WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:38 PM GMT

PDB ID	:	3UEL
Title	:	Crystal structure of the catalytic domain of rat poly (ADP-ribose) glycohydrolase bound to ADP-HPD
Authors	:	Kim, I.K.; Kiefer, J.R.; Stegemann, R.A.; Classen, S.; Tainer, J.A.; Ellenberger, T.
Deposited on	:	2011-10-30
Resolution	:	3.00 Å(reported)

The following versions of software and data (see references ⓘ) 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 ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	Percentile Ranks	Value
Rfree		0.278
Clashscore		10
Ramachandran outliers		1.2%
Sidechain outliers		5.5%
RSRZ outliers		2.9%

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
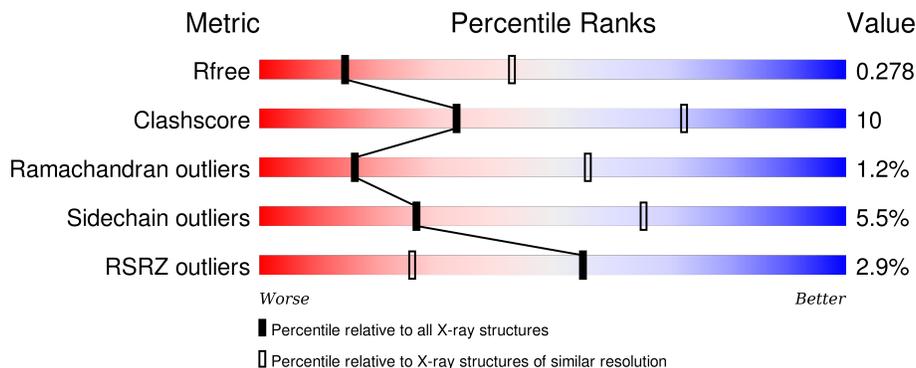
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	588	% 65% 23% · 11%
1	B	588	2% 66% 21% · 11%
1	C	588	5% 72% 15% · 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11952 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	521	Total	C	N	O	S	0	0	0
			4048	2590	692	743	23			
1	B	521	Total	C	N	O	S	0	0	0
			4027	2574	683	747	23			
1	C	521	Total	C	N	O	S	0	0	0
			3772	2386	647	719	20			

- 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: $C_{15}H_{24}N_6O_{12}P_2$).

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		

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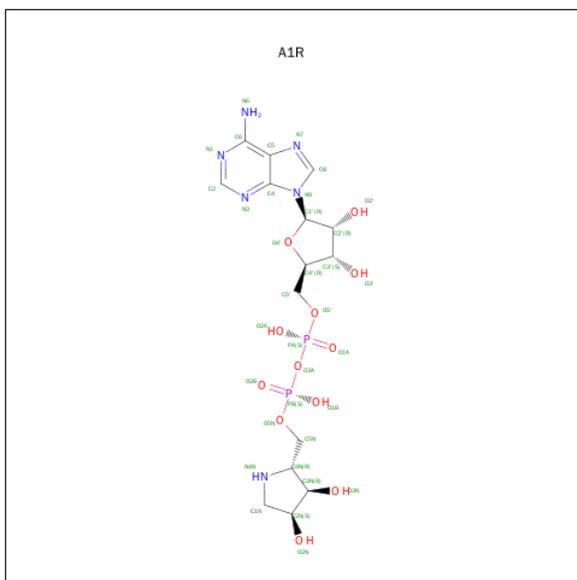
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	35	15	6	12	2	0	0

3 Residue-property plots ⓘ

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.
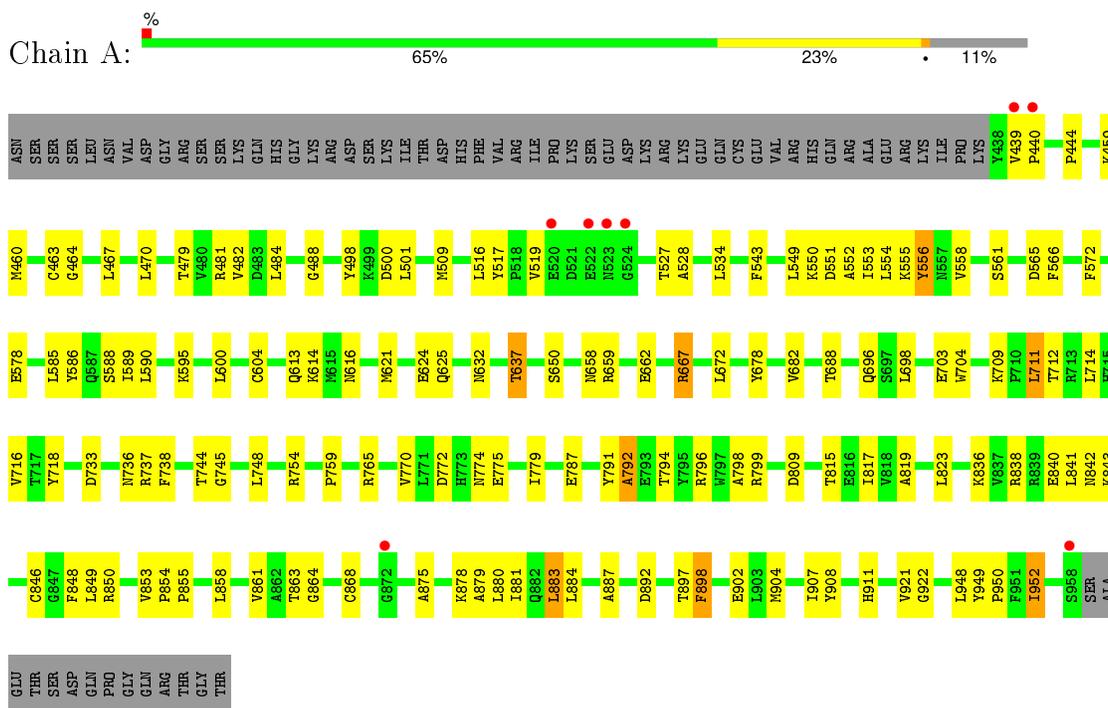
• Molecule 1: Poly(ADP-ribose) glycohydrolase

• Molecule 1: Poly(ADP-ribose) glycohydrolase

R850 V853 P854 P855 E856 V861 A862 T863 G864 N865 C868 A875 R876 L877 L880 I881 F898 E902 T912 E916 R917 K918 Y932 C936 R937 D938 S941 P942 G943 L948 I952 S958 SER ALA GLU THR SER ASP GLN PRO GLY GLN ARG THR GLY

THR

● Molecule 1: Poly(ADP-ribose) glycohydrolase

Chain C:

5%

72%   15%   •   11%

ASN SER SER SER LEU ASN VAL ASP GLY ARG SER SER LYS GLN HIS GLY LYS ARG ASP SER LYS ILE THR ASP HIS PHE VAL ARG ILE PRO LYS SER GLU ASP LYS ARG LYS GLU GLN CYS GLU VAL ARG HIS GLN ARG ALA GLU ARG LYS ILE PRO LYS Y438 V439 P440 P441 N442 L443 P444

P445 D446 K447 C463 L470 T479 V482 G488 Y498 K499 D500 L501 M509 L516 Y517 P518 V519 E520 D521 E522 N523 T527 A528 E533 F543 P546 L549 I553 L554 K555 Y556 N557 V558 S561 D565 F566 F572 W573 L577 E578 E581

L585 Y586 Q587 S588 I589 L590 P591 L600 C604 N616 Q623 E624 Q625 L630 A631 N632 A633 T637 S650 N658 E662 R667 K668 K671 L672 Y678 F679 V682 T683 T688 G689 R695 Q696 P702 E703 W704 D733 R737 G745 A746

G747 L748 R754 P759 E769 D772 H773 N774 E787 Y791 A792 E793 T794 A798 R799 D809 W810 Q811 I817 V818 A819 L823 K836 V837 R838 L841 N842 K843 G852 V853 P854 T863 G864 N865 C868 A875 I881 Y895 T915 Y932

E935 C936 R937 D938 C939 S940 S941 P942 G943 P944 D945 T946 A956 E957 S958 SER ALA GLU THR SER ASP GLN PRO GLY GLN ARG THR GLY THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	130.77Å 195.99Å 163.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.47 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.9 (30.00-3.00) 90.0 (29.47-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.27 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.245 , 0.274 0.248 , 0.278	Depositor DCC
R_{free} test set	1945 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	78.7	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 58.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Outliers	13 of 37891 reflections (0.034%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	11952	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.81	4/4154 (0.1%)	0.74	5/5656 (0.1%)
1	B	0.66	4/4133 (0.1%)	0.73	0/5638
1	C	0.64	4/3867 (0.1%)	0.66	0/5299
All	All	0.71	12/12154 (0.1%)	0.71	5/16593 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	566	PHE	CG-CD1	-19.54	1.09	1.38
1	A	566	PHE	CG-CD2	-18.97	1.10	1.38
1	A	566	PHE	CE2-CZ	-13.15	1.12	1.37
1	A	566	PHE	CE1-CZ	-12.36	1.13	1.37
1	C	566	PHE	CG-CD2	-10.19	1.23	1.38
1	B	566	PHE	CG-CD1	-10.17	1.23	1.38
1	C	566	PHE	CG-CD1	-10.11	1.23	1.38
1	B	566	PHE	CG-CD2	-9.98	1.23	1.38
1	C	566	PHE	CE2-CZ	-6.64	1.24	1.37
1	C	566	PHE	CE1-CZ	-6.60	1.24	1.37
1	B	566	PHE	CE1-CZ	-6.48	1.25	1.37
1	B	566	PHE	CE2-CZ	-6.47	1.25	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
1	A	566	PHE	CE1-CZ-CE2	-7.38	106.71	120.00
1	A	566	PHE	CD1-CG-CD2	-6.37	110.02	118.30
1	A	566	PHE	CB-CG-CD1	6.34	125.23	120.80
1	A	566	PHE	CB-CG-CD2	5.62	124.73	120.80
1	A	566	PHE	CD1-CE1-CZ	5.55	126.76	120.10

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	4048	0	3858	89	0
1	B	4027	0	3798	87	0
1	C	3772	0	3311	59	0
2	A	35	0	22	3	0
2	B	35	0	22	4	0
2	C	35	0	22	0	0
All	All	11952	0	11033	235	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 10.

All (235) 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:A:632:ASN:OD1	1:A:637:THR:HG21	1.70	0.90
1:A:509:MET:HE3	1:A:600:LEU:HD21	1.53	0.88
1:B:948:LEU:O	1:B:952:ILE:HG23	1.79	0.80
1:A:509:MET:CE	1:A:600:LEU:HD21	2.13	0.79
1:B:470:LEU:O	1:B:482:VAL:HG21	1.83	0.79
1:A:898:PHE:HD2	2:A:1001:A1R:C4	1.96	0.79
1:A:879:ALA:HB1	1:A:907:ILE:CD1	2.13	0.79
1:C:572:PHE:CD2	1:C:672:LEU:HD12	2.22	0.75
1:B:952:ILE:C	1:B:952:ILE:HD12	2.08	0.74
1:B:632:ASN:OD1	1:B:637:THR:HG21	1.88	0.73
1:C:632:ASN:OD1	1:C:637:THR:HG21	1.89	0.72
1:B:509:MET:HE1	1:B:600:LEU:HD21	1.71	0.72
1:B:754:ARG:NH1	1:B:817:ILE:CD1	2.53	0.72
1:C:509:MET:HE3	1:C:600:LEU:HD21	1.72	0.71
1:C:500:ASP:O	1:C:501:LEU:HD23	1.90	0.71
1:B:470:LEU:HD13	1:B:810:TRP:CD2	2.27	0.69
1:A:709:LYS:O	1:A:921:VAL:HG23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:LEU:O	1:C:482:VAL:HG21	1.92	0.69
1:A:838:ARG:O	1:A:842:ASN:ND2	2.27	0.68
1:B:865:ASN:HD22	2:B:1001:A1R:H1'	1.60	0.67
1:A:534:LEU:HD12	1:A:556:TYR:HB3	1.77	0.66
1:A:949:TYR:HA	1:A:952:ILE:HG23	1.78	0.65
1:C:585:LEU:HD11	1:C:590:LEU:HD21	1.78	0.65
1:B:517:TYR:CZ	1:B:534:LEU:HD12	2.30	0.65
1:C:754:ARG:NH1	1:C:817:ILE:CD1	2.59	0.64
1:B:509:MET:CE	1:B:600:LEU:HD21	2.27	0.64
1:A:554:LEU:HD22	1:A:561:SER:HA	1.79	0.64
1:B:898:PHE:HD2	2:B:1001:A1R:C4	2.10	0.64
1:C:585:LEU:HG	1:C:590:LEU:HD23	1.79	0.63
1:A:879:ALA:CB	1:A:907:ILE:CD1	2.76	0.63
1:C:585:LEU:CD1	1:C:590:LEU:CD2	2.77	0.63
1:B:856:GLU:N	1:B:856:GLU:OE1	2.31	0.62
1:A:879:ALA:CB	1:A:907:ILE:HD11	2.28	0.62
1:B:554:LEU:HD22	1:B:561:SER:HA	1.82	0.61
1:C:585:LEU:HD11	1:C:590:LEU:CD2	2.30	0.61
1:B:500:ASP:O	1:B:501:LEU:HD23	2.01	0.61
1:A:543:PHE:O	1:A:586:TYR:HB2	2.01	0.61
1:B:572:PHE:CE1	1:B:577:LEU:HG	2.36	0.61
1:B:543:PHE:O	1:B:586:TYR:HB2	2.02	0.60
1:A:549:LEU:O	1:A:553:ILE:HD12	2.01	0.60
1:A:884:LEU:HD22	1:A:921:VAL:HG13	1.82	0.60
1:A:488:GLY:O	1:A:688:THR:HG21	2.01	0.59
1:C:585:LEU:HG	1:C:590:LEU:CD2	2.33	0.59
1:C:554:LEU:HD22	1:C:561:SER:HA	1.85	0.59
1:B:850:ARG:O	1:B:853:VAL:HG13	2.03	0.58
1:B:868:CYS:SG	1:B:875:ALA:HA	2.43	0.58
1:B:516:LEU:HD13	1:B:528:ALA:HB1	1.85	0.58
1:C:863:THR:OG1	1:C:864:GLY:N	2.37	0.58
1:C:838:ARG:O	1:C:842:ASN:ND2	2.37	0.57
1:B:863:THR:OG1	1:B:864:GLY:N	2.36	0.57
1:A:500:ASP:O	1:A:501:LEU:HD23	2.03	0.57
1:C:549:LEU:O	1:C:553:ILE:HD12	2.05	0.57
1:B:516:LEU:HD13	1:B:528:ALA:CB	2.34	0.57
1:B:485:LEU:CD1	1:B:811:GLN:HE21	2.17	0.56
1:B:439:VAL:HG22	1:B:440:PRO:O	2.05	0.56
1:C:543:PHE:O	1:C:586:TYR:HB2	2.05	0.56
1:A:585:LEU:HD12	1:A:589:ILE:HD12	1.86	0.56
1:A:470:LEU:O	1:A:482:VAL:HG21	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:ARG:NH1	1:A:817:ILE:CD1	2.69	0.56
1:C:509:MET:CE	1:C:600:LEU:HD21	2.34	0.55
1:B:736:ASN:HB2	2:B:1001:A1R:O3N	2.06	0.55
1:A:712:THR:HB	1:A:892:ASP:OD1	2.07	0.54
1:B:517:TYR:OH	1:B:534:LEU:HD12	2.08	0.54
1:C:546:PRO:HG3	1:C:573:TRP:CG	2.43	0.53
1:A:517:TYR:CE2	1:A:519:VAL:HG22	2.44	0.53
1:A:572:PHE:C	1:A:572:PHE:CD1	2.82	0.53
1:B:764:SER:HB2	1:B:777:LEU:HD21	1.89	0.53
1:B:698:LEU:HD12	1:B:846:CYS:HA	1.91	0.53
1:B:948:LEU:O	1:B:952:ILE:CG2	2.54	0.53
1:A:948:LEU:O	1:A:952:ILE:HG22	2.09	0.53
1:B:845:TYR:OH	1:B:849:LEU:HD22	2.08	0.53
1:C:517:TYR:CE2	1:C:519:VAL:HG22	2.44	0.52
1:A:868:CYS:SG	1:A:875:ALA:HA	2.50	0.52
1:A:616:ASN:ND2	1:A:696:GLN:HA	2.26	0.51
1:A:714:LEU:HB2	1:A:911:HIS:CE1	2.45	0.51
1:B:678:TYR:HB2	1:B:759:PRO:HG2	1.92	0.51
1:C:488:GLY:O	1:C:688:THR:HG21	2.10	0.51
1:A:853:VAL:HG11	1:A:858:LEU:CD2	2.41	0.51
1:A:467:LEU:HD23	1:A:809:ASP:OD2	2.10	0.51
1:C:516:LEU:HD13	1:C:528:ALA:CB	2.41	0.51
1:A:898:PHE:CD2	2:A:1001:A1R:C4	2.85	0.50
1:A:863:THR:OG1	1:A:864:GLY:N	2.44	0.50
1:C:616:ASN:ND2	1:C:696:GLN:HA	2.25	0.50
1:B:572:PHE:CD1	1:B:572:PHE:C	2.85	0.50
1:C:678:TYR:HB2	1:C:759:PRO:HG2	1.94	0.50
1:B:546:PRO:HA	1:B:573:TRP:CZ3	2.47	0.50
1:C:516:LEU:HD13	1:C:528:ALA:HB1	1.93	0.49
1:B:791:TYR:O	1:B:792:ALA:C	2.51	0.49
1:B:455:GLU:CD	1:B:455:GLU:H	2.15	0.49
1:B:488:GLY:O	1:B:688:THR:HG21	2.12	0.49
1:A:841:LEU:CD2	1:A:881:ILE:HG23	2.43	0.49
1:A:704:TRP:O	1:A:922:GLY:HA2	2.13	0.49
1:A:481:ARG:NH2	1:A:484:LEU:HD11	2.27	0.48
1:A:733:ASP:HB3	1:A:819:ALA:HA	1.95	0.48
1:C:865:ASN:HA	1:C:895:TYR:OH	2.13	0.48
1:B:549:LEU:O	1:B:553:ILE:HD12	2.14	0.48
1:C:585:LEU:CD1	1:C:590:LEU:HD22	2.42	0.48
1:A:841:LEU:HG	1:A:881:ILE:HG23	1.95	0.48
1:A:467:LEU:HD23	1:A:809:ASP:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:LEU:HD12	1:A:846:CYS:HA	1.94	0.48
1:B:787:GLU:O	1:B:798:ALA:HB3	2.11	0.48
1:C:572:PHE:CG	1:C:672:LEU:HD12	2.49	0.48
1:A:481:ARG:CZ	1:A:484:LEU:HD11	2.44	0.48
1:A:678:TYR:HB2	1:A:759:PRO:HG2	1.96	0.48
1:A:460:MET:SD	1:A:464:GLY:HA3	2.53	0.48
1:A:516:LEU:HD13	1:A:528:ALA:HB1	1.95	0.48
1:C:841:LEU:HG	1:C:881:ILE:HG23	1.95	0.48
1:A:516:LEU:HD13	1:A:528:ALA:CB	2.43	0.48
1:B:733:ASP:HB3	1:B:819:ALA:HA	1.95	0.48
1:A:549:LEU:O	1:A:552:ALA:HB3	2.14	0.48
1:A:711:LEU:CD2	1:A:711:LEU:N	2.77	0.47
1:B:841:LEU:HG	1:B:881:ILE:HG23	1.95	0.47
1:B:616:ASN:ND2	1:B:696:GLN:HA	2.29	0.47
1:B:845:TYR:CZ	1:B:849:LEU:HD22	2.48	0.47
1:C:774:ASN:H	1:C:774:ASN:HD22	1.61	0.47
1:C:585:LEU:CG	1:C:590:LEU:CD2	2.93	0.47
1:B:577:LEU:HD22	1:B:581:GLU:OE1	2.14	0.47
1:B:838:ARG:O	1:B:842:ASN:ND2	2.48	0.47
1:B:774:ASN:HD22	1:B:774:ASN:H	1.62	0.47
1:C:733:ASP:HB3	1:C:819:ALA:HA	1.97	0.47
1:A:848:PHE:CE1	1:A:861:VAL:HG11	2.50	0.46
1:B:829:LEU:O	1:B:831:GLN:N	2.48	0.46
1:B:622:SER:HA	1:B:690:LEU:HD23	1.97	0.46
1:C:577:LEU:HD22	1:C:581:GLU:CB	2.44	0.46
1:A:791:TYR:O	1:A:792:ALA:C	2.53	0.46
1:C:772:ASP:O	1:C:843:LYS:NZ	2.49	0.46
1:B:841:LEU:CD2	1:B:881:ILE:HG23	2.45	0.46
1:C:572:PHE:CD1	1:C:572:PHE:C	2.88	0.46
1:B:565:ASP:HB3	1:B:662:GLU:HB2	1.97	0.46
1:B:754:ARG:NH1	1:B:817:ILE:HD11	2.29	0.46
1:A:550:LYS:O	1:A:551:ASP:C	2.54	0.45
1:B:477:THR:HB	1:B:619:VAL:HG13	1.99	0.45
1:C:565:ASP:HB3	1:C:662:GLU:HB2	1.99	0.45
1:B:577:LEU:HD13	1:B:581:GLU:HB3	1.98	0.45
1:A:551:ASP:O	1:A:555:LYS:HG3	2.15	0.45
1:A:572:PHE:CE2	1:A:672:LEU:HB2	2.50	0.45
1:A:823:LEU:HD13	1:A:836:LYS:HD2	1.97	0.45
1:B:768:THR:HG21	1:B:777:LEU:HD22	1.97	0.45
1:A:565:ASP:HB3	1:A:662:GLU:HB2	1.97	0.45
1:C:787:GLU:O	1:C:798:ALA:HB3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:841:LEU:CD2	1:C:881:ILE:HG23	2.47	0.45
1:A:459:LYS:C	1:A:463:CYS:SG	2.95	0.45
1:A:884:LEU:O	1:A:887:ALA:HB3	2.16	0.45
1:A:498:TYR:CE2	1:A:500:ASP:HB2	2.52	0.45
1:C:577:LEU:HD22	1:C:581:GLU:HB3	1.98	0.45
1:A:678:TYR:O	1:A:682:VAL:HG22	2.17	0.45
1:B:479:THR:HB	1:B:625:GLN:HE22	1.82	0.45
1:A:948:LEU:O	1:A:952:ILE:CG2	2.66	0.44
1:B:917:ARG:HB2	1:B:917:ARG:HH11	1.82	0.44
1:B:485:LEU:HD11	1:B:811:GLN:HE21	1.80	0.44
1:B:678:TYR:O	1:B:682:VAL:HG22	2.17	0.44
1:A:879:ALA:HB2	1:A:907:ILE:HD11	1.98	0.44
1:A:744:THR:HG23	1:A:765:ARG:NH2	2.33	0.44
1:B:848:PHE:CE1	1:B:861:VAL:HG11	2.53	0.44
1:C:549:LEU:HD12	1:C:553:ILE:HD12	1.99	0.44
1:C:868:CYS:SG	1:C:875:ALA:HA	2.57	0.44
1:B:711:LEU:N	1:B:711:LEU:HD23	2.33	0.44
1:B:517:TYR:CE2	1:B:519:VAL:HG22	2.53	0.44
1:A:439:VAL:HA	1:A:440:PRO:HD3	1.66	0.44
1:A:883:LEU:HD11	1:A:911:HIS:ND1	2.33	0.43
1:B:807:LYS:HD3	1:B:811:GLN:HB2	2.00	0.43
1:B:932:TYR:O	1:B:936:CYS:N	2.47	0.43
1:A:712:THR:HG23	1:A:887:ALA:HA	2.01	0.43
1:C:623:GLN:OE1	1:C:689:GLY:HA3	2.18	0.43
1:C:498:TYR:CE2	1:C:500:ASP:HB2	2.54	0.43
1:B:549:LEU:O	1:B:552:ALA:HB3	2.19	0.43
1:B:706:ARG:HG2	1:B:706:ARG:O	2.17	0.43
1:A:787:GLU:O	1:A:798:ALA:HB3	2.19	0.43
1:A:479:THR:OG1	1:A:621:MET:HB3	2.19	0.43
1:B:714:LEU:HD12	1:B:715:HIS:N	2.34	0.43
1:A:949:TYR:O	1:A:950:PRO:C	2.57	0.43
1:B:498:TYR:CE2	1:B:500:ASP:HB2	2.53	0.43
1:A:738:PHE:CE1	1:A:770:VAL:HB	2.53	0.43
1:A:849:LEU:HD12	1:A:850:ARG:H	1.83	0.43
1:B:937:ARG:C	1:B:938:ASP:OD1	2.56	0.43
1:B:623:GLN:OE1	1:B:689:GLY:HA3	2.19	0.43
1:C:577:LEU:HD22	1:C:581:GLU:CD	2.39	0.42
1:C:479:THR:HB	1:C:625:GLN:HE22	1.82	0.42
1:A:718:TYR:HA	1:A:897:THR:OG1	2.18	0.42
1:C:440:PRO:HA	1:C:441:PRO:HD3	1.92	0.42
1:C:823:LEU:HD13	1:C:836:LYS:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:ILE:N	1:A:779:ILE:HD12	2.34	0.42
1:A:659:ARG:O	1:A:662:GLU:HG2	2.20	0.42
1:A:716:VAL:HG22	1:A:904:MET:HG3	2.01	0.42
1:A:479:THR:HB	1:A:625:GLN:HE22	1.84	0.42
1:A:880:LEU:O	1:A:881:ILE:C	2.58	0.42
1:B:714:LEU:HD12	1:B:715:HIS:H	1.85	0.42
1:B:590:LEU:HB2	1:B:591:PRO:HD3	2.02	0.42
1:B:701:PHE:CG	1:B:842:ASN:OD1	2.73	0.42
1:B:898:PHE:HD2	2:B:1001:A1R:C5	2.33	0.42
1:C:590:LEU:HB2	1:C:591:PRO:HD3	2.02	0.42
1:A:696:GLN:O	1:A:775:GLU:HA	2.20	0.42
1:C:678:TYR:O	1:C:682:VAL:HG22	2.19	0.42
1:B:667:ARG:HB3	1:B:748:LEU:HD12	2.02	0.42
1:B:668:LYS:O	1:B:671:LYS:HB2	2.19	0.42
1:C:668:LYS:O	1:C:671:LYS:HB2	2.19	0.42
1:A:632:ASN:CG	1:A:637:THR:HG21	2.38	0.41
1:B:854:PRO:HA	1:B:855:PRO:HD2	1.77	0.41
1:B:698:LEU:CD1	1:B:846:CYS:HA	2.49	0.41
1:C:604:CYS:HA	1:C:625:GLN:HE21	1.85	0.41
1:B:839:ARG:NH1	1:B:840:GLU:OE1	2.45	0.41
1:C:791:TYR:O	1:C:792:ALA:C	2.57	0.41
1:A:772:ASP:O	1:A:843:LYS:NZ	2.51	0.41
1:C:572:PHE:CE1	1:C:577:LEU:HG	2.55	0.41
1:B:675:LEU:O	1:B:678:TYR:HB3	2.21	0.41
1:B:470:LEU:HD13	1:B:810:TRP:CE3	2.55	0.41
1:A:736:ASN:HB2	2:A:1001:A1R:O3N	2.20	0.41
1:A:854:PRO:HA	1:A:855:PRO:HD2	1.73	0.41
1:A:613:GLN:O	1:A:614:LYS:HB2	2.21	0.41
1:A:460:MET:SD	1:A:464:GLY:CA	3.08	0.41
1:A:840:GLU:OE2	1:A:878:LYS:HE2	2.20	0.41
1:C:630:LEU:O	1:C:633:ALA:HB3	2.20	0.41
1:A:884:LEU:HD23	1:A:884:LEU:HA	1.84	0.41
1:A:585:LEU:HG	1:A:590:LEU:CD2	2.51	0.41
1:A:907:ILE:HG22	1:A:908:TYR:N	2.35	0.41
1:A:879:ALA:HB1	1:A:907:ILE:HD12	1.98	0.41
1:C:572:PHE:CE2	1:C:672:LEU:HB2	2.56	0.41
1:B:546:PRO:HA	1:B:573:TRP:CE3	2.55	0.41
1:A:604:CYS:HA	1:A:625:GLN:HE21	1.86	0.41
1:C:810:TRP:O	1:C:811:GLN:C	2.58	0.41
1:B:479:THR:OG1	1:B:621:MET:HB3	2.21	0.41
1:C:600:LEU:HD22	1:C:632:ASN:ND2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:VAL:HG11	1:A:858:LEU:HD21	2.03	0.40
1:B:877:LEU:O	1:B:877:LEU:HD12	2.21	0.40
1:C:679:PHE:O	1:C:683:THR:HG23	2.21	0.40
1:B:517:TYR:CZ	1:B:534:LEU:CD1	3.02	0.40
1:A:572:PHE:CD2	1:A:672:LEU:HD12	2.56	0.40
1:B:616:ASN:HD21	1:B:697:SER:H	1.69	0.40
1:C:695:ARG:NH2	1:C:769:GLU:O	2.54	0.40
1:B:754:ARG:CZ	1:B:817:ILE:HD11	2.51	0.40
1:C:791:TYR:O	1:C:794:THR:N	2.40	0.40
1:B:912:THR:O	1:B:916:GLU:HB2	2.21	0.40
1:B:738:PHE:CE1	1:B:770:VAL:HB	2.57	0.40
1:B:667:ARG:HA	1:B:667:ARG:HD2	1.69	0.40
1:A:667:ARG:HA	1:A:667:ARG:HD2	1.72	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	519/588 (88%)	481 (93%)	34 (7%)	4 (1%)	24	66
1	B	519/588 (88%)	483 (93%)	30 (6%)	6 (1%)	16	56
1	C	519/588 (88%)	466 (90%)	44 (8%)	9 (2%)	11	46
All	All	1557/1764 (88%)	1430 (92%)	108 (7%)	19 (1%)	16	56

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	811	GLN
1	C	935	GLU
1	A	792	ALA
1	B	658	ASN

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Mol	Chain	Res	Type
1	B	792	ALA
1	B	830	ASP
1	C	658	ASN
1	A	444	PRO
1	A	658	ASN
1	B	746	ALA
1	C	704	TRP
1	C	746	ALA
1	C	792	ALA
1	C	932	TYR
1	C	865	ASN
1	A	745	GLY
1	B	745	GLY
1	C	745	GLY
1	C	444	PRO

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	417/520 (80%)	394 (94%)	23 (6%)	27	65
1	B	414/520 (80%)	387 (94%)	27 (6%)	21	58
1	C	349/520 (67%)	334 (96%)	15 (4%)	35	75
All	All	1180/1560 (76%)	1115 (94%)	65 (6%)	27	65

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	527	THR
1	A	556	TYR
1	A	558	VAL
1	A	578	GLU
1	A	588	SER
1	A	595	LYS
1	A	624	GLU

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Mol	Chain	Res	Type
1	A	637	THR
1	A	650	SER
1	A	667	ARG
1	A	703	GLU
1	A	711	LEU
1	A	737	ARG
1	A	748	LEU
1	A	774	ASN
1	A	794	THR
1	A	796	ARG
1	A	799	ARG
1	A	815	THR
1	A	883	LEU
1	A	898	PHE
1	A	902	GLU
1	A	952	ILE
1	B	527	THR
1	B	556	TYR
1	B	558	VAL
1	B	577	LEU
1	B	578	GLU
1	B	588	SER
1	B	637	THR
1	B	650	SER
1	B	667	ARG
1	B	711	LEU
1	B	737	ARG
1	B	748	LEU
1	B	774	ASN
1	B	793	GLU
1	B	794	THR
1	B	799	ARG
1	B	809	ASP
1	B	815	THR
1	B	853	VAL
1	B	880	LEU
1	B	898	PHE
1	B	902	GLU
1	B	917	ARG
1	B	918	LYS
1	B	938	ASP
1	B	941	SER

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Mol	Chain	Res	Type
1	B	952	ILE
1	C	527	THR
1	C	533	GLU
1	C	556	TYR
1	C	558	VAL
1	C	578	GLU
1	C	588	SER
1	C	637	THR
1	C	650	SER
1	C	667	ARG
1	C	737	ARG
1	C	748	LEU
1	C	774	ASN
1	C	794	THR
1	C	799	ARG
1	C	811	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	536	GLN
1	A	557	ASN
1	A	616	ASN
1	A	625	GLN
1	A	658	ASN
1	A	774	ASN
1	A	784	GLN
1	A	824	HIS
1	A	842	ASN
1	B	504	ASN
1	B	557	ASN
1	B	616	ASN
1	B	658	ASN
1	B	774	ASN
1	B	824	HIS
1	B	865	ASN
1	B	911	HIS
1	C	557	ASN
1	C	616	ASN
1	C	625	GLN
1	C	658	ASN
1	C	774	ASN

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Mol	Chain	Res	Type
1	C	824	HIS
1	C	842	ASN

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 ⓘ

3 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	A1R	A	1001	-	30,38,38	0.95	1 (3%)	32,58,58	2.16	10 (31%)
2	A1R	B	1001	-	30,38,38	0.98	1 (3%)	32,58,58	2.47	9 (28%)
2	A1R	C	1001	-	30,38,38	0.89	1 (3%)	32,58,58	1.93	7 (21%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	A1R	C5-C4	2.59	1.46	1.40
2	C	1001	A1R	C5-C4	2.85	1.46	1.40
2	A	1001	A1R	C5-C4	3.22	1.47	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	A1R	N3-C2-N1	-7.64	123.04	128.89
2	B	1001	A1R	N3-C2-N1	-7.58	123.09	128.89
2	A	1001	A1R	N3-C2-N1	-6.07	124.25	128.89
2	B	1001	A1R	PB-O3A-PA	-5.55	117.15	132.73
2	A	1001	A1R	C4-C5-N7	-4.21	105.60	109.48
2	B	1001	A1R	C2'-C1'-N9	-4.00	108.18	114.29
2	B	1001	A1R	C5N-C4N-C3N	-3.79	107.58	114.11
2	A	1001	A1R	O3A-PA-O5'	-3.54	93.55	102.94
2	C	1001	A1R	C4-C5-N7	-3.07	106.66	109.48
2	B	1001	A1R	C1'-N9-C4	-2.91	122.55	126.94
2	A	1001	A1R	PB-O3A-PA	-2.71	125.12	132.73
2	C	1001	A1R	C1'-N9-C4	-2.65	122.94	126.94
2	A	1001	A1R	C5N-C4N-C3N	-2.41	109.97	114.11
2	C	1001	A1R	C5N-C4N-C3N	-2.15	110.41	114.11
2	A	1001	A1R	O3N-C3N-C2N	-2.07	106.75	111.68
2	C	1001	A1R	PB-O3A-PA	-2.07	126.93	132.73
2	A	1001	A1R	C1'-N9-C4	-2.07	123.82	126.94
2	B	1001	A1R	N6-C6-N1	2.02	123.53	119.20
2	B	1001	A1R	C2-N1-C6	2.04	122.41	118.77
2	A	1001	A1R	O4'-C1'-N9	2.07	112.43	108.10
2	C	1001	A1R	O4'-C4'-C3'	2.20	109.57	105.15
2	A	1001	A1R	O2A-PA-O3A	2.24	115.24	105.09
2	C	1001	A1R	C2-N1-C6	2.51	123.26	118.77
2	B	1001	A1R	O5N-C5N-C4N	3.36	113.80	108.33
2	A	1001	A1R	O5N-C5N-C4N	5.34	117.02	108.33
2	B	1001	A1R	O4'-C1'-N9	5.53	119.68	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	A1R	3	0
2	B	1001	A1R	4	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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	521/588 (88%)	-0.22	8 (1%)	76	49	49, 87, 145, 199	0
1	B	521/588 (88%)	-0.11	9 (1%)	73	45	56, 99, 162, 210	0
1	C	521/588 (88%)	0.23	28 (5%)	29	11	65, 124, 205, 256	0
All	All	1563/1764 (88%)	-0.03	45 (2%)	55	26	49, 101, 186, 256	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	440	PRO	7.1
1	C	704	TRP	5.0
1	B	525	GLU	4.9
1	C	852	GLY	4.4
1	A	523	ASN	4.4
1	C	942	PRO	4.3
1	C	956	ALA	3.7
1	C	463	CYS	3.5
1	C	520	GLU	3.4
1	C	941	SER	3.3
1	A	524	GLY	3.2
1	C	702	PRO	3.1
1	B	958	SER	3.1
1	C	703	GLU	3.0
1	C	938	ASP	3.0
1	C	522	GLU	3.0
1	C	523	ASN	2.9
1	C	447	LYS	2.9
1	A	522	GLU	2.8
1	C	943	GLY	2.8
1	A	520	GLU	2.8
1	B	942	PRO	2.8
1	C	915	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	524	GLY	2.7
1	B	941	SER	2.7
1	A	958	SER	2.5
1	B	943	GLY	2.5
1	C	939	CYS	2.5
1	C	940	SER	2.5
1	A	440	PRO	2.4
1	B	664	ARG	2.4
1	C	442	ASN	2.4
1	C	944	PRO	2.4
1	A	872	GLY	2.4
1	B	487	ALA	2.3
1	C	945	ASP	2.3
1	C	853	VAL	2.2
1	A	439	VAL	2.2
1	C	446	ASP	2.2
1	B	482	VAL	2.1
1	C	946	THR	2.1
1	C	809	ASP	2.0
1	C	441	PRO	2.0
1	C	936	CYS	2.0
1	C	854	PRO	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(Å²)	Q<0.9
2	A1R	C	1001	35/35	0.91	0.18	-0.76	70,88,97,112	0
2	A1R	A	1001	35/35	0.96	0.11	-1.29	64,76,85,90	0
2	A1R	B	1001	35/35	0.95	0.15	-1.69	61,67,75,78	0

6.5 Other polymers (i)

There are no such residues in this entry.