Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:18 PM GMT

PDB ID	:	1A4M
Title	:	ADA STRUCTURE COMPLEXED WITH PURINE RIBOSIDE AT PH 7.0
Authors	:	Wang, Z.; Quiocho, F.A.
Deposited on	:	1998-01-31
Resolution	:	1.95 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:

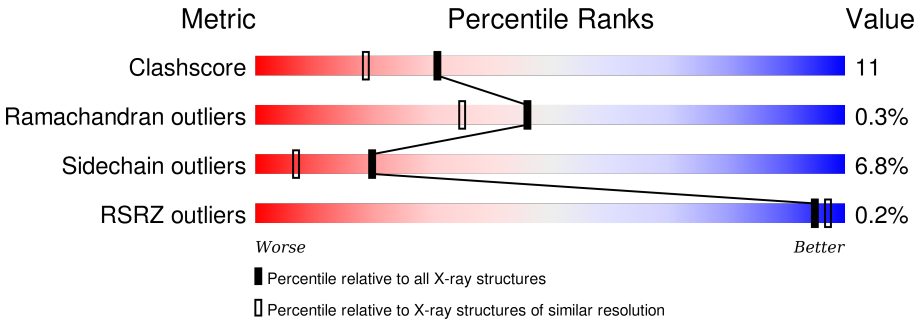
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 1.95 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))
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	349	79% 19% .
1	B	349	71% 26% .
1	C	349	% 71% 24% 5%
1	D	349	73% 23% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12313 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.

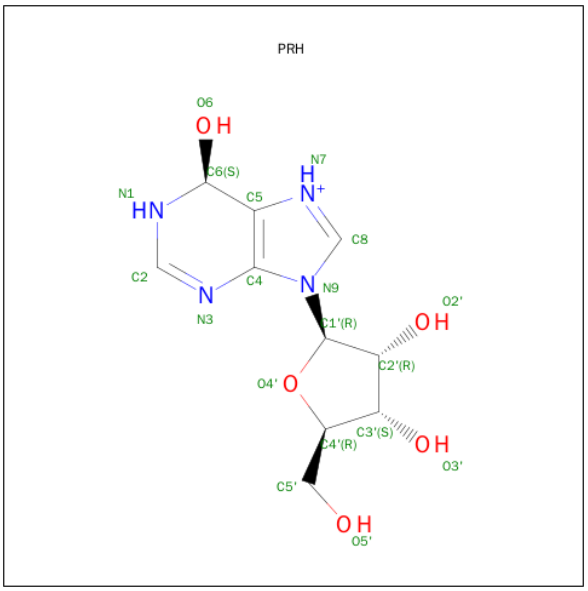
- Molecule 1 is a protein called ADENOSINE DEAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2792	1778	470	530	14			
1	B	349	Total	C	N	O	S	0	0	0
			2792	1778	470	530	14			
1	C	349	Total	C	N	O	S	0	0	0
			2792	1778	470	530	14			
1	D	349	Total	C	N	O	S	0	0	0
			2792	1778	470	530	14			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 6-HYDROXY-1,6-DIHYDRO PURINE NUCLEOSIDE (three-letter code: PRH) (formula: $C_{10}H_{15}N_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 19 10 4 5	0	0
3	B	1	Total C N O 19 10 4 5	0	0
3	C	1	Total C N O 19 10 4 5	0	0
3	D	1	Total C N O 19 10 4 5	0	0

- Molecule 4 is water.

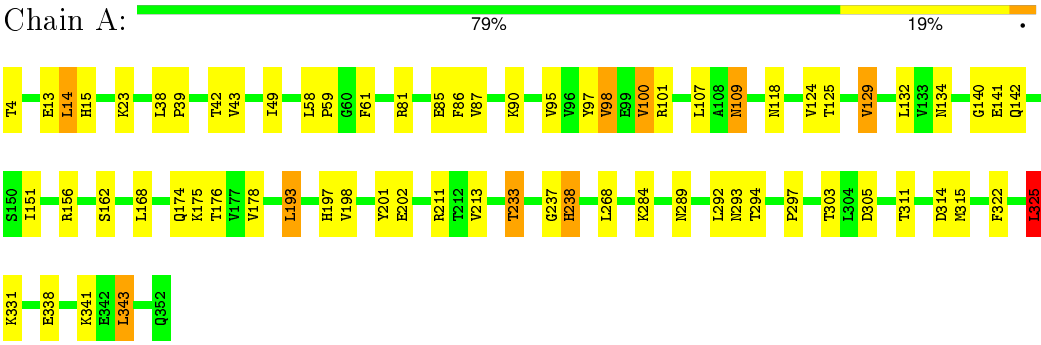
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	287	Total O 287 287	0	0
4	B	269	Total O 269 269	0	0
4	C	242	Total O 242 242	0	0
4	D	267	Total O 267 267	0	0

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.

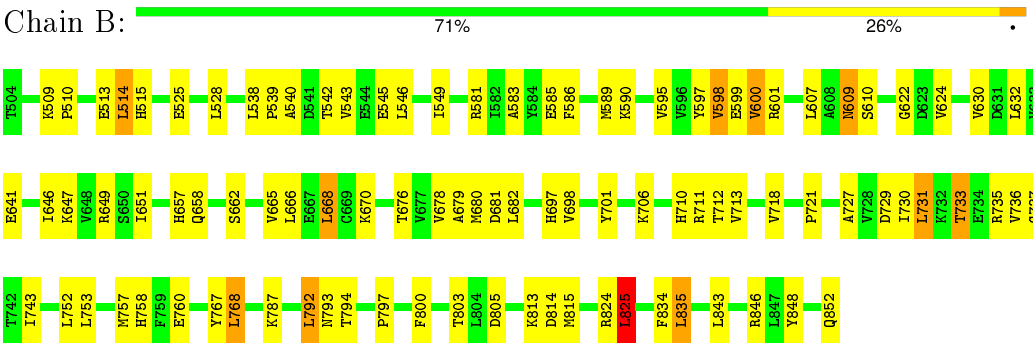
- Molecule 1: ADENOSINE DEAMINASE

Chain A:



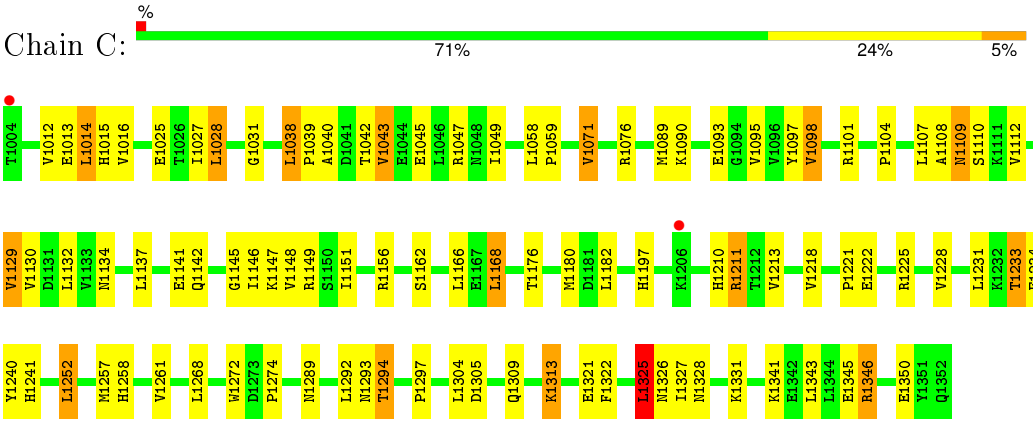
- Molecule 1: ADENOSINE DEAMINASE

Chain B:



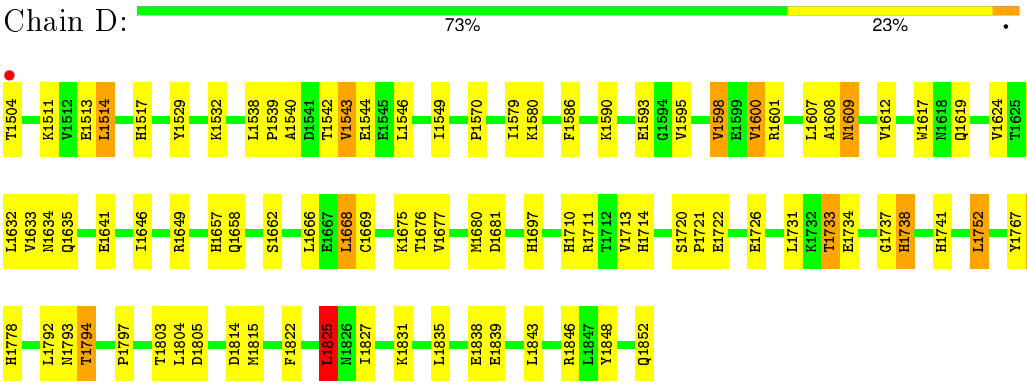
- Molecule 1: ADENOSINE DEAMINASE

Chain C:



• Molecule 1: ADENOSINE DEAMINASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.69Å 93.64Å 102.18Å 90.00° 102.84° 90.00°	Depositor
Resolution (Å)	10.00 – 1.95 39.56 – 1.95	Depositor EDS
% Data completeness (in resolution range)	70.2 (10.00-1.95) 65.7 (39.56-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 1.95Å)	Xtriage
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.193 , 0.281 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	16.3	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	2 of 77949 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12313	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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 62.96 % 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 1.0400e-05.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: ZN, PRH

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	0/2856	0.69	1/3864 (0.0%)
1	B	0.42	0/2856	0.70	3/3864 (0.1%)
1	C	0.41	0/2856	0.69	1/3864 (0.0%)
1	D	0.42	0/2856	0.68	1/3864 (0.0%)
All	All	0.42	0/11424	0.69	6/15456 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1825	LEU	CA-CB-CG	8.66	135.22	115.30
1	A	325	LEU	CA-CB-CG	8.64	135.16	115.30
1	C	1325	LEU	CA-CB-CG	7.89	133.44	115.30
1	B	825	LEU	CA-CB-CG	7.54	132.63	115.30
1	B	835	LEU	CA-CB-CG	5.98	129.06	115.30
1	B	598	VAL	CB-CA-C	-5.07	101.76	111.40

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	2792	0	2757	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2792	0	2757	69	0
1	C	2792	0	2757	66	0
1	D	2792	0	2757	62	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	19	0	14	2	0
3	B	19	0	14	0	0
3	C	19	0	14	0	0
3	D	19	0	14	1	0
4	A	287	0	0	10	0
4	B	269	0	0	2	0
4	C	242	0	0	10	0
4	D	267	0	0	3	0
All	All	12313	0	11084	244	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 11.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:LEU:HD13	1:B:546:LEU:HD22	1.55	0.89
1:C:1109:ASN:HD21	1:C:1124:VAL:H	1.22	0.87
1:A:294:THR:HG23	1:A:297:PRO:HD3	1.59	0.83
1:C:1294:THR:HG23	1:C:1297:PRO:HD3	1.62	0.80
1:B:792:LEU:HD22	1:B:825:LEU:HD11	1.66	0.77
1:B:542:THR:OG1	1:B:545:GLU:HG2	1.84	0.77
1:D:1539:PRO:HB2	1:D:1549:ILE:HD13	1.67	0.74
3:A:354:PRH:H6	4:A:2348:HOH:O	1.87	0.73
1:A:175:LYS:HG3	4:A:2869:HOH:O	1.91	0.71
1:D:1609:ASN:HD21	1:D:1624:VAL:H	1.39	0.70
1:B:641:GLU:HG3	1:B:646:ILE:O	1.91	0.70
1:C:1213:VAL:HG23	1:C:1233:THR:HG23	1.73	0.70
1:A:213:VAL:HG23	1:A:233:THR:HG23	1.72	0.70
1:D:1657:HIS:CD2	1:D:1658:GLN:HG2	2.27	0.69
1:B:729:ASP:HB3	1:D:1532:LYS:HE3	1.75	0.69
1:C:1042:THR:OG1	1:C:1045:GLU:HG2	1.91	0.69
1:A:14:LEU:H	1:A:293:ASN:HD21	1.40	0.68
1:A:95:VAL:HG11	1:A:98:VAL:HG22	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1794:THR:HG23	1:D:1797:PRO:HD3	1.75	0.67
1:A:141:GLU:HG3	1:A:146:ILE:O	1.93	0.67
1:A:95:VAL:CG1	1:A:98:VAL:HG22	2.25	0.67
1:C:1341:LYS:O	1:C:1345:GLU:HG3	1.96	0.65
1:A:109:ASN:HD21	1:A:124:VAL:H	1.42	0.65
1:B:813:LYS:HG3	4:B:2417:HOH:O	1.96	0.65
1:B:586:PHE:CZ	1:B:600:VAL:HG13	2.32	0.65
1:B:595:VAL:HG11	1:B:598:VAL:HG22	1.79	0.64
1:C:1014:LEU:H	1:C:1293:ASN:ND2	1.95	0.64
1:B:803:THR:HG23	1:B:805:ASP:H	1.61	0.64
1:B:768:LEU:HD23	1:B:800:PHE:CD1	2.34	0.63
1:D:1713:VAL:HG23	1:D:1733:THR:HG23	1.79	0.63
1:B:768:LEU:HD23	1:B:800:PHE:HD1	1.61	0.63
1:B:609:ASN:HD21	1:B:624:VAL:H	1.46	0.63
1:D:1649:ARG:HD3	1:D:1676:THR:HA	1.80	0.63
1:D:1517:HIS:HD1	3:D:1854:PRH:HO5'	1.46	0.63
1:A:4:THR:HB	4:A:2563:HOH:O	1.99	0.62
1:B:515:HIS:H	1:B:793:ASN:ND2	1.98	0.61
1:C:1109:ASN:ND2	1:C:1124:VAL:H	1.95	0.61
1:C:1012:VAL:H	1:C:1326:ASN:ND2	1.98	0.61
1:A:14:LEU:H	1:A:293:ASN:ND2	1.98	0.61
1:B:595:VAL:CG1	1:B:598:VAL:HG22	2.31	0.61
1:D:1794:THR:CG2	1:D:1797:PRO:HD3	2.30	0.60
1:A:213:VAL:HG23	1:A:233:THR:CG2	2.32	0.60
1:D:1540:ALA:HB3	1:D:1546:LEU:HD13	1.84	0.60
1:B:634:ASN:ND2	1:B:676:THR:OG1	2.35	0.59
1:C:1141:GLU:HG3	1:C:1146:ILE:O	2.02	0.59
1:C:1221:PRO:HG3	1:C:1241:HIS:O	2.02	0.59
1:D:1710:HIS:HE1	4:D:2694:HOH:O	1.86	0.58
1:A:42:THR:HG22	4:A:2820:HOH:O	2.04	0.57
1:D:1511:LYS:HD2	1:D:1804:LEU:HD23	1.87	0.57
1:C:1218:VAL:HG21	4:C:3010:HOH:O	2.04	0.57
1:D:1669:CYS:HA	1:D:1677:VAL:HG11	1.86	0.57
1:B:730:ILE:HD11	1:D:1529:TYR:HA	1.85	0.57
1:A:322:PHE:HA	1:A:325:LEU:HD13	1.87	0.57
1:A:201:TYR:CD2	1:A:211:ARG:HG2	2.39	0.57
1:C:1166:LEU:HB2	1:C:1180:MET:HE1	1.86	0.57
3:A:354:PRH:C6	4:A:2348:HOH:O	2.48	0.57
1:B:735:ARG:HD3	1:B:758:HIS:CD2	2.39	0.56
1:D:1586:PHE:CZ	1:D:1600:VAL:HG13	2.40	0.56
1:B:701:TYR:CD2	1:B:711:ARG:HG2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1608:ALA:HB3	1:D:1612:VAL:HG21	1.87	0.56
1:C:1294:THR:CG2	1:C:1297:PRO:HD3	2.32	0.56
1:C:1028:LEU:HD23	1:C:1043:VAL:HG12	1.88	0.56
1:C:1321:GLU:O	1:C:1325:LEU:HD13	2.06	0.56
1:D:1514:LEU:H	1:D:1793:ASN:ND2	2.03	0.56
1:D:1814:ASP:O	1:D:1815:MET:HB2	2.06	0.56
1:C:1145:GLY:HA2	4:C:2163:HOH:O	2.06	0.55
1:D:1634:ASN:ND2	1:D:1676:THR:OG1	2.40	0.55
1:C:1134:ASN:ND2	1:C:1176:THR:OG1	2.39	0.55
1:D:1737:GLY:O	1:D:1738:HIS:HB2	2.07	0.55
1:C:1014:LEU:H	1:C:1293:ASN:HD21	1.53	0.55
1:A:294:THR:CG2	1:A:297:PRO:HD3	2.35	0.55
1:B:713:VAL:HG23	1:B:733:THR:HG23	1.88	0.55
1:D:1504:THR:N	4:D:2317:HOH:O	2.40	0.55
1:B:662:SER:OG	1:B:697:HIS:HD2	1.90	0.55
1:A:4:THR:N	4:A:2299:HOH:O	2.39	0.54
1:A:58:LEU:HB3	1:A:59:PRO:HD3	1.89	0.54
1:B:682:LEU:HB3	1:B:713:VAL:HG13	1.90	0.54
1:A:303:THR:HG23	1:A:305:ASP:H	1.73	0.54
1:C:1047:ARG:HD3	4:C:2151:HOH:O	2.07	0.54
1:D:1513:GLU:HB3	1:D:1598:VAL:HG13	1.90	0.53
1:A:15:HIS:H	1:A:293:ASN:ND2	2.07	0.53
1:C:1013:GLU:OE2	1:C:1294:THR:HB	2.09	0.53
1:C:1309:GLN:O	1:C:1313:LYS:HD3	2.08	0.53
1:C:1031:GLY:HA2	1:C:1071:VAL:HG22	1.91	0.53
1:D:1514:LEU:H	1:D:1793:ASN:HD21	1.57	0.53
1:C:1162:SER:OG	1:C:1197:HIS:HD2	1.92	0.53
1:C:1095:VAL:HG11	1:C:1098:VAL:HG22	1.90	0.52
1:C:1093:GLU:OE1	1:C:1304:LEU:HB2	2.09	0.52
1:B:649:ARG:HD3	1:B:676:THR:HA	1.91	0.52
1:B:609:ASN:ND2	1:B:624:VAL:H	2.07	0.52
1:A:13:GLU:HB3	1:A:98:VAL:HG13	1.92	0.52
1:B:666:LEU:HA	1:B:680:MET:CE	2.41	0.51
1:B:794:THR:HG23	1:B:797:PRO:HD3	1.91	0.51
1:B:813:LYS:HB3	1:B:813:LYS:NZ	2.24	0.51
1:C:1322:PHE:HA	1:C:1325:LEU:HD13	1.92	0.51
1:B:727:ALA:HA	1:B:731:LEU:HD23	1.91	0.51
1:D:1835:LEU:HG	1:D:1839:GLU:HB2	1.93	0.51
1:B:721:PRO:HG3	1:B:741:HIS:O	2.11	0.51
1:D:1827:ILE:HG22	1:D:1831:LYS:HE2	1.93	0.51
1:C:1013:GLU:HB3	1:C:1098:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:LYS:HB3	1:B:510:PRO:HD2	1.92	0.51
1:A:109:ASN:C	1:A:109:ASN:HD22	2.13	0.51
1:C:1210:HIS:HE1	4:C:3040:HOH:O	1.94	0.50
1:C:1134:ASN:ND2	4:C:2164:HOH:O	2.45	0.50
1:D:1767:TYR:CD2	1:D:1768:LEU:HD13	2.46	0.50
1:B:513:GLU:OE2	1:B:794:THR:HG22	2.12	0.50
1:B:513:GLU:HB3	1:B:598:VAL:HG13	1.93	0.50
1:B:539:PRO:HB2	1:B:549:ILE:HD13	1.92	0.50
1:B:814:ASP:O	1:B:815:MET:HB2	2.12	0.50
1:C:1089:MET:HE1	4:C:2996:HOH:O	2.11	0.50
1:C:1305:ASP:O	1:C:1309:GLN:HG2	2.12	0.49
1:C:1027:ILE:HG22	1:C:1038:LEU:HD21	1.95	0.49
1:B:540:ALA:HB1	1:B:545:GLU:HB2	1.93	0.49
1:B:630:VAL:HG21	1:B:668:LEU:HG	1.93	0.49
1:C:1110:SER:O	1:C:1112:VAL:HG23	2.12	0.49
1:A:4:THR:N	4:A:2563:HOH:O	2.46	0.49
1:D:1662:SER:OG	1:D:1697:HIS:HD2	1.95	0.49
1:C:1095:VAL:CG1	1:C:1098:VAL:HG22	2.42	0.49
1:B:514:LEU:H	1:B:793:ASN:HD21	1.61	0.49
1:A:162:SER:OG	1:A:197:HIS:HD2	1.94	0.49
1:B:681:ASP:HA	1:B:712:THR:O	2.12	0.49
1:B:597:TYR:HD1	1:B:647:LYS:HB3	1.78	0.49
1:C:1240:TYR:HE1	1:C:1261:VAL:HG13	1.78	0.48
1:D:1822:PHE:HA	1:D:1825:LEU:HD13	1.96	0.48
1:D:1641:GLU:HG3	1:D:1646:ILE:O	2.13	0.48
1:B:729:ASP:HB3	1:D:1532:LYS:CE	2.43	0.48
1:A:134:ASN:ND2	1:A:176:THR:OG1	2.47	0.48
1:B:586:PHE:O	1:B:589:MET:HB2	2.14	0.48
1:C:1313:LYS:HG3	4:C:3066:HOH:O	2.14	0.48
1:B:601:ARG:HA	1:B:651:ILE:O	2.14	0.48
1:A:174:GLN:NE2	1:A:178:VAL:HG12	2.29	0.48
1:C:1346:ARG:HD3	1:C:1350:GLU:OE2	2.14	0.47
1:D:1609:ASN:HD22	1:D:1609:ASN:C	2.18	0.47
1:A:125:THR:O	1:A:129:VAL:HG13	2.14	0.47
1:D:1595:VAL:CG1	1:D:1598:VAL:HG22	2.45	0.47
1:D:1721:PRO:HG3	1:D:1741:HIS:O	2.15	0.47
1:B:666:LEU:HG	1:B:670:LYS:HE3	1.95	0.47
1:B:599:GLU:HA	1:B:649:ARG:O	2.15	0.47
1:A:86:PHE:CZ	1:A:100:VAL:HG13	2.50	0.47
1:B:657:HIS:CD2	1:B:658:GLN:HG2	2.50	0.47
1:B:848:TYR:O	1:B:852:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:698:VAL:HG11	1:D:1543:VAL:HG11	1.97	0.47
1:A:193:LEU:HG	1:C:1025:GLU:HG2	1.97	0.47
1:D:1626:PRO:O	1:D:1630:VAL:HG23	2.15	0.46
1:C:1252:LEU:HG	1:C:1257:MET:HG2	1.97	0.46
1:C:1237:GLY:O	1:C:1238:HIS:HB2	2.14	0.46
1:D:1681:ASP:OD2	1:D:1714:HIS:HE1	1.98	0.46
1:C:1108:ALA:HB3	1:C:1112:VAL:HG21	1.97	0.46
1:C:1327:ILE:HG22	1:C:1331:LYS:HE2	1.96	0.46
1:B:767:TYR:CD2	1:B:768:LEU:HD13	2.51	0.46
1:B:590:LYS:HA	1:B:590:LYS:HD3	1.72	0.46
1:C:1039:PRO:HB2	1:C:1049:ILE:HD13	1.96	0.46
1:B:737:GLY:O	1:B:738:HIS:HB2	2.15	0.46
1:C:1104:PRO:O	1:C:1129:VAL:HG11	2.16	0.46
1:D:1593:GLU:OE1	1:D:1804:LEU:HB2	2.15	0.46
1:A:87:VAL:HG11	1:A:140:GLY:C	2.36	0.46
1:C:1313:LYS:HB3	4:C:2756:HOH:O	2.16	0.46
1:C:1149:ARG:HD3	1:C:1176:THR:HA	1.98	0.45
1:C:1126:PRO:O	1:C:1129:VAL:HG13	2.15	0.45
1:B:787:LYS:HA	1:B:787:LYS:HD3	1.77	0.45
1:B:662:SER:OG	1:B:697:HIS:CD2	2.70	0.45
1:A:327:ILE:HG22	1:A:331:LYS:HE2	1.98	0.45
1:A:97:TYR:HD1	1:A:147:LYS:HB3	1.81	0.45
1:A:330:ALA:HB1	1:A:343:LEU:HD13	1.99	0.45
1:A:156:ARG:O	1:A:197:HIS:HE1	2.00	0.45
1:A:338:GLU:HG3	4:A:2095:HOH:O	2.16	0.45
1:C:1097:TYR:HD1	1:C:1147:LYS:HB3	1.82	0.45
1:C:1228:VAL:HG21	1:C:1252:LEU:HD11	1.99	0.45
1:B:737:GLY:HA2	1:B:760:GLU:HB2	1.99	0.45
1:C:1222:GLU:OE1	1:C:1225:ARG:HD2	2.17	0.45
1:C:1076:ARG:NH1	4:C:3029:HOH:O	2.50	0.45
1:D:1590:LYS:HD3	1:D:1590:LYS:HA	1.76	0.45
1:B:581:ARG:HD3	1:B:585:GLU:OE2	2.16	0.45
1:D:1752:LEU:HA	1:D:1752:LEU:HD12	1.86	0.44
1:A:175:LYS:HE2	1:A:175:LYS:HB3	1.88	0.44
1:B:706:LYS:HE3	4:B:2959:HOH:O	2.17	0.44
1:C:1182:LEU:HB3	1:C:1213:VAL:HG13	2.00	0.44
1:B:665:VAL:HG12	1:B:680:MET:HE2	1.99	0.44
1:B:651:ILE:HG12	1:B:679:ALA:HB3	2.00	0.44
1:D:1710:HIS:HD2	1:D:1734:GLU:OE1	2.00	0.44
1:C:1289:ASN:ND2	1:C:1328:ASN:HB3	2.32	0.44
1:D:1630:VAL:HG21	1:D:1668:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASN:ND2	1:A:124:VAL:H	2.12	0.44
1:B:515:HIS:H	1:B:793:ASN:HD22	1.64	0.44
1:C:1130:VAL:HG21	1:C:1168:LEU:HG	2.00	0.44
1:D:1542:THR:O	1:D:1546:LEU:HB2	2.17	0.43
1:C:1101:ARG:HA	1:C:1151:ILE:O	2.18	0.43
1:C:1258:HIS:HA	1:C:1289:ASN:O	2.17	0.43
1:C:1015:HIS:CE1	1:C:1101:ARG:NH1	2.86	0.43
1:A:118:ASN:ND2	4:A:2850:HOH:O	2.51	0.43
1:D:1803:THR:HG23	1:D:1805:ASP:H	1.82	0.43
1:C:1058:LEU:HB3	1:C:1059:PRO:HD3	2.01	0.43
1:C:1040:ALA:HB1	1:C:1045:GLU:HB2	2.01	0.43
1:D:1595:VAL:HG11	1:D:1598:VAL:HG22	1.99	0.43
1:D:1629:VAL:O	1:D:1633:VAL:HG23	2.19	0.43
1:A:13:GLU:HG3	1:A:293:ASN:HD22	1.83	0.43
1:D:1601:ARG:HH11	1:D:1714:HIS:CE1	2.37	0.43
1:D:1722:GLU:O	1:D:1726:GLU:HG3	2.17	0.43
1:A:341:LYS:HB2	1:A:341:LYS:HE3	1.73	0.43
1:C:1156:ARG:HA	1:C:1197:HIS:CE1	2.53	0.43
1:A:198:VAL:O	1:A:202:GLU:HG3	2.19	0.43
1:C:1137:LEU:HD22	1:C:1148:VAL:HG11	2.00	0.43
1:B:679:ALA:HB2	1:B:834:PHE:CD2	2.54	0.43
1:C:1090:LYS:HA	1:C:1090:LYS:HD3	1.77	0.43
1:D:1720:SER:HB2	1:D:1721:PRO:CD	2.49	0.43
1:D:1609:ASN:ND2	1:D:1624:VAL:H	2.11	0.42
1:B:787:LYS:C	1:B:824:ARG:HH22	2.23	0.42
1:B:583:ALA:HB3	1:B:636:GLY:HA3	2.01	0.42
1:B:525:GLU:HG3	1:B:543:VAL:HG11	2.02	0.42
1:A:39:PRO:HB2	1:A:49:ILE:HD13	2.00	0.42
1:B:528:LEU:HA	1:B:528:LEU:HD12	1.93	0.42
1:A:101:ARG:HA	1:A:151:ILE:O	2.19	0.42
1:D:1848:TYR:O	1:D:1852:GLN:HG2	2.20	0.42
1:B:678:VAL:O	1:B:710:HIS:HB2	2.19	0.42
1:D:1579:ILE:HD13	1:D:1629:VAL:HB	2.02	0.42
1:D:1570:PRO:HG3	1:D:1617:TRP:HB3	2.01	0.42
1:B:740:TYR:O	1:B:743:ILE:HG12	2.19	0.42
1:B:610:SER:HB2	1:B:622:GLY:O	2.20	0.42
1:A:23:LYS:HD3	1:A:85:GLU:OE1	2.20	0.42
1:D:1609:ASN:HB3	1:D:1619:GLN:NE2	2.35	0.41
1:A:303:THR:HG23	1:A:305:ASP:N	2.36	0.41
1:B:736:VAL:HG23	1:B:757:MET:SD	2.59	0.41
1:D:1580:LYS:HE2	1:D:1635:GLN:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:THR:O	1:A:314:ASP:O	2.38	0.41
1:D:1838:GLU:CD	1:D:1838:GLU:H	2.23	0.41
1:B:803:THR:HG23	1:B:805:ASP:N	2.33	0.41
1:A:314:ASP:O	1:A:315:MET:HB2	2.21	0.41
1:C:1211:ARG:NH1	1:C:1234:GLU:HG3	2.36	0.41
1:C:1016:VAL:HG23	1:C:1294:THR:HG22	2.02	0.41
1:B:514:LEU:H	1:B:793:ASN:ND2	2.19	0.41
1:A:284:LYS:HD3	4:A:2340:HOH:O	2.21	0.41
1:A:90:LYS:HD3	1:A:90:LYS:HA	1.73	0.41
1:C:1272:TRP:CZ2	1:C:1274:PRO:HA	2.56	0.41
1:B:666:LEU:CA	1:B:680:MET:HE1	2.51	0.41
1:D:1720:SER:HB2	1:D:1721:PRO:HD2	2.02	0.41
1:D:1666:LEU:HA	1:D:1680:MET:HE3	2.03	0.41
1:D:1772:TRP:CD2	1:D:1778:HIS:HD2	2.39	0.41
1:D:1609:ASN:ND2	1:D:1609:ASN:C	2.74	0.41
1:D:1675:LYS:HE2	1:D:1675:LYS:HB3	1.89	0.41
1:A:237:GLY:O	1:A:238:HIS:HB2	2.20	0.40
1:C:1141:GLU:HG2	4:C:2170:HOH:O	2.20	0.40
1:A:109:ASN:ND2	1:A:109:ASN:C	2.75	0.40
1:D:1713:VAL:HG23	1:D:1733:THR:CG2	2.47	0.40
1:D:1777:THR:HG22	4:D:2440:HOH:O	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	347/349 (99%)	334 (96%)	12 (4%)	1 (0%)	46	35
1	B	347/349 (99%)	335 (96%)	11 (3%)	1 (0%)	46	35
1	C	347/349 (99%)	333 (96%)	13 (4%)	1 (0%)	46	35
1	D	347/349 (99%)	334 (96%)	12 (4%)	1 (0%)	46	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1388/1396 (99%)	1336 (96%)	48 (4%)	4 (0%)	46 35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1238	HIS
1	A	238	HIS
1	B	738	HIS
1	D	1738	HIS

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	304/304 (100%)	283 (93%)	21 (7%)	19 7
1	B	304/304 (100%)	286 (94%)	18 (6%)	24 10
1	C	304/304 (100%)	281 (92%)	23 (8%)	16 5
1	D	304/304 (100%)	283 (93%)	21 (7%)	19 7
All	All	1216/1216 (100%)	1133 (93%)	83 (7%)	20 7

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	38	LEU
1	A	43	VAL
1	A	61	PHE
1	A	81	ARG
1	A	98	VAL
1	A	100	VAL
1	A	107	LEU
1	A	109	ASN
1	A	129	VAL
1	A	132	LEU

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Mol	Chain	Res	Type
1	A	142	GLN
1	A	149	ARG
1	A	168	LEU
1	A	193	LEU
1	A	233	THR
1	A	268	LEU
1	A	289	ASN
1	A	292	LEU
1	A	325	LEU
1	A	343	LEU
1	B	514	LEU
1	B	538	LEU
1	B	600	VAL
1	B	607	LEU
1	B	609	ASN
1	B	632	LEU
1	B	668	LEU
1	B	718	VAL
1	B	731	LEU
1	B	733	THR
1	B	752	LEU
1	B	753	LEU
1	B	768	LEU
1	B	792	LEU
1	B	825	LEU
1	B	835	LEU
1	B	843	LEU
1	B	846	ARG
1	C	1014	LEU
1	C	1028	LEU
1	C	1038	LEU
1	C	1043	VAL
1	C	1071	VAL
1	C	1098	VAL
1	C	1107	LEU
1	C	1109	ASN
1	C	1129	VAL
1	C	1132	LEU
1	C	1142	GLN
1	C	1168	LEU
1	C	1211	ARG
1	C	1231	LEU

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Mol	Chain	Res	Type
1	C	1233	THR
1	C	1252	LEU
1	C	1268	LEU
1	C	1292	LEU
1	C	1294	THR
1	C	1313	LYS
1	C	1325	LEU
1	C	1343	LEU
1	C	1346	ARG
1	D	1514	LEU
1	D	1538	LEU
1	D	1543	VAL
1	D	1544	GLU
1	D	1598	VAL
1	D	1600	VAL
1	D	1607	LEU
1	D	1609	ASN
1	D	1629	VAL
1	D	1632	LEU
1	D	1668	LEU
1	D	1711	ARG
1	D	1731	LEU
1	D	1733	THR
1	D	1752	LEU
1	D	1768	LEU
1	D	1792	LEU
1	D	1794	THR
1	D	1825	LEU
1	D	1843	LEU
1	D	1846	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	118	ASN
1	A	119	GLN
1	A	134	ASN
1	A	158	GLN
1	A	174	GLN
1	A	197	HIS
1	A	214	HIS

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Mol	Chain	Res	Type
1	A	250	ASN
1	A	256	ASN
1	A	289	ASN
1	A	293	ASN
1	A	326	ASN
1	B	609	ASN
1	B	619	GLN
1	B	634	ASN
1	B	697	HIS
1	B	710	HIS
1	B	741	HIS
1	B	750	ASN
1	B	756	ASN
1	B	789	ASN
1	B	793	ASN
1	B	826	ASN
1	C	1109	ASN
1	C	1119	GLN
1	C	1134	ASN
1	C	1197	HIS
1	C	1210	HIS
1	C	1214	HIS
1	C	1250	ASN
1	C	1256	ASN
1	C	1289	ASN
1	C	1293	ASN
1	C	1326	ASN
1	D	1609	ASN
1	D	1619	GLN
1	D	1634	ASN
1	D	1658	GLN
1	D	1697	HIS
1	D	1710	HIS
1	D	1714	HIS
1	D	1756	ASN
1	D	1789	ASN
1	D	1793	ASN
1	D	1826	ASN

5.3.3 RNA

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, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	PRH	A	354	2	13,21,21	2.24	3 (23%)	13,31,31	2.38	3 (23%)
3	PRH	B	854	2	13,21,21	2.24	3 (23%)	13,31,31	2.43	4 (30%)
3	PRH	C	1354	2	13,21,21	2.20	4 (30%)	13,31,31	2.15	3 (23%)
3	PRH	D	1854	2	13,21,21	2.21	3 (23%)	13,31,31	2.52	4 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PRH	A	354	2	-	0/2/32/32	0/3/3/3
3	PRH	B	854	2	-	0/2/32/32	0/3/3/3
3	PRH	C	1354	2	-	0/2/32/32	0/3/3/3
3	PRH	D	1854	2	-	0/2/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	354	PRH	O4'-C4'	-2.98	1.38	1.45
3	C	1354	PRH	O4'-C4'	-2.75	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	854	PRH	O4'-C4'	-2.72	1.38	1.45
3	D	1854	PRH	O4'-C4'	-2.70	1.38	1.45
3	C	1354	PRH	C6-N1	-2.00	1.39	1.45
3	A	354	PRH	C3'-C4'	2.73	1.60	1.53
3	C	1354	PRH	C3'-C4'	2.89	1.60	1.53
3	B	854	PRH	C3'-C4'	2.96	1.61	1.53
3	D	1854	PRH	C3'-C4'	3.12	1.61	1.53
3	C	1354	PRH	O6-C6	6.35	1.60	1.40
3	D	1854	PRH	O6-C6	6.37	1.60	1.40
3	B	854	PRH	O6-C6	6.44	1.61	1.40
3	A	354	PRH	O6-C6	6.48	1.61	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	854	PRH	C2'-C3'-C4'	-6.57	89.11	102.61
3	A	354	PRH	C2'-C3'-C4'	-6.53	89.18	102.61
3	D	1854	PRH	C2'-C3'-C4'	-6.45	89.35	102.61
3	C	1354	PRH	C2'-C3'-C4'	-5.61	91.09	102.61
3	D	1854	PRH	C4'-O4'-C1'	-3.85	105.49	109.72
3	A	354	PRH	C4'-O4'-C1'	-3.52	105.85	109.72
3	B	854	PRH	C4'-O4'-C1'	-3.28	106.12	109.72
3	D	1854	PRH	C2'-C1'-N9	-3.02	108.81	114.17
3	C	1354	PRH	C4'-O4'-C1'	-2.97	106.45	109.72
3	B	854	PRH	C2'-C1'-N9	-2.27	110.14	114.17
3	A	354	PRH	O4'-C4'-C3'	3.10	111.40	105.15
3	D	1854	PRH	O4'-C4'-C3'	3.24	111.67	105.15
3	B	854	PRH	O4'-C4'-C3'	3.25	111.69	105.15
3	C	1354	PRH	O4'-C4'-C3'	3.35	111.90	105.15

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
3	A	354	PRH	2	0
3	D	1854	PRH	1	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	349/349 (100%)	-0.39	0	100	100	8, 16, 29, 44	0
1	B	349/349 (100%)	-0.39	0	100	100	7, 15, 29, 44	0
1	C	349/349 (100%)	-0.35	2 (0%)	90	94	7, 16, 28, 44	0
1	D	349/349 (100%)	-0.31	1 (0%)	94	96	8, 16, 29, 43	0
All	All	1396/1396 (100%)	-0.36	3 (0%)	95	97	7, 16, 29, 44	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1504	THR	2.4
1	C	1206	LYS	2.2
1	C	1004	THR	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
3	PRH	B	854	19/19	0.96	0.08	-0.34	5,9,13,14	0
3	PRH	D	1854	19/19	0.97	0.08	-0.41	3,8,11,12	0
3	PRH	A	354	19/19	0.97	0.08	-0.58	5,10,15,19	0
3	PRH	C	1354	19/19	0.97	0.08	-0.64	2,10,14,17	0
2	ZN	B	900	1/1	1.00	0.09	-0.96	16,16,16,16	0
2	ZN	D	1900	1/1	0.99	0.07	-1.71	16,16,16,16	0
2	ZN	A	400	1/1	1.00	0.07	-1.72	13,13,13,13	0
2	ZN	C	1400	1/1	1.00	0.07	-1.74	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.