Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:57 PM 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 (i) symbol.

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

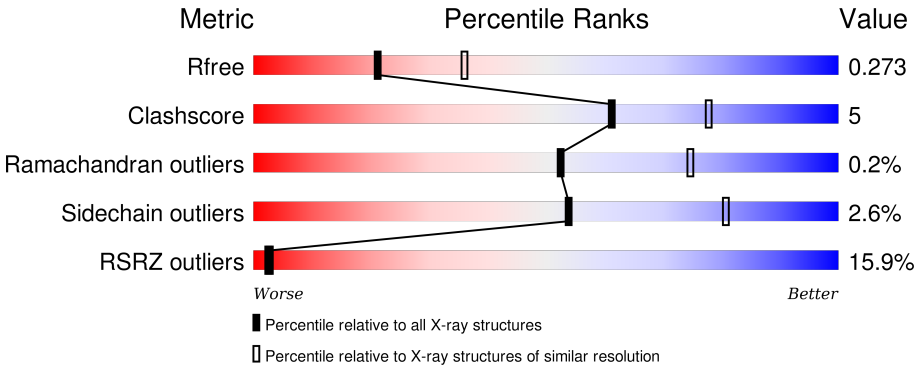
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 <=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	14% 87% 9% • •
1	B	522	21% 80% 14% 5%
1	C	522	10% 84% 11% • •

2 Entry composition

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.

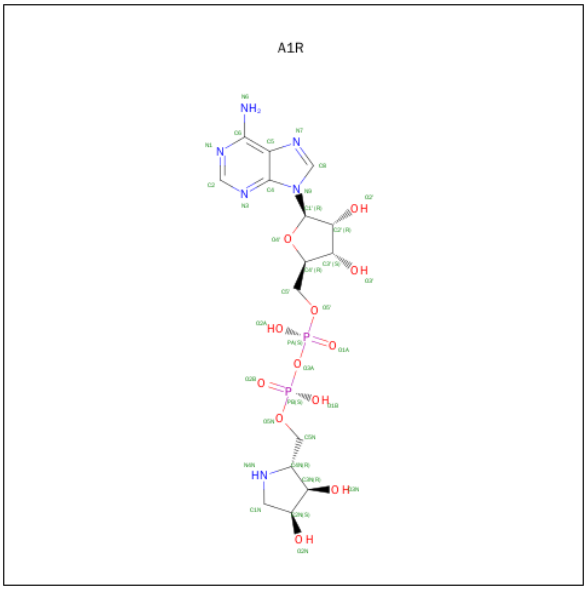
- Molecule 1 is a protein called Poly(ADP-ribose) glycohydrolase.

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]METHOXY}(HYDROXY)PHOSPHORYL]OXY}(HYDROXY)PHOSPHORYL]ADENOSINE (three-letter code: A1R) (formula: $C_{15}H_{24}N_6O_{12}P_2$).



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.

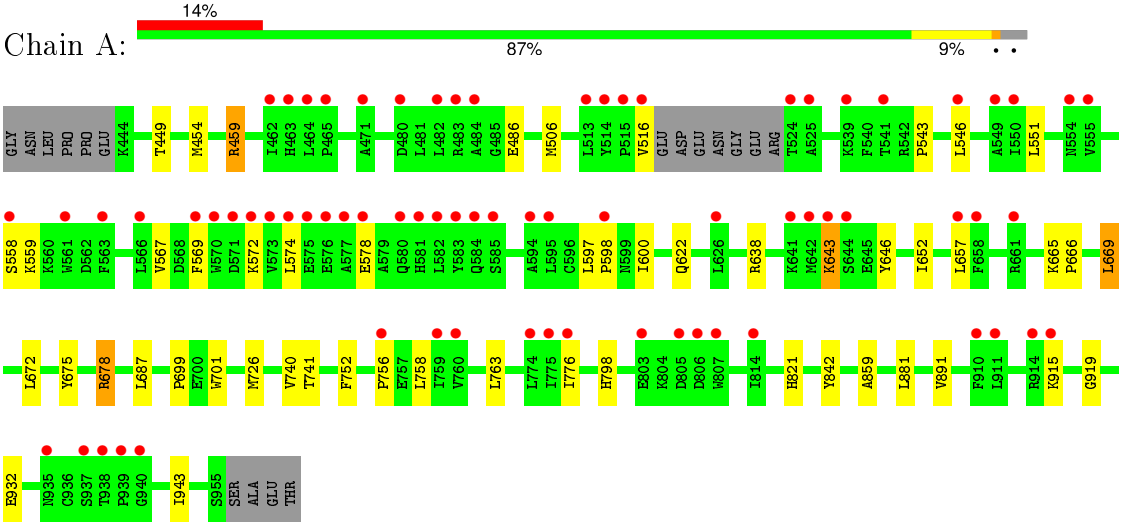
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	45	Total	O	0	0
			45	45		
4	B	6	Total	O	0	0
			6	6		
4	C	41	Total	O	0	0
			41	41		

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 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.

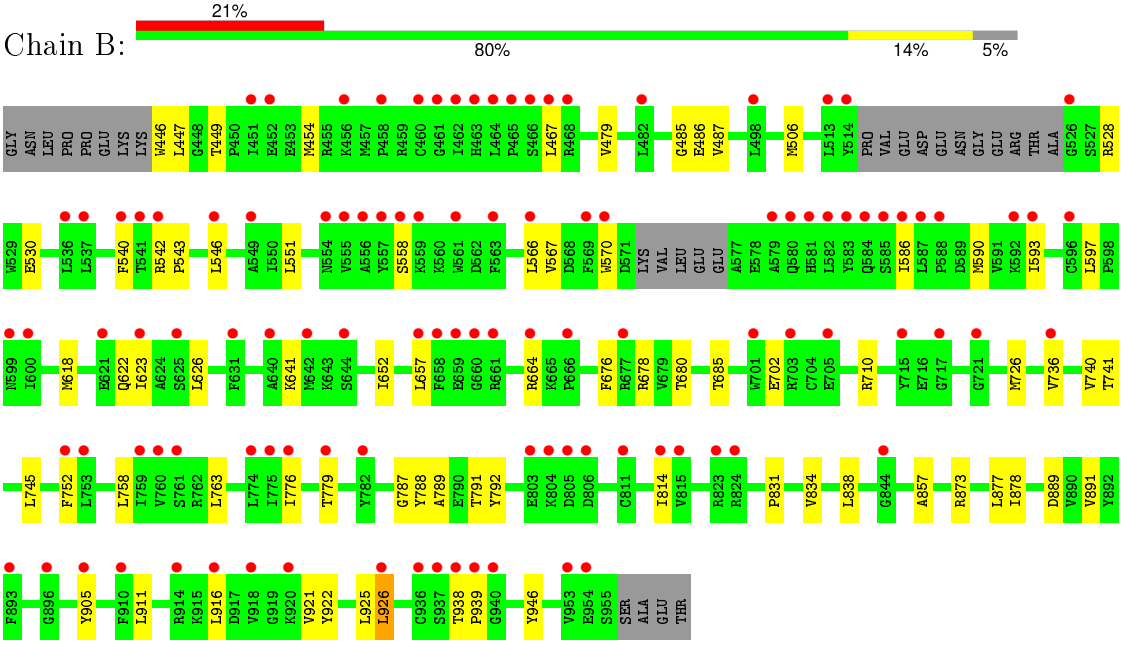
- Molecule 1: Poly(ADP-ribose) glycohydrolase

Chain A:



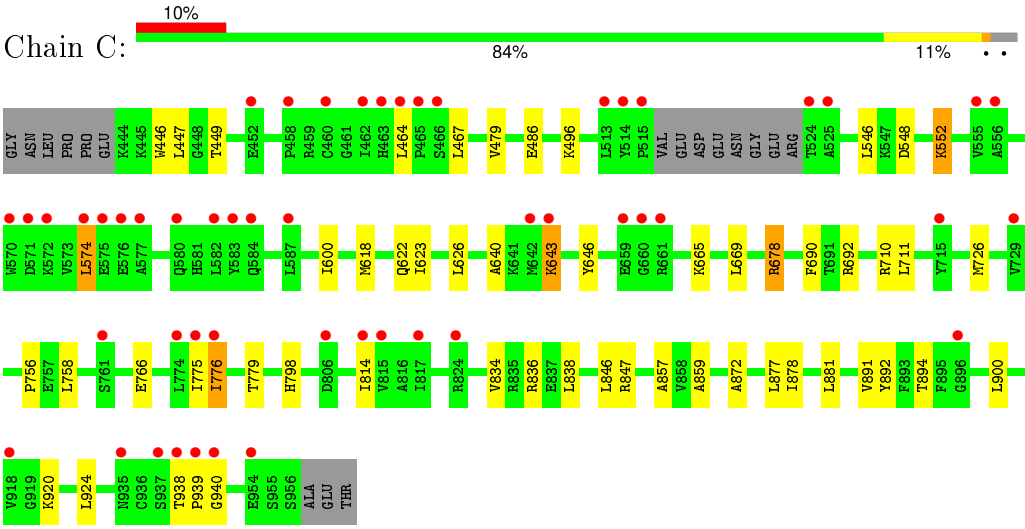
- Molecule 1: Poly(ADP-ribose) glycohydrolase

Chain B:



- Molecule 1: Poly(ADP-ribose) glycohydrolase

Chain C:


10%
84%
11%
GLY ASN LEU PRO PRO GLU K444 K445 W446 L447 G448 T449 E452 P458 R459 C460 G461 I462 H463 L464 P465 S466 L467 V479 E486 K496 L513 Y514 P515 VAL GLU ASP GLU ASN GLY GLU ARG T524 A525 L546 K547 D548 K552 V555 A556 K559 V567 D568 F569
W570 D571 K572 V573 L574 E575 E576 A577 Q580 H581 L582 Y583 Q584 L587 I600 M618 Q622 I623 L626 A640 K641 M642 K643 Y646 E659 G660 R661 K665 L669 R678 F690 T691 R692 R710 L711 Y715 M726 V729 V746 Q747 F752
P756 E757 L758 S761 E766 L774 I775 I776 T779 H798 D806 I814 V815 A816 I817 R824 V834 R835 R836 E837 L838 L846 R847 A857 Y858 A859 A872 L877 I878 L881 V891 Y892 F893 T894 F895 G896 L900 L911 K915 L916 D917
V918 G919 K920 L924 N935 C936 S937 T938 P939 G940 E954 S955 S956 ALA GLU THR

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	3096 reflections (5.33%)	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 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	11 of 62008 reflections (0.018%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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

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

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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

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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:C:618:MSE:HE2	1:C:623:ILE:HG12	1.84	0.59
1:C:618:MSE:HE1	1:C:626:LEU:CD1	2.31	0.59
1:B:726:MSE:HE3	1:B:857:ALA:CB	2.33	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:569:PHE:CE1	1:C:574:LEU:HD13	2.39	0.57
1:C:467:LEU:O	1:C:479:VAL:HG11	2.04	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:C:752:PHE:O	1:C:756:PRO:HA	2.10	0.52
1:B:454:MSE:HE1	1:B:889:ASP:HB3	1.92	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:B:618:MSE:HE2	1:B:623:ILE:CG1	2.40	0.51
1:A:643:LYS:HD3	1:A:646:TYR:HB2	1.93	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

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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:C:746:VAL:CG1	1:C:747:GLN:N	2.80	0.44
1:B:922:TYR:CE1	1:B:926:LEU:HD21	2.52	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:C:834:VAL:O	1:C:838:LEU:HD23	2.17	0.43
1:C:678:ARG:NH2	1:C:798:HIS:O	2.51	0.43
1:A:449:THR:HB	1:A:454:MSE:HE2	1.99	0.43
1:B:487:VAL:HG22	1:B:685:THR:HG22	1.99	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:516:VAL:O	1:A:516:VAL:HG12	2.17	0.43
1:B:873:ARG:HB3	1:B:946:TYR:CE1	2.54	0.43
1:A:569:PHE:CZ	1:A:574:LEU:HD11	2.54	0.43
1:B:447:LEU:HD22	1:B:905:TYR:CD2	2.53	0.43
1:B:726:MSE:HE1	1:B:891:VAL:CB	2.49	0.43
1:A:506:MSE:HE1	1:A:597:LEU:HD11	2.01	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

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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:C:775:ILE:HD13	1:C:847:ARG:CZ	2.52	0.40
1:B:938:THR:HG23	1:B:939:PRO:HD2	2.03	0.40
1:C:911:LEU:CD2	1:C:916:LEU:HD12	2.47	0.40
1:B:454:MSE:CE	1:B:889:ASP:HB3	2.51	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 (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	501/522 (96%)	487 (97%)	13 (3%)	1 (0%)	52	75
1	B	488/522 (94%)	459 (94%)	28 (6%)	1 (0%)	52	75
1	C	501/522 (96%)	485 (97%)	15 (3%)	1 (0%)	52	75
All	All	1490/1566 (95%)	1431 (96%)	56 (4%)	3 (0%)	52	75

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%)	55	82
1	B	435/450 (97%)	424 (98%)	11 (2%)	55	82
1	C	445/450 (99%)	432 (97%)	13 (3%)	50	77
All	All	1325/1350 (98%)	1290 (97%)	35 (3%)	54	81

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

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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

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 carbohydrates in this entry.

5.6 Ligand geometry

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	-	30,38,38	0.85	1 (3%)	32,58,58	2.18	3 (9%)
2	A1R	B	1001	-	30,38,38	0.79	1 (3%)	32,58,58	2.20	3 (9%)
2	A1R	C	1001	-	30,38,38	0.77	0	32,58,58	2.01	5 (15%)

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'	2.37	1.44	1.41
2	B	1001	A1R	O4'-C1'	2.38	1.44	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	A1R	N3-C2-N1	-10.76	120.66	128.89
2	B	1001	A1R	N3-C2-N1	-10.32	120.99	128.89
2	C	1001	A1R	N3-C2-N1	-9.67	121.49	128.89
2	B	1001	A1R	PB-O3A-PA	-4.62	119.76	132.73
2	A	1001	A1R	C4-C5-N7	-2.74	106.96	109.48
2	C	1001	A1R	PB-O3A-PA	-2.70	125.14	132.73
2	A	1001	A1R	PB-O3A-PA	-2.41	125.97	132.73
2	C	1001	A1R	C1'-N9-C4	-2.39	123.34	126.94
2	C	1001	A1R	O3A-PA-O5'	-2.28	96.88	102.94
2	C	1001	A1R	C4-C5-N7	-2.28	107.38	109.48
2	B	1001	A1R	O3A-PA-O5'	-2.04	97.54	102.94

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

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	496/522 (95%)	0.70	73 (14%) 3 3	27, 53, 101, 137	0
1	B	485/522 (92%)	1.24	109 (22%) 1 1	40, 106, 225, 331	0
1	C	496/522 (95%)	0.49	53 (10%) 8 8	26, 51, 92, 136	0
All	All	1477/1566 (94%)	0.81	235 (15%) 3 2	26, 62, 173, 331	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	582	LEU	17.7
1	C	939	PRO	13.4
1	A	939	PRO	12.7
1	B	658	PHE	12.1
1	B	555	VAL	11.7
1	B	939	PRO	9.9
1	A	515	PRO	9.6
1	B	583	TYR	7.8
1	C	582	LEU	7.8
1	A	582	LEU	7.3
1	A	577	ALA	7.3
1	B	916	LEU	7.1
1	B	466	SER	6.8
1	B	580	GLN	6.8
1	A	516	VAL	6.5
1	A	578	GLU	6.4
1	B	540	PHE	6.2
1	B	584	GLN	6.2
1	A	546	LEU	6.1
1	A	463	HIS	5.8
1	A	566	LEU	5.7
1	C	580	GLN	5.6
1	C	938	THR	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	905	TYR	5.4
1	B	806	ASP	5.4
1	B	570	TRP	5.3
1	A	580	GLN	5.3
1	C	576	GLU	5.3
1	B	463	HIS	5.2
1	B	587	LEU	5.1
1	B	660	GLY	5.1
1	A	575	GLU	5.1
1	B	938	THR	5.1
1	B	566	LEU	5.1
1	B	513	LEU	5.0
1	B	918	VAL	4.9
1	B	705	GLU	4.7
1	A	803	GLU	4.6
1	B	556	ALA	4.6
1	A	658	PHE	4.6
1	B	554	ASN	4.6
1	B	586	ILE	4.6
1	B	561	TRP	4.6
1	B	659	GLU	4.6
1	C	660	GLY	4.5
1	A	940	GLY	4.4
1	B	644	SER	4.3
1	B	579	ALA	4.3
1	B	588	PRO	4.3
1	A	574	LEU	4.2
1	A	524	THR	4.2
1	B	557	TYR	4.1
1	A	464	LEU	4.1
1	C	940	GLY	4.1
1	B	458	PRO	4.1
1	B	677	ARG	4.1
1	A	938	THR	4.0
1	A	572	LYS	3.9
1	B	467	LEU	3.9
1	B	814	ILE	3.9
1	B	526	GLY	3.9
1	C	643	LYS	3.8
1	A	480	ASP	3.8
1	B	805	ASP	3.8
1	A	550	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	759	ILE	3.8
1	A	462	ILE	3.7
1	C	513	LEU	3.7
1	A	555	VAL	3.7
1	C	584	GLN	3.7
1	B	563	PHE	3.7
1	B	631	PHE	3.7
1	C	937	SER	3.7
1	A	570	TRP	3.6
1	B	803	GLU	3.6
1	C	918	VAL	3.6
1	C	463	HIS	3.6
1	B	926	LEU	3.6
1	B	936	CYS	3.6
1	C	556	ALA	3.6
1	A	806	ASP	3.6
1	C	572	LYS	3.5
1	A	561	TRP	3.5
1	C	570	TRP	3.5
1	C	583	TYR	3.5
1	A	583	TYR	3.5
1	A	642	MET	3.5
1	B	774	LEU	3.5
1	B	717	GLY	3.5
1	B	896	GLY	3.5
1	A	483	ARG	3.4
1	A	643	LYS	3.4
1	B	661	ARG	3.4
1	C	515	PRO	3.4
1	B	666	PRO	3.4
1	B	546	LEU	3.4
1	C	464	LEU	3.4
1	A	776	ILE	3.4
1	B	920	LYS	3.3
1	B	460	CYS	3.3
1	C	555	VAL	3.3
1	A	644	SER	3.3
1	B	452	GLU	3.3
1	B	464	LEU	3.3
1	A	585	SER	3.3
1	A	805	ASP	3.2
1	A	915	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	542	ARG	3.2
1	B	514	TYR	3.2
1	A	576	GLU	3.2
1	B	482	LEU	3.1
1	B	779	THR	3.1
1	A	910	PHE	3.1
1	A	514	TYR	3.1
1	A	581	HIS	3.1
1	A	935	ASN	3.1
1	B	451	ILE	3.0
1	C	577	ALA	3.0
1	C	575	GLU	3.0
1	B	954	GLU	3.0
1	A	584	GLN	2.9
1	B	592	LYS	2.9
1	A	539	LYS	2.9
1	A	774	LEU	2.9
1	A	558	SER	2.9
1	A	814	ILE	2.9
1	A	598	PRO	2.9
1	C	571	ASP	2.9
1	A	937	SER	2.9
1	C	661	ARG	2.9
1	A	471	ALA	2.8
1	A	914	ARG	2.8
1	A	549	ALA	2.8
1	C	458	PRO	2.8
1	A	554	ASN	2.8
1	B	537	LEU	2.8
1	B	815	VAL	2.8
1	B	776	ILE	2.8
1	B	558	SER	2.8
1	B	462	ILE	2.7
1	C	659	GLU	2.7
1	B	721	GLY	2.7
1	B	715	TYR	2.7
1	C	642	MET	2.7
1	A	594	ALA	2.7
1	B	585	SER	2.7
1	B	953	VAL	2.7
1	B	640	ALA	2.7
1	B	596	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	774	LEU	2.7
1	C	935	ASN	2.7
1	A	525	ALA	2.7
1	B	824	ARG	2.7
1	A	661	ARG	2.6
1	B	642	MET	2.6
1	B	752	PHE	2.6
1	B	468	ARG	2.6
1	C	460	CYS	2.6
1	B	657	LEU	2.6
1	B	465	PRO	2.6
1	B	753	LEU	2.6
1	B	937	SER	2.6
1	C	775	ILE	2.6
1	C	715	TYR	2.6
1	B	599	ASN	2.5
1	C	574	LEU	2.5
1	A	641	LYS	2.5
1	A	657	LEU	2.5
1	B	761	SER	2.5
1	A	484	ALA	2.5
1	C	729	VAL	2.5
1	C	525	ALA	2.5
1	A	465	PRO	2.5
1	B	559	LYS	2.4
1	C	462	ILE	2.4
1	B	910	PHE	2.4
1	C	916	LEU	2.4
1	A	573	VAL	2.4
1	B	541	THR	2.4
1	A	482	LEU	2.4
1	C	824	ARG	2.4
1	B	593	ILE	2.4
1	A	569	PHE	2.4
1	C	954	GLU	2.4
1	A	775	ILE	2.3
1	B	600	ILE	2.3
1	C	814	ILE	2.3
1	C	452	GLU	2.3
1	B	760	VAL	2.3
1	C	815	VAL	2.3
1	B	823	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	806	ASP	2.3
1	B	775	ILE	2.3
1	B	456	LYS	2.3
1	B	581	HIS	2.3
1	B	940	GLY	2.3
1	B	736	VAL	2.3
1	B	664	ARG	2.3
1	A	807	TRP	2.2
1	B	461	GLY	2.2
1	B	782	TYR	2.2
1	A	563	PHE	2.2
1	A	595	LEU	2.2
1	C	524	THR	2.2
1	C	817	ILE	2.2
1	A	626	LEU	2.2
1	A	541	THR	2.2
1	B	623	ILE	2.1
1	B	759	ILE	2.1
1	B	811	CYS	2.1
1	B	893	PHE	2.1
1	C	465	PRO	2.1
1	B	914	ARG	2.1
1	B	844	GLY	2.1
1	B	703	ARG	2.1
1	B	701	TRP	2.1
1	B	549	ALA	2.1
1	C	567	VAL	2.1
1	B	804	LYS	2.1
1	C	776	ILE	2.1
1	B	536	LEU	2.1
1	B	625	SER	2.1
1	A	571	ASP	2.1
1	A	760	VAL	2.1
1	A	756	PRO	2.1
1	B	498	LEU	2.1
1	C	587	LEU	2.1
1	C	761	SER	2.1
1	B	621	GLU	2.1
1	A	911	LEU	2.1
1	B	569	PHE	2.1
1	C	466	SER	2.1
1	A	513	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	514	TYR	2.0
1	C	896	GLY	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, 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	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.