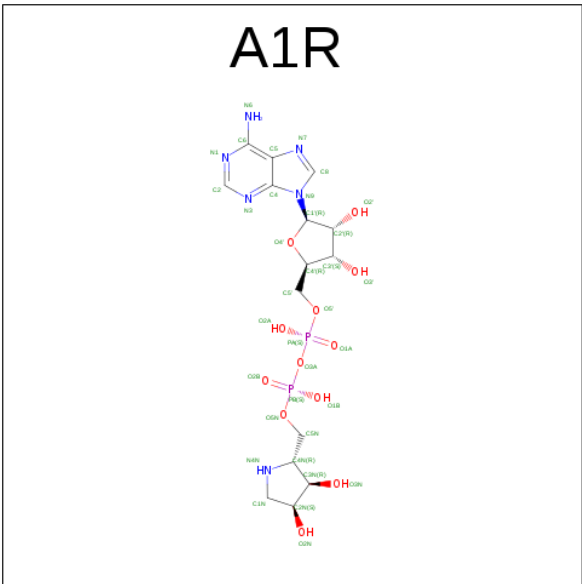
- Molecule 1 is a protein called Poly(ADP-ribose) glycohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	Se	0	0	0
			4102	2621	714	744	14	9			
1	B	494	Total	C	N	O	S	Se	0	0	0
			4016	2565	700	728	14	9			
1	C	505	Total	C	N	O	S	Se	0	0	0
			4101	2619	714	745	14	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	GLY	-	EXPRESSION TAG	UNP O88622
B	438	GLY	-	EXPRESSION TAG	UNP O88622
C	438	GLY	-	EXPRESSION TAG	UNP O88622

- Molecule 2 is 5'-O-[(S)-{[(S)-{[(2R,3R,4S)-3,4-DIHYDROXYPYRROLIDIN-2-YL]MET HOXY}(HYDROXY)PHOSPHORYL]OXY}(HYDROXY)PHOSPHORYL]ADENOSINE (three-letter code: A1R) (formula: C₁₅H₂₄N₆O₁₂P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			35	15	6	12	2		
2	B	1	Total	C	N	O	P	0	0
			35	15	6	12	2		
2	C	1	Total	C	N	O	P	0	0
			35	15	6	12	2		

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	I	0	0
			1	1		
3	A	2	Total	I	0	0
			2	2		
3	C	2	Total	I	0	0
			2	2		

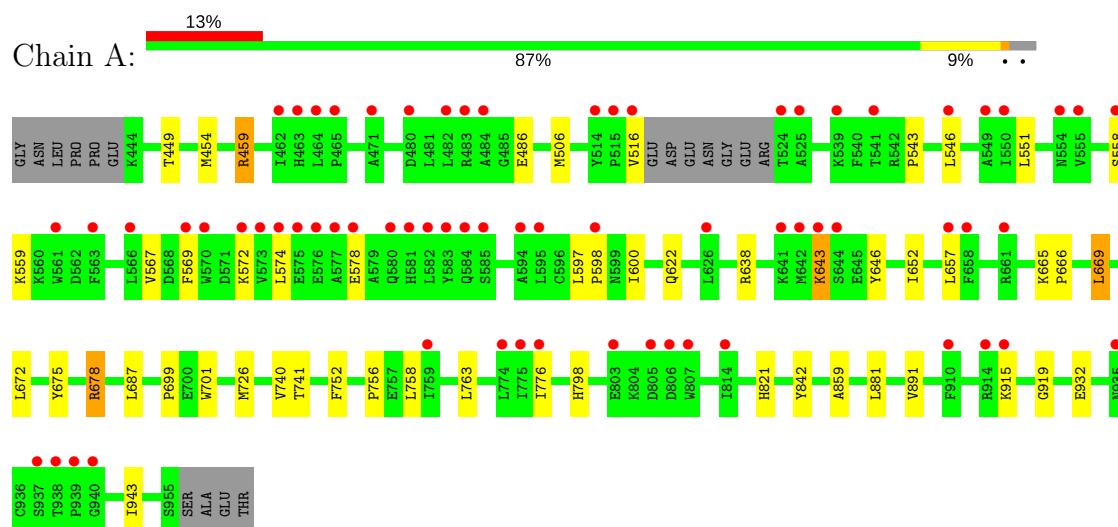
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	45	Total	O	0	0
			45	45		
4	B	6	Total	O	0	0
			6	6		
4	C	41	Total	O	0	0
			41	41		

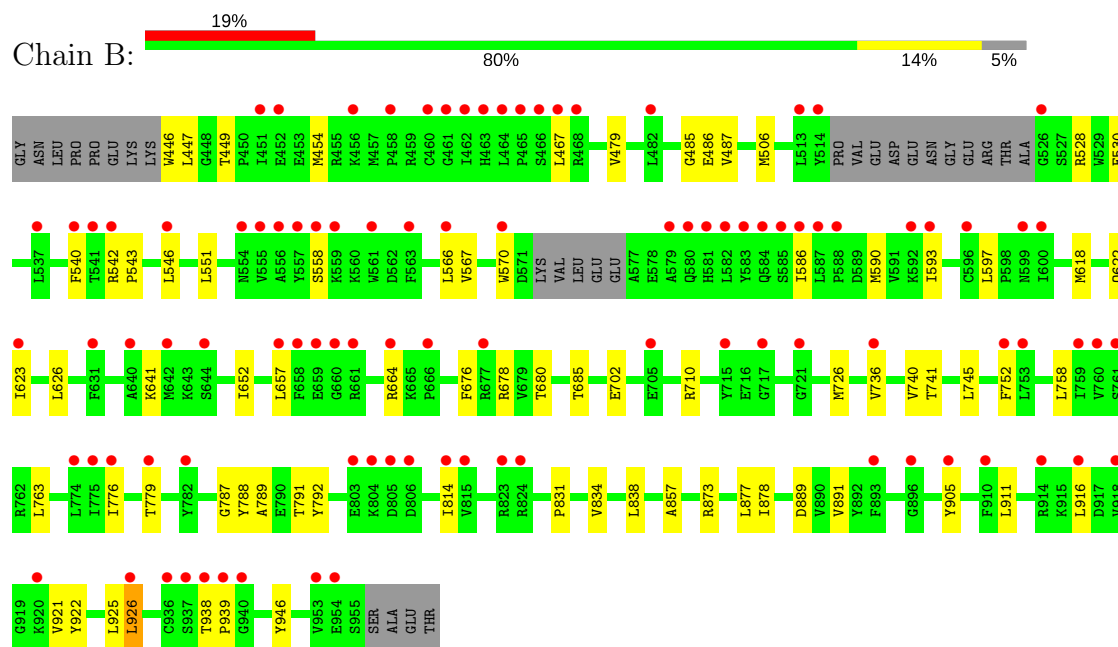
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

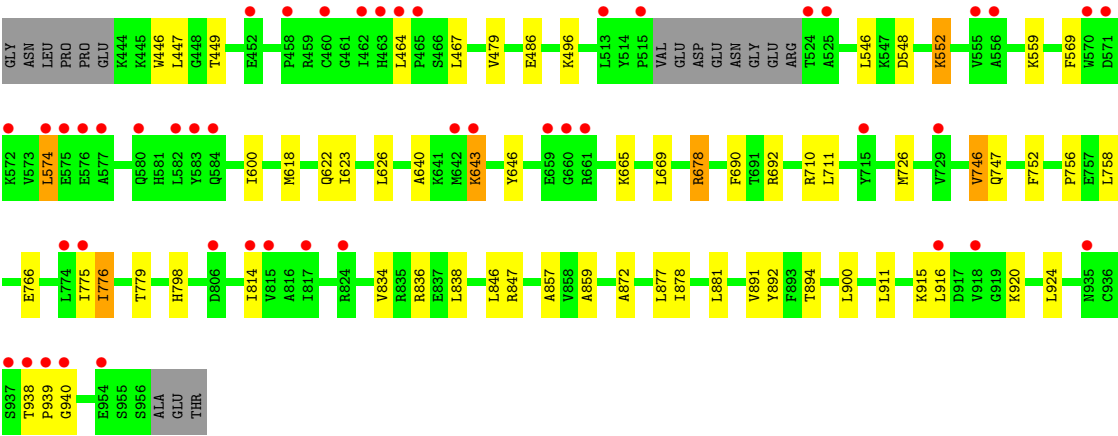
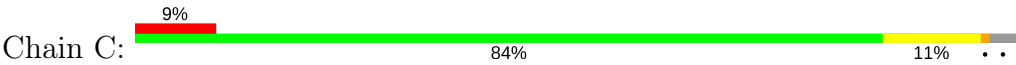
- Molecule 1: Poly(ADP-ribose) glycohydrolase



- Molecule 1: Poly(ADP-ribose) glycohydrolase



- Molecule 1: Poly(ADP-ribose) glycohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	188.95Å 55.57Å 165.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50 37.99 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.00-2.50) 98.7 (37.99-2.49)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.242 , 0.282 0.236 , 0.273	Depositor DCC
R_{free} test set	3091 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12421	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.61 % 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 4.2432e-06. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, A1R

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	0.38	0/4195	0.54	0/5663
1	B	0.31	0/4107	0.48	0/5543
1	C	0.37	0/4194	0.53	0/5661
All	All	0.35	0/12496	0.52	0/16867

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4102	0	4072	31	0
1	B	4016	0	3972	55	0
1	C	4101	0	4068	48	0
2	A	35	0	22	0	0
2	B	35	0	22	1	0
2	C	35	0	22	2	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
4	A	45	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	0	1	0
4	C	41	0	0	1	0
All	All	12421	0	12178	134	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 (134) 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:779:THR:HG22	4:C:1107:HOH:O	1.72	0.89
1:B:618:MSE:HE1	1:B:626:LEU:HD12	1.56	0.87
1:C:726:MSE:HE2	1:C:859:ALA:HB2	1.56	0.85
1:C:618:MSE:CE	1:C:626:LEU:HD12	2.08	0.82
1:B:726:MSE:HE3	1:B:857:ALA:HB3	1.62	0.81
1:C:746:VAL:HG13	2:C:1001:A1R:O1A	1.80	0.80
1:A:726:MSE:HE1	1:A:891:VAL:HB	1.64	0.78
1:A:726:MSE:HE2	1:A:859:ALA:HB2	1.69	0.75
1:C:726:MSE:HE1	1:C:891:VAL:HB	1.68	0.75
1:B:618:MSE:HE1	1:B:626:LEU:CD1	2.16	0.74
1:C:938:THR:HG22	1:C:940:GLY:H	1.52	0.74
1:C:838:LEU:HD22	1:C:878:ILE:HG23	1.70	0.74
1:C:726:MSE:HE1	1:C:891:VAL:CG2	2.19	0.72
1:C:911:LEU:HD23	1:C:916:LEU:HD12	1.73	0.71
1:B:877:LEU:HD23	1:B:925:LEU:HD21	1.74	0.69
1:B:590:MSE:HE2	1:B:676:PHE:HB3	1.75	0.69
1:C:618:MSE:CE	1:C:626:LEU:CD1	2.71	0.69
1:B:838:LEU:HD13	1:B:878:ILE:HG23	1.75	0.68
1:C:618:MSE:HE3	1:C:626:LEU:HD12	1.76	0.68
1:B:726:MSE:HE1	1:B:891:VAL:CG2	2.26	0.66
1:C:746:VAL:HG13	1:C:747:GLN:H	1.61	0.65
1:A:932:GLU:HG2	1:A:943:ILE:HG22	1.77	0.65
1:C:726:MSE:HE1	1:C:891:VAL:CB	2.26	0.64
1:B:618:MSE:HE2	1:B:623:ILE:HG13	1.80	0.63
1:B:758:LEU:HD22	1:B:776:ILE:HD12	1.81	0.63
1:C:618:MSE:HE3	1:C:626:LEU:CD1	2.30	0.61
1:C:618:MSE:HE2	1:C:623:ILE:CG1	2.30	0.61
1:B:449:THR:HG21	1:B:710:ARG:HD2	1.80	0.61
1:B:467:LEU:O	1:B:479:VAL:HG11	2.00	0.61
1:A:678:ARG:NH2	1:A:798:HIS:O	2.34	0.60
1:C:877:LEU:O	1:C:881:LEU:HD13	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:LEU:HD23	1:B:566:LEU:HD21	1.83	0.60
1:A:726:MSE:HE1	1:A:891:VAL:CB	2.31	0.59
1:B:726:MSE:HE3	1:B:857:ALA:CB	2.33	0.59
1:C:618:MSE:HE1	1:C:626:LEU:CD1	2.31	0.59
1:C:618:MSE:HE2	1:C:623:ILE:HG12	1.84	0.59
1:B:740:VAL:HG13	1:B:741:THR:HG23	1.82	0.59
1:A:638:ARG:NH2	1:A:763:LEU:O	2.35	0.59
1:C:692:ARG:NH2	1:C:766:GLU:O	2.36	0.58
1:C:467:LEU:O	1:C:479:VAL:HG11	2.04	0.57
1:C:569:PHE:CE1	1:C:574:LEU:HD13	2.39	0.57
1:C:618:MSE:HE1	1:C:626:LEU:HD12	1.86	0.57
1:B:745:LEU:HD21	1:B:792:TYR:CD1	2.40	0.57
1:B:657:LEU:HD11	1:B:741:THR:HA	1.87	0.57
1:A:600:ILE:HG22	1:A:622:GLN:HG2	1.87	0.56
1:C:690:PHE:CD2	1:C:776:ILE:HD13	2.41	0.56
1:C:726:MSE:HE3	1:C:857:ALA:HB3	1.88	0.55
1:C:872:ALA:HB1	1:C:900:LEU:HD21	1.87	0.55
1:A:543:PRO:HB2	1:A:567:VAL:HG12	1.88	0.55
1:B:922:TYR:O	1:B:926:LEU:HD23	2.07	0.55
1:A:665:LYS:O	1:A:669:LEU:HD22	2.07	0.54
1:B:593:ILE:HD13	1:B:680:THR:HG22	1.89	0.54
1:C:746:VAL:CG1	2:C:1001:A1R:O1A	2.53	0.54
1:C:746:VAL:HG13	1:C:747:GLN:N	2.22	0.54
1:A:726:MSE:HE1	1:A:891:VAL:CG2	2.37	0.54
1:B:485:GLY:O	1:B:685:THR:HG21	2.07	0.54
1:B:758:LEU:HD11	1:B:814:ILE:CD1	2.38	0.53
1:A:657:LEU:HD21	1:A:672:LEU:HD12	1.90	0.53
1:B:831:PRO:HG3	1:B:926:LEU:HD13	1.90	0.53
1:A:752:PHE:O	1:A:756:PRO:HA	2.08	0.52
1:B:788:TYR:H	1:B:791:THR:HG23	1.73	0.52
1:B:454:MSE:HE1	1:B:889:ASP:HB3	1.92	0.52
1:C:752:PHE:O	1:C:756:PRO:HA	2.10	0.52
1:A:740:VAL:HG13	1:A:741:THR:HG23	1.91	0.51
1:C:779:THR:HG21	1:C:814:ILE:HD12	1.93	0.51
1:B:779:THR:HG21	1:B:814:ILE:HD12	1.92	0.51
1:C:640:ALA:HB3	1:C:643:LYS:HB2	1.93	0.51
1:C:726:MSE:HE1	1:C:891:VAL:HG21	1.92	0.51
1:A:643:LYS:HD3	1:A:646:TYR:HB2	1.93	0.51
1:B:618:MSE:HE2	1:B:623:ILE:CG1	2.40	0.51
1:B:551:LEU:HD22	1:B:558:SER:HA	1.93	0.50
1:C:920:LYS:O	1:C:924:LEU:HD13	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:PRO:CB	1:A:567:VAL:HG12	2.41	0.49
1:A:459:ARG:HD3	1:A:459:ARG:N	2.27	0.49
1:B:726:MSE:HE1	1:B:891:VAL:HB	1.94	0.49
1:B:487:VAL:CG2	1:B:685:THR:HG22	2.44	0.48
1:C:449:THR:HG21	1:C:710:ARG:HD2	1.94	0.48
1:B:506:MSE:HE1	1:B:597:LEU:HD11	1.95	0.48
1:B:922:TYR:CZ	1:B:926:LEU:HD21	2.48	0.47
1:A:699:PRO:HD3	1:A:842:TYR:CE2	2.50	0.47
1:A:551:LEU:HD22	1:A:558:SER:HA	1.96	0.47
1:A:675:TYR:CG	1:A:756:PRO:HG2	2.51	0.46
1:C:938:THR:HG23	1:C:939:PRO:HD2	1.96	0.46
1:B:543:PRO:HD3	1:B:570:TRP:CD2	2.51	0.46
1:B:726:MSE:HE1	1:B:891:VAL:HG23	1.97	0.46
1:C:446:TRP:O	1:C:447:LEU:HD12	2.16	0.46
1:B:911:LEU:HD22	1:B:916:LEU:HD12	1.98	0.46
1:B:788:TYR:N	1:B:791:THR:HG23	2.32	0.45
1:C:665:LYS:O	1:C:669:LEU:HD23	2.17	0.45
1:C:726:MSE:HE3	1:C:857:ALA:CB	2.47	0.45
1:B:543:PRO:HB2	1:B:567:VAL:HG22	1.98	0.45
1:B:758:LEU:HD23	1:B:776:ILE:HG21	1.99	0.44
1:B:586:ILE:CG2	1:B:590:MSE:HE1	2.47	0.44
1:B:922:TYR:CE1	1:B:926:LEU:HD21	2.52	0.44
1:C:746:VAL:CG1	1:C:747:GLN:N	2.80	0.44
1:B:911:LEU:CD2	1:B:916:LEU:HD12	2.48	0.44
1:A:652:ILE:HG12	1:A:763:LEU:HD13	2.00	0.44
1:A:449:THR:HB	1:A:454:MSE:HE2	1.99	0.43
1:C:678:ARG:NH2	1:C:798:HIS:O	2.51	0.43
1:C:834:VAL:O	1:C:838:LEU:HD23	2.17	0.43
1:B:487:VAL:HG22	1:B:685:THR:HG22	1.99	0.43
1:A:516:VAL:O	1:A:516:VAL:HG12	2.17	0.43
1:B:586:ILE:HG22	1:B:590:MSE:CE	2.49	0.43
1:C:758:LEU:HD23	1:C:776:ILE:HG21	2.01	0.43
1:A:569:PHE:CZ	1:A:574:LEU:HD11	2.54	0.43
1:B:873:ARG:HB3	1:B:946:TYR:CE1	2.54	0.43
1:B:447:LEU:HD22	1:B:905:TYR:CD2	2.53	0.43
1:A:506:MSE:HE1	1:A:597:LEU:HD11	2.01	0.43
1:B:726:MSE:HE1	1:B:891:VAL:CB	2.49	0.43
1:C:548:ASP:O	1:C:552:LYS:HD3	2.19	0.42
1:A:574:LEU:HD22	1:A:578:GLU:HB3	2.01	0.42
1:A:597:LEU:N	1:A:598:PRO:HD2	2.35	0.42
1:A:701:TRP:O	1:A:919:GLY:HA2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:LEU:HD21	1:A:672:LEU:CD1	2.50	0.42
1:C:600:ILE:HG22	1:C:622:GLN:HG2	2.02	0.41
1:A:758:LEU:HD23	1:A:776:ILE:HG21	2.02	0.41
1:B:652:ILE:HG12	1:B:763:LEU:HD13	2.02	0.41
1:B:618:MSE:HE3	1:B:622:GLN:HB3	2.03	0.41
1:B:740:VAL:HG21	1:B:752:PHE:HB3	2.03	0.41
1:C:643:LYS:HD2	1:C:646:TYR:HB2	2.03	0.41
1:B:736:VAL:HG22	4:B:1102:HOH:O	2.20	0.41
1:B:834:VAL:O	1:B:838:LEU:HD23	2.20	0.41
1:B:788:TYR:OH	2:B:1001:A1R:H5'1	2.21	0.41
1:B:911:LEU:HD13	1:B:921:VAL:HG21	2.02	0.41
1:B:447:LEU:HD13	1:B:905:TYR:HB3	2.03	0.40
1:B:787:GLY:CA	1:B:791:THR:HG23	2.52	0.40
1:C:892:TYR:CE2	1:C:894:THR:HG22	2.56	0.40
1:A:726:MSE:HE2	1:A:859:ALA:CB	2.46	0.40
1:B:938:THR:HG23	1:B:939:PRO:HD2	2.03	0.40
1:C:775:ILE:HD13	1:C:847:ARG:CZ	2.52	0.40
1:B:454:MSE:CE	1:B:889:ASP:HB3	2.51	0.40
1:C:911:LEU:CD2	1:C:916:LEU:HD12	2.47	0.40
1:A:665:LYS:N	1:A:666:PRO:CD	2.85	0.40
1:C:836:ARG:HD3	1:C:836:ARG:C	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	501/522 (96%)	487 (97%)	13 (3%)	1 (0%)	51	73
1	B	488/522 (94%)	459 (94%)	28 (6%)	1 (0%)	51	73
1	C	501/522 (96%)	485 (97%)	15 (3%)	1 (0%)	51	73
All	All	1490/1566 (95%)	1431 (96%)	56 (4%)	3 (0%)	51	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	643	LYS
1	C	643	LYS
1	B	789	ALA

5.3.2 Protein sidechains ⓘ

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	445/450 (99%)	434 (98%)	11 (2%)	53	79
1	B	435/450 (97%)	424 (98%)	11 (2%)	53	79
1	C	445/450 (99%)	432 (97%)	13 (3%)	48	75
All	All	1325/1350 (98%)	1290 (97%)	35 (3%)	51	78

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	459	ARG
1	A	486	GLU
1	A	546	LEU
1	A	559	LYS
1	A	572	LYS
1	A	669	LEU
1	A	678	ARG
1	A	687	LEU
1	A	821	HIS
1	A	881	LEU
1	A	915	LYS
1	B	446	TRP
1	B	486	GLU
1	B	528	ARG
1	B	530	GLU
1	B	540	PHE
1	B	542	ARG
1	B	641	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	664	ARG
1	B	678	ARG
1	B	702	GLU
1	B	926	LEU
1	C	464	LEU
1	C	486	GLU
1	C	496	LYS
1	C	546	LEU
1	C	552	LYS
1	C	559	LYS
1	C	574	LEU
1	C	678	ARG
1	C	711	LEU
1	C	746	VAL
1	C	776	ILE
1	C	846	LEU
1	C	915	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

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	A1R	A	1001	-	32,38,38	0.82	1 (3%)	29,58,58	1.98	2 (6%)
2	A1R	B	1001	-	32,38,38	0.77	1 (3%)	29,58,58	1.91	1 (3%)
2	A1R	C	1001	-	32,38,38	0.76	0	29,58,58	1.76	2 (6%)

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	A1R	A	1001	-	-	0/18/51/51	0/4/4/4
2	A1R	B	1001	-	-	0/18/51/51	0/4/4/4
2	A1R	C	1001	-	-	0/18/51/51	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	A1R	O4'-C1'	2.12	1.44	1.41
2	B	1001	A1R	O4'-C1'	2.13	1.44	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	A1R	N3-C2-N1	-9.42	120.66	128.86
2	B	1001	A1R	N3-C2-N1	-9.03	120.99	128.86
2	C	1001	A1R	N3-C2-N1	-8.46	121.49	128.86
2	A	1001	A1R	C4-C5-N7	-2.54	106.96	109.41
2	C	1001	A1R	C4-C5-N7	-2.10	107.38	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	A1R	1	0
2	C	1001	A1R	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	496/522 (95%)	0.63	68 (13%) 3 3	27, 53, 101, 137	0
1	B	485/522 (92%)	1.15	99 (20%) 1 1	40, 106, 225, 331	0
1	C	496/522 (95%)	0.42	46 (9%) 9 9	26, 51, 92, 136	0
All	All	1477/1566 (94%)	0.73	213 (14%) 3 2	26, 62, 173, 331	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	582	LEU	17.1
1	C	939	PRO	12.8
1	A	939	PRO	12.1
1	B	658	PHE	11.8
1	B	555	VAL	11.2
1	B	939	PRO	9.4
1	A	515	PRO	9.1
1	B	583	TYR	7.6
1	C	582	LEU	7.5
1	A	582	LEU	7.0
1	A	577	ALA	7.0
1	B	916	LEU	6.9
1	B	466	SER	6.6
1	B	580	GLN	6.5
1	A	578	GLU	6.2
1	A	516	VAL	6.2
1	B	540	PHE	6.0
1	B	584	GLN	5.9
1	A	546	LEU	5.8
1	A	463	HIS	5.6
1	A	566	LEU	5.5
1	C	580	GLN	5.4
1	B	905	TYR	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	938	THR	5.2
1	B	570	TRP	5.2
1	B	806	ASP	5.2
1	A	580	GLN	5.1
1	C	576	GLU	5.1
1	B	463	HIS	5.0
1	B	587	LEU	4.9
1	A	575	GLU	4.9
1	B	566	LEU	4.9
1	B	660	GLY	4.9
1	B	938	THR	4.9
1	B	513	LEU	4.8
1	B	918	VAL	4.7
1	B	705	GLU	4.5
1	A	658	PHE	4.5
1	A	803	GLU	4.5
1	B	561	TRP	4.4
1	B	554	ASN	4.4
1	B	556	ALA	4.4
1	B	659	GLU	4.4
1	B	586	ILE	4.4
1	C	660	GLY	4.3
1	A	940	GLY	4.2
1	B	644	SER	4.2
1	B	579	ALA	4.1
1	B	588	PRO	4.1
1	A	574	LEU	4.0
1	A	524	THR	4.0
1	B	557	TYR	4.0
1	A	464	LEU	3.9
1	B	677	ARG	3.9
1	C	940	GLY	3.9
1	B	458	PRO	3.9
1	A	938	THR	3.8
1	A	572	LYS	3.8
1	B	467	LEU	3.7
1	B	814	ILE	3.7
1	C	643	LYS	3.7
1	B	526	GLY	3.7
1	A	550	ILE	3.6
1	A	759	ILE	3.6
1	A	480	ASP	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	805	ASP	3.6
1	A	462	ILE	3.6
1	C	513	LEU	3.6
1	A	555	VAL	3.5
1	B	563	PHE	3.5
1	B	631	PHE	3.5
1	C	584	GLN	3.5
1	C	937	SER	3.5
1	A	570	TRP	3.5
1	B	803	GLU	3.5
1	C	463	HIS	3.5
1	B	926	LEU	3.4
1	C	918	VAL	3.4
1	C	572	LYS	3.4
1	C	556	ALA	3.4
1	A	561	TRP	3.4
1	B	936	CYS	3.4
1	C	570	TRP	3.4
1	C	583	TYR	3.4
1	A	806	ASP	3.4
1	A	583	TYR	3.4
1	A	643	LYS	3.3
1	B	774	LEU	3.3
1	A	483	ARG	3.3
1	B	661	ARG	3.3
1	A	642	MET	3.3
1	B	717	GLY	3.3
1	B	896	GLY	3.3
1	B	546	LEU	3.2
1	B	920	LYS	3.2
1	C	515	PRO	3.2
1	C	464	LEU	3.2
1	A	776	ILE	3.2
1	B	666	PRO	3.2
1	A	644	SER	3.1
1	B	452	GLU	3.1
1	A	585	SER	3.1
1	B	460	CYS	3.1
1	B	464	LEU	3.1
1	C	555	VAL	3.1
1	A	915	LYS	3.1
1	B	542	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	514	TYR	3.1
1	A	805	ASP	3.0
1	A	576	GLU	3.0
1	B	482	LEU	3.0
1	A	910	PHE	3.0
1	A	514	TYR	3.0
1	B	779	THR	3.0
1	A	581	HIS	2.9
1	A	935	ASN	2.9
1	B	451	ILE	2.9
1	C	575	GLU	2.8
1	B	954	GLU	2.8
1	A	539	LYS	2.8
1	B	592	LYS	2.8
1	A	584	GLN	2.8
1	C	577	ALA	2.8
1	A	774	LEU	2.8
1	A	558	SER	2.8
1	A	814	ILE	2.7
1	A	937	SER	2.7
1	C	661	ARG	2.7
1	A	914	ARG	2.7
1	C	571	ASP	2.7
1	A	598	PRO	2.7
1	A	471	ALA	2.7
1	A	549	ALA	2.7
1	A	554	ASN	2.7
1	B	537	LEU	2.6
1	C	458	PRO	2.6
1	B	558	SER	2.6
1	B	776	ILE	2.6
1	C	659	GLU	2.6
1	B	715	TYR	2.6
1	B	815	VAL	2.6
1	B	462	ILE	2.6
1	B	585	SER	2.6
1	B	721	GLY	2.6
1	A	594	ALA	2.6
1	C	774	LEU	2.6
1	C	642	MET	2.6
1	C	935	ASN	2.6
1	B	640	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	953	VAL	2.5
1	B	824	ARG	2.5
1	A	661	ARG	2.5
1	B	596	CYS	2.5
1	B	752	PHE	2.5
1	A	525	ALA	2.5
1	B	468	ARG	2.5
1	B	657	LEU	2.5
1	B	642	MET	2.5
1	B	753	LEU	2.5
1	B	937	SER	2.5
1	B	465	PRO	2.5
1	C	460	CYS	2.4
1	C	715	TYR	2.4
1	C	775	ILE	2.4
1	A	641	LYS	2.4
1	B	599	ASN	2.4
1	C	574	LEU	2.4
1	A	657	LEU	2.4
1	B	761	SER	2.4
1	A	484	ALA	2.4
1	B	559	LYS	2.3
1	C	729	VAL	2.3
1	C	525	ALA	2.3
1	B	910	PHE	2.3
1	A	465	PRO	2.3
1	C	462	ILE	2.3
1	C	916	LEU	2.3
1	C	824	ARG	2.3
1	A	569	PHE	2.3
1	B	541	THR	2.3
1	A	482	LEU	2.3
1	C	954	GLU	2.3
1	A	573	VAL	2.2
1	B	593	ILE	2.2
1	A	775	ILE	2.2
1	B	600	ILE	2.2
1	C	814	ILE	2.2
1	C	452	GLU	2.2
1	B	823	ARG	2.2
1	B	456	LYS	2.2
1	B	760	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	815	VAL	2.2
1	B	581	HIS	2.1
1	B	664	ARG	2.1
1	B	775	ILE	2.1
1	C	806	ASP	2.1
1	B	736	VAL	2.1
1	A	807	TRP	2.1
1	B	782	TYR	2.1
1	B	940	GLY	2.1
1	A	563	PHE	2.1
1	B	461	GLY	2.1
1	A	595	LEU	2.1
1	C	524	THR	2.1
1	C	817	ILE	2.0
1	A	626	LEU	2.0
1	B	893	PHE	2.0
1	A	541	THR	2.0
1	B	623	ILE	2.0
1	B	759	ILE	2.0
1	C	465	PRO	2.0
1	B	914	ARG	2.0
1	B	804	LYS	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 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	A1R	C	1001	35/35	0.96	0.15	-0.18	26,34,39,41	0
2	A1R	B	1001	35/35	0.92	0.17	-0.30	45,62,67,71	0
2	A1R	A	1001	35/35	0.96	0.14	-0.44	27,34,41,48	0
3	IOD	B	1002	1/1	0.85	0.07	-2.46	113,113,113,113	0
3	IOD	A	1003	1/1	0.98	0.03	-2.98	66,66,66,66	0
3	IOD	C	1002	1/1	0.96	0.06	-3.42	68,68,68,68	0
3	IOD	A	1002	1/1	0.99	0.21	-	88,88,88,88	0
3	IOD	C	1003	1/1	0.95	0.42	-	121,121,121,121	0

6.5 Other polymers [i](#)

There are no such residues in this entry.