Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:03 PM GMT

PDB ID	:	4QSK
Title	:	Crystal Structure of L. monocytogenes Pyruvate Carboxylase in complex with Cyclic-di-AMP
Authors	:	Choi, P.H.; Tong, L.
Deposited on	:	2014-07-04
Resolution	:	2.70 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:

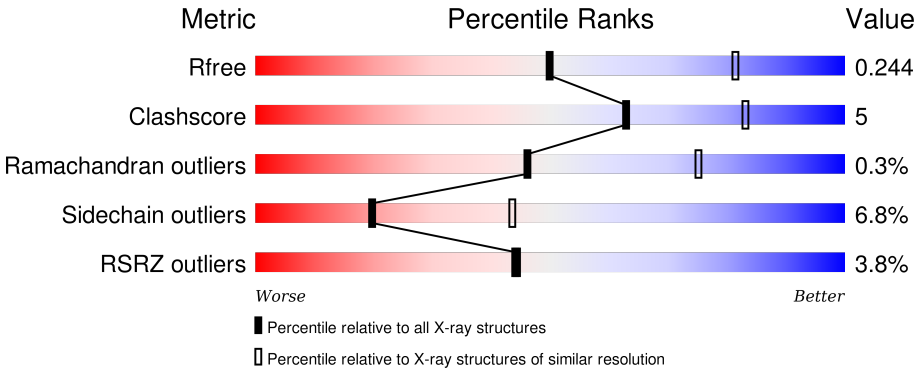
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	1147	4% 79% 13% • 6%
1	B	1147	3% 78% 14% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16959 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.

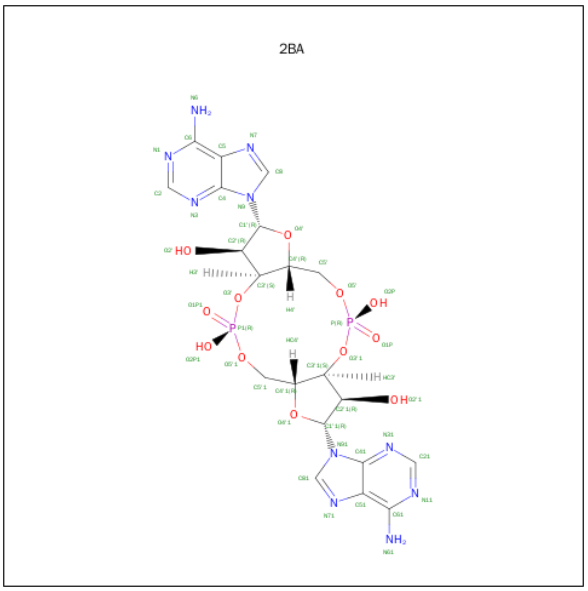
- Molecule 1 is a protein called Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1073	Total	C	N	O	S	0	0	0
			8438	5355	1433	1609	41			
1	B	1073	Total	C	N	O	S	0	0	0
			8449	5362	1433	1613	41			

There are 2 discrepancies between the modelled and reference sequences:

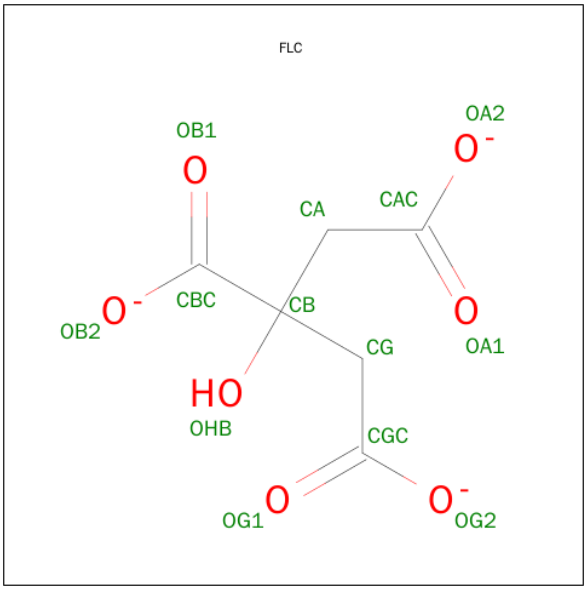
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP W6G6F5
B	0	MET	-	EXPRESSION TAG	UNP W6G6F5

- Molecule 2 is (2R,3R,3AS,5R,7AR,9R,10R,10AS,12R,14AR)-2,9-BIS(6-AMINO-9H-PURIN-9-YL)OCTAHYDRO-2H,7H-DIFURO[3,2-D:3',2'-J][1,3,7,9,2,8]TETRAOXADIPHOSPHACYCLODODECINE-3,5,10,12-TETROL 5,12-DIOXIDE (three-letter code: 2BA) (formula: $C_{20}H_{24}N_{10}O_{12}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P 22 10 5 6 1	0	0
2	B	1	Total C N O P 22 10 5 6 1	0	0

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

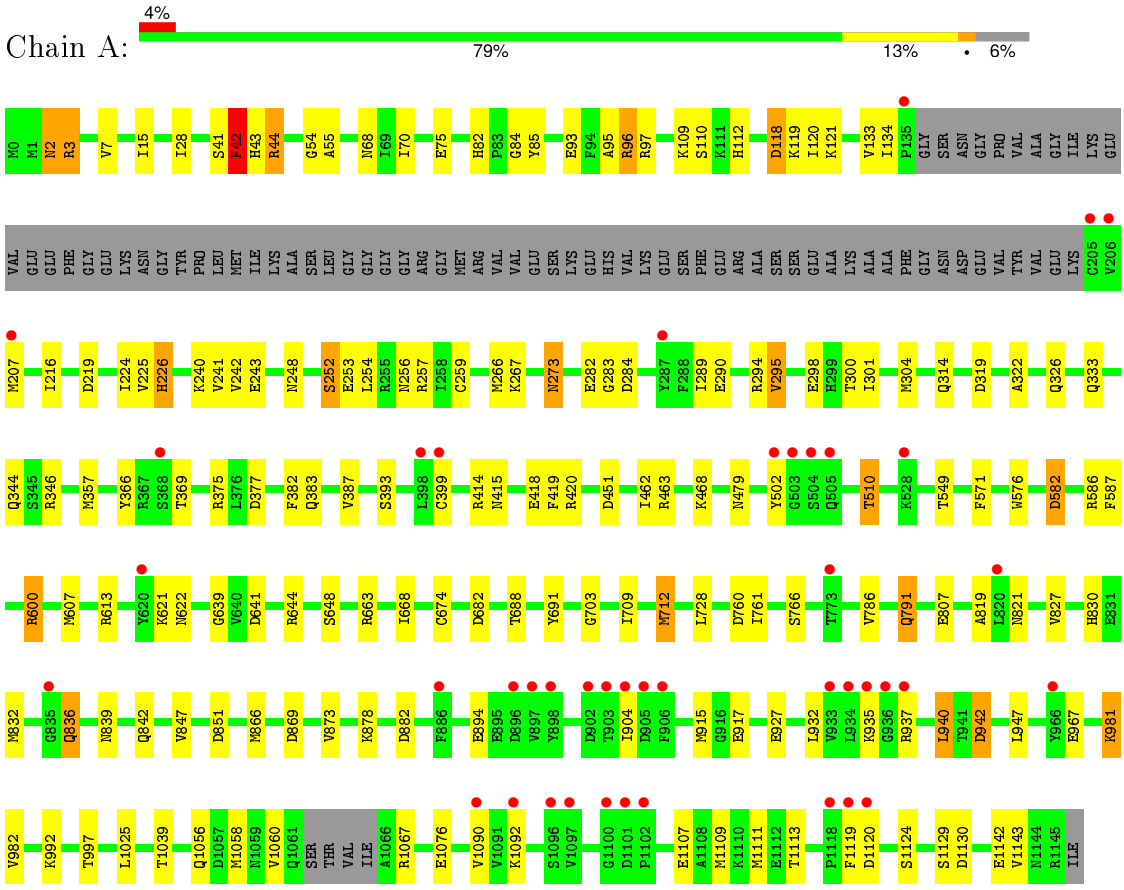
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mn 1 1	0	0
4	A	1	Total Mn 1 1	0	0

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.

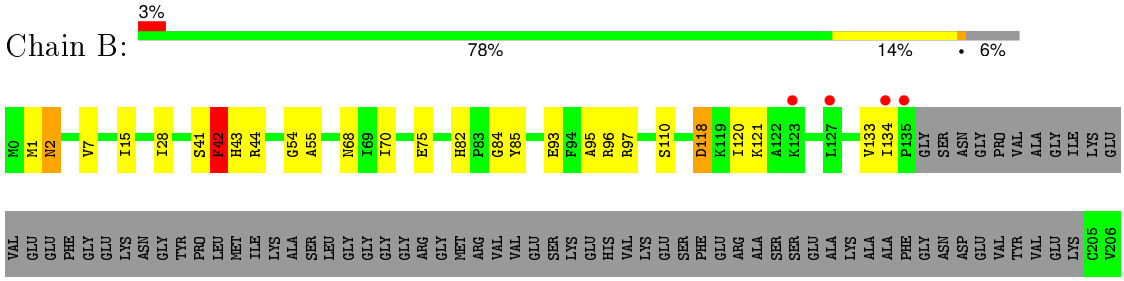
- Molecule 1: Pyruvate carboxylase

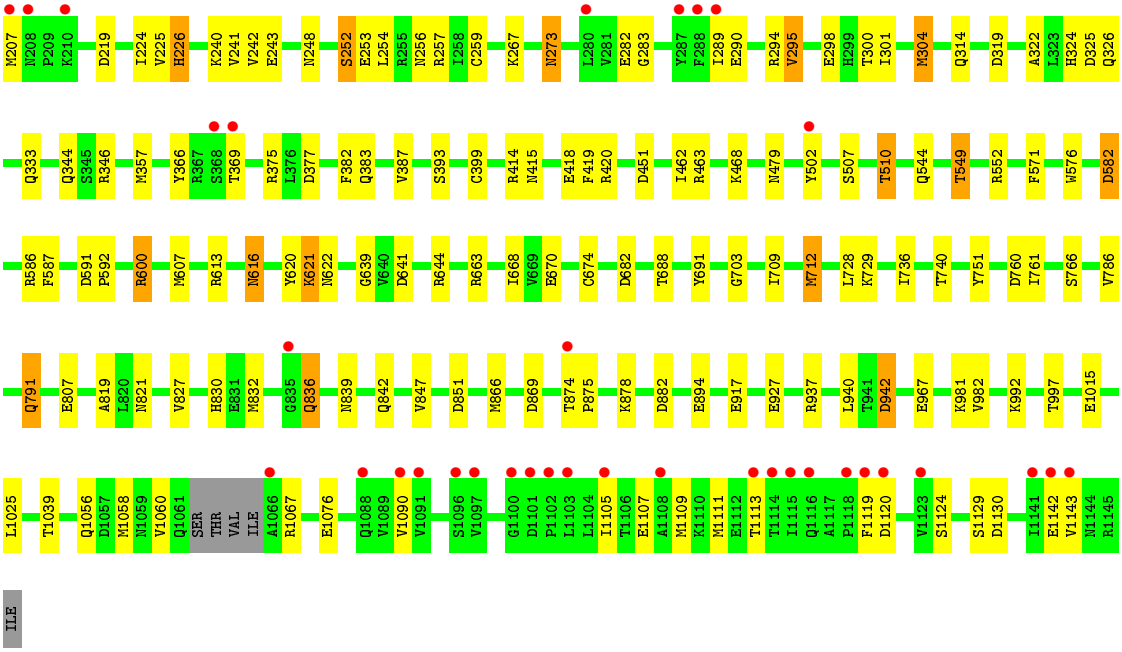
Chain A:



- Molecule 1: Pyruvate carboxylase

Chain B:




W207 N208 P209 K210 D219 I224 V225 H226 K240 V241 Y242 E243 N248 S252 E253 L254 R255 N256 R257 I258 C259 K267 N273 L280 V281 E282 G283 Y287 F288 I289 E290 R294 V295 E298 H299 T300 I301 M304 Q314 D319 A322 L323 H324 D325 Q326
Q333 Q344 S345 R346 M357 Y366 R367 S368 T369 R375 L376 D377 F382 Q383 V387 S393 C399 R414 N415 E418 F419 R420 D451 I462 R463 K468 N479 Y502 S507 T510 Q544 T549 R552 F571 W576 D582
R586 F587 D591 P592 R600 M607 R613 N616 Y620 K621 M622 G639 V640 D641 R644 R663 I668 V669 E670 C674 D682 T688 Y691 G703 I709 M712 L728 K729 I736 T740 Y751 D760 I761 S766 V786
Q791 E807 A819 L820 N821 V827 H830 E831 M832 G835 Q836 N839 Q842 V847 D851 M866 D869 T874 P875 K878 D882 E894 E917 E927 R937 L940 T941 D942 E967 K981 V982 K992 T997 E1015
L1025 T1039 Q1056 D1057 M1058 N1059 V1060 Q1061 SER THR VAL ILE A1066 R1067 E1076 Q1088 V1089 V1090 V1091 S1096 V1097 G1100 D1101 P1102 L1103 L1104 I1105 T1106 E1107 A1108 M1109 K1110 M1111 E1112 T1113 T1114 I1115 Q1116 A1117 P1118 F1119 D1120 V1123 S1124 S1129 D1130 I1141 E1142 V1143 N1144 R1145
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	227.00Å 146.86Å 96.06Å 90.00° 103.54° 90.00°	Depositor
Resolution (Å)	45.68 – 2.70 45.64 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.9 (45.68-2.70) 96.9 (45.64-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.198 , 0.242 0.198 , 0.244	Depositor DCC
R_{free} test set	4071 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	65.2	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 81819 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16959	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: FLC, MN, 2BA

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	0.61	0/8605	0.80	4/11659 (0.0%)
1	B	0.68	0/8616	0.82	3/11673 (0.0%)
All	All	0.64	0/17221	0.81	7/23332 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	42	PHE	CB-CA-C	6.27	122.93	110.40
1	A	420	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	42	PHE	CB-CA-C	5.36	121.11	110.40
1	A	420	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	304	MET	CG-SD-CE	-5.06	92.10	100.20
1	A	96	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	552	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	621	LYS	Peptide

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	8438	0	8361	92	0
1	B	8449	0	8378	88	0
2	A	22	0	11	0	1
2	B	22	0	11	0	1
3	A	13	0	5	0	0
3	B	13	0	5	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	16959	0	16771	177	2

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 (177) 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:582:ASP:OD2	1:B:586:ARG:NH1	2.01	0.92
1:A:582:ASP:OD2	1:A:586:ARG:NH1	2.03	0.91
1:A:663:ARG:NH1	1:A:703:GLY:O	2.13	0.81
1:B:663:ARG:NH1	1:B:703:GLY:O	2.14	0.80
1:B:510:THR:HG21	1:B:571:PHE:O	1.82	0.80
1:A:904:ILE:O	1:A:935:LYS:NZ	2.14	0.80
1:A:510:THR:HG21	1:A:571:PHE:O	1.86	0.76
1:B:644:ARG:NH1	1:B:670:GLU:OE2	2.21	0.72
1:B:42:PHE:HB3	1:B:382:PHE:CE1	2.25	0.72
1:A:226:HIS:CD2	1:A:259:CYS:HB3	2.25	0.72
1:B:226:HIS:CD2	1:B:259:CYS:HB3	2.25	0.71
1:A:295:VAL:HG22	1:A:314:GLN:NE2	2.06	0.70
1:A:366:TYR:H	1:A:383:GLN:HE21	1.40	0.69
1:B:819:ALA:O	1:B:821:ASN:ND2	2.25	0.69
1:B:616:ASN:HB3	1:B:621:LYS:O	1.93	0.69
1:A:42:PHE:HB3	1:A:382:PHE:CE1	2.28	0.68
1:B:295:VAL:HG22	1:B:314:GLN:NE2	2.08	0.68
1:A:819:ALA:O	1:A:821:ASN:ND2	2.26	0.68
1:A:942:ASP:OD1	1:A:942:ASP:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:TYR:H	1:B:383:GLN:HE21	1.41	0.67
1:A:932:LEU:O	1:A:935:LYS:HE3	1.95	0.67
1:B:830:HIS:HD2	1:B:832:MET:H	1.42	0.67
1:A:830:HIS:HD2	1:A:832:MET:H	1.43	0.67
1:A:93:GLU:O	1:A:97:ARG:HB2	1.95	0.66
1:A:54:GLY:H	1:A:68:ASN:HD22	1.43	0.66
1:B:93:GLU:O	1:B:97:ARG:HB2	1.97	0.64
1:A:82:HIS:HD2	1:A:84:GLY:H	1.46	0.64
1:B:942:ASP:N	1:B:942:ASP:OD1	2.31	0.64
1:B:82:HIS:HD2	1:B:84:GLY:H	1.46	0.64
1:B:54:GLY:H	1:B:68:ASN:HD22	1.46	0.64
1:B:253:GLU:OE2	1:B:257:ARG:HD3	1.97	0.63
1:A:304:MET:CE	1:A:399:CYS:HB3	2.29	0.63
1:A:253:GLU:OE2	1:A:257:ARG:HD3	1.98	0.62
1:B:118:ASP:HB3	1:B:121:LYS:HG3	1.82	0.62
1:B:252:SER:O	1:B:256:ASN:ND2	2.31	0.61
1:B:420:ARG:NH1	3:B:1203:FLC:OA1	2.32	0.61
1:A:304:MET:HE3	1:A:399:CYS:HB3	1.82	0.61
1:B:304:MET:CE	1:B:399:CYS:HB3	2.31	0.60
1:B:304:MET:HE3	1:B:399:CYS:HB3	1.83	0.60
1:A:295:VAL:HG22	1:A:314:GLN:HE22	1.65	0.60
1:A:674:CYS:HB3	1:A:712:MET:HE1	1.84	0.59
1:A:674:CYS:CB	1:A:712:MET:HE1	2.33	0.59
1:A:252:SER:O	1:A:256:ASN:ND2	2.33	0.59
1:B:226:HIS:H	1:B:333:GLN:HE22	1.49	0.59
1:B:2:ASN:HB2	1:B:319:ASP:OD2	2.04	0.57
1:B:709:ILE:HD11	1:B:728:LEU:CD1	2.34	0.57
1:A:226:HIS:H	1:A:333:GLN:HE22	1.52	0.56
1:A:2:ASN:HB2	1:A:319:ASP:OD2	2.05	0.56
1:A:709:ILE:HD11	1:A:728:LEU:CD1	2.35	0.56
1:B:369:THR:CG2	1:B:415:ASN:HD22	2.18	0.56
1:A:369:THR:CG2	1:A:415:ASN:HD22	2.19	0.56
1:B:295:VAL:HG22	1:B:314:GLN:HE22	1.69	0.56
1:B:847:VAL:O	1:B:847:VAL:CG1	2.53	0.56
1:A:847:VAL:CG1	1:A:847:VAL:O	2.54	0.56
1:B:878:LYS:NZ	1:B:882:ASP:OD2	2.39	0.55
1:B:243:GLU:OE2	1:B:346:ARG:NH2	2.39	0.55
1:A:369:THR:HG21	1:A:415:ASN:HD22	1.72	0.55
1:B:369:THR:HG21	1:B:415:ASN:HD22	1.72	0.55
1:A:82:HIS:HE1	1:A:314:GLN:OE1	1.89	0.55
1:A:298:GLU:N	1:A:298:GLU:OE2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLY:O	1:B:55:ALA:C	2.46	0.54
1:A:622:ASN:ND2	1:A:917:GLU:O	2.41	0.53
1:B:118:ASP:CB	1:B:121:LYS:HG3	2.39	0.53
1:A:243:GLU:OE2	1:A:346:ARG:NH2	2.41	0.53
1:A:3:ARG:NH1	1:A:319:ASP:O	2.41	0.52
1:B:298:GLU:O	1:B:301:ILE:HG12	2.09	0.52
1:B:82:HIS:HE1	1:B:314:GLN:OE1	1.92	0.52
1:B:298:GLU:N	1:B:298:GLU:OE2	2.42	0.52
1:A:82:HIS:CE1	1:A:314:GLN:OE1	2.63	0.52
1:B:468:LYS:HG2	1:B:992:LYS:O	2.09	0.51
1:A:298:GLU:O	1:A:301:ILE:HG12	2.11	0.51
1:A:15:ILE:HB	1:A:85:TYR:CE2	2.45	0.51
1:A:878:LYS:NZ	1:A:882:ASP:OD2	2.42	0.51
1:B:836:GLN:O	1:B:836:GLN:HG3	2.10	0.50
1:A:468:LYS:HG2	1:A:992:LYS:O	2.10	0.50
1:B:82:HIS:CE1	1:B:314:GLN:OE1	2.64	0.50
1:A:118:ASP:HB3	1:A:121:LYS:HG2	1.92	0.50
1:A:479:ASN:HD21	1:A:1058:MET:H	1.60	0.50
1:A:836:GLN:HG3	1:A:836:GLN:O	2.11	0.50
1:A:915:MET:O	1:A:940:LEU:HD12	2.12	0.50
1:A:510:THR:HG23	1:A:607:MET:HG3	1.93	0.50
1:A:915:MET:O	1:A:940:LEU:CD1	2.60	0.49
1:B:479:ASN:HD21	1:B:1058:MET:H	1.61	0.49
1:A:600:ARG:NH2	1:A:641:ASP:OD2	2.45	0.49
1:B:586:ARG:HD3	1:B:587:PHE:CZ	2.47	0.49
1:B:607:MET:HE1	1:B:668:ILE:HD12	1.94	0.48
1:B:600:ARG:NH2	1:B:641:ASP:OD2	2.46	0.48
1:A:241:VAL:HG12	1:A:242:VAL:HG23	1.94	0.47
1:A:289:ILE:HG13	1:A:290:GLU:HB2	1.95	0.47
1:B:133:VAL:HG12	1:B:134:ILE:N	2.30	0.47
1:B:15:ILE:HB	1:B:85:TYR:CE2	2.49	0.47
1:A:133:VAL:HG12	1:A:134:ILE:N	2.30	0.47
1:B:622:ASN:ND2	1:B:917:GLU:O	2.43	0.47
1:A:301:ILE:HA	1:A:304:MET:HE2	1.96	0.47
1:B:241:VAL:HG12	1:B:242:VAL:HG23	1.95	0.46
1:A:1090:VAL:O	1:A:1090:VAL:HG12	2.16	0.46
1:B:301:ILE:HA	1:B:304:MET:HE2	1.98	0.46
1:B:289:ILE:HG13	1:B:290:GLU:HB2	1.97	0.46
1:B:1090:VAL:O	1:B:1090:VAL:HG12	2.16	0.46
1:B:510:THR:HG23	1:B:607:MET:HG3	1.98	0.45
1:B:847:VAL:O	1:B:847:VAL:HG12	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:MET:HE1	1:A:668:ILE:HD12	1.97	0.45
1:A:225:VAL:CG1	1:A:226:HIS:N	2.80	0.45
1:A:942:ASP:OD2	1:A:947:LEU:HD21	2.17	0.45
1:A:712:MET:HB3	1:A:712:MET:HE3	1.73	0.45
1:B:1124:SER:HB3	1:B:1142:GLU:HB3	1.99	0.45
1:A:600:ARG:HG2	1:A:639:GLY:HA3	1.99	0.45
1:B:96:ARG:HH11	1:B:96:ARG:HG2	1.82	0.45
1:A:847:VAL:O	1:A:847:VAL:HG12	2.16	0.45
1:A:96:ARG:HG2	1:A:96:ARG:HH11	1.82	0.45
1:A:786:VAL:O	1:A:791:GLN:NE2	2.48	0.45
1:B:225:VAL:CG1	1:B:226:HIS:N	2.81	0.44
1:B:369:THR:OG1	1:B:415:ASN:ND2	2.50	0.44
1:A:54:GLY:O	1:A:55:ALA:C	2.56	0.44
1:B:760:ASP:C	1:B:761:ILE:HG13	2.38	0.44
1:A:1124:SER:HB3	1:A:1142:GLU:HB3	2.00	0.44
1:B:300:THR:HG22	1:B:375:ARG:CZ	2.47	0.44
1:A:41:SER:OG	1:A:43:HIS:HD2	2.00	0.44
1:B:786:VAL:O	1:B:791:GLN:NE2	2.50	0.43
1:B:620:TYR:CZ	1:B:621:LYS:HD3	2.53	0.43
1:A:95:ALA:O	1:A:96:ARG:C	2.56	0.43
1:A:502:TYR:CE1	1:B:75:GLU:HG2	2.53	0.43
1:B:95:ALA:O	1:B:96:ARG:C	2.56	0.43
1:B:219:ASP:OD2	1:B:322:ALA:HA	2.18	0.43
1:B:1076:GLU:HG3	1:B:1143:VAL:O	2.19	0.43
1:B:224:ILE:HD12	1:B:267:LYS:HA	2.00	0.43
1:A:44:ARG:NH2	1:B:1015:GLU:OE2	2.51	0.43
1:A:3:ARG:NH1	1:A:3:ARG:HB2	2.34	0.43
1:B:1039:THR:HA	1:B:1056:GLN:HA	2.00	0.43
1:B:544:GLN:HG3	1:B:549:THR:OG1	2.19	0.43
1:B:41:SER:OG	1:B:43:HIS:HD2	2.01	0.43
1:B:295:VAL:CG2	1:B:314:GLN:HE22	2.32	0.43
1:A:240:LYS:HB2	1:A:346:ARG:HH22	1.84	0.43
1:A:760:ASP:C	1:A:761:ILE:HG13	2.40	0.43
1:A:344:GLN:HG3	1:A:399:CYS:SG	2.59	0.42
1:A:300:THR:HG22	1:A:375:ARG:CZ	2.49	0.42
1:A:414:ARG:NH1	1:A:418:GLU:OE1	2.50	0.42
1:A:75:GLU:HG2	1:B:502:TYR:CE1	2.54	0.42
1:B:240:LYS:HB2	1:B:346:ARG:HH22	1.85	0.42
1:B:729:LYS:HD3	1:B:736:ILE:HD12	2.02	0.42
1:B:600:ARG:HG2	1:B:639:GLY:HA3	2.01	0.42
1:A:7:VAL:HG23	1:A:28:ILE:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:VAL:HG23	1:B:28:ILE:HG21	2.00	0.42
1:A:207:MET:HB2	1:A:282:GLU:OE2	2.20	0.42
1:A:981:LYS:HE3	1:A:981:LYS:HB2	1.88	0.42
1:A:1076:GLU:HG3	1:A:1143:VAL:O	2.20	0.42
1:B:616:ASN:CB	1:B:621:LYS:O	2.63	0.41
1:A:830:HIS:CD2	1:A:832:MET:HG3	2.55	0.41
1:A:304:MET:HE1	1:A:399:CYS:CB	2.50	0.41
1:A:224:ILE:HD12	1:A:267:LYS:HA	2.01	0.41
1:A:866:MET:SD	1:A:894:GLU:HG3	2.60	0.41
1:A:586:ARG:HD3	1:A:587:PHE:CZ	2.54	0.41
1:A:369:THR:OG1	1:A:415:ASN:ND2	2.53	0.41
1:A:219:ASP:OD2	1:A:322:ALA:HA	2.19	0.41
1:B:830:HIS:CD2	1:B:832:MET:HG3	2.55	0.41
1:B:344:GLN:HG3	1:B:399:CYS:SG	2.61	0.41
1:B:414:ARG:NH1	1:B:418:GLU:OE1	2.52	0.41
1:B:324:HIS:O	1:B:325:ASP:C	2.59	0.41
1:B:591:ASP:HA	1:B:592:PRO:HD2	1.92	0.41
1:A:1039:THR:HA	1:A:1056:GLN:HA	2.02	0.41
1:A:226:HIS:NE2	1:A:259:CYS:HB3	2.35	0.41
1:B:226:HIS:NE2	1:B:259:CYS:HB3	2.35	0.41
1:A:295:VAL:CG2	1:A:314:GLN:HE22	2.29	0.41
1:B:674:CYS:CB	1:B:712:MET:HE1	2.51	0.41
1:B:688:THR:O	1:B:691:TYR:HB3	2.20	0.41
1:A:109:LYS:H	1:A:112:HIS:HD2	1.69	0.41
1:B:740:THR:HG22	1:B:751:TYR:CE1	2.55	0.41
1:B:874:THR:HA	1:B:875:PRO:HA	1.91	0.41
1:B:866:MET:SD	1:B:894:GLU:HG3	2.61	0.41
1:B:207:MET:HB2	1:B:282:GLU:OE2	2.21	0.41
1:A:118:ASP:CB	1:A:121:LYS:HG2	2.50	0.41
1:A:607:MET:HE2	1:A:641:ASP:HB3	2.03	0.40
1:B:712:MET:HB3	1:B:712:MET:HE3	1.52	0.40
1:A:216:ILE:HG13	1:A:266:MET:HG3	2.04	0.40
1:A:282:GLU:O	1:A:284:ASP:N	2.54	0.40
1:A:688:THR:O	1:A:691:TYR:HB3	2.21	0.40
1:A:648:SER:HA	1:A:873:VAL:HG13	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2000:2BA:P	2:A:2000:2BA:O3'[2_757]	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1202:2BA:P	2:B:1202:2BA:O3'[2_757]	1.82	0.38

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	1067/1147 (93%)	1004 (94%)	60 (6%)	3 (0%)	46 75
1	B	1067/1147 (93%)	1007 (94%)	57 (5%)	3 (0%)	46 75
All	All	2134/2294 (93%)	2011 (94%)	117 (6%)	6 (0%)	46 75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	GLY
1	B	283	GLY
1	A	273	ASN
1	B	273	ASN
1	A	869	ASP
1	B	869	ASP

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	917/982 (93%)	855 (93%)	62 (7%)	20 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	920/982 (94%)	857 (93%)	63 (7%)	20 43
All	All	1837/1964 (94%)	1712 (93%)	125 (7%)	20 43

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	3	ARG
1	A	42	PHE
1	A	44	ARG
1	A	70	ILE
1	A	110	SER
1	A	118	ASP
1	A	119	LYS
1	A	120	ILE
1	A	226	HIS
1	A	248	ASN
1	A	252	SER
1	A	254	LEU
1	A	273	ASN
1	A	294	ARG
1	A	295	VAL
1	A	326	GLN
1	A	357	MET
1	A	377	ASP
1	A	387	VAL
1	A	393	SER
1	A	419	PHE
1	A	451	ASP
1	A	462	ILE
1	A	463	ARG
1	A	510	THR
1	A	549	THR
1	A	576	TRP
1	A	582	ASP
1	A	600	ARG
1	A	613	ARG
1	A	644	ARG
1	A	682	ASP
1	A	712	MET
1	A	766	SER
1	A	791	GLN

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Mol	Chain	Res	Type
1	A	807	GLU
1	A	827	VAL
1	A	836	GLN
1	A	839	ASN
1	A	842	GLN
1	A	851	ASP
1	A	927	GLU
1	A	937	ARG
1	A	940	LEU
1	A	942	ASP
1	A	967	GLU
1	A	981	LYS
1	A	982	VAL
1	A	997	THR
1	A	1025	LEU
1	A	1060	VAL
1	A	1067	ARG
1	A	1092	LYS
1	A	1107	GLU
1	A	1109	MET
1	A	1111	MET
1	A	1113	THR
1	A	1119	PHE
1	A	1120	ASP
1	A	1129	SER
1	A	1130	ASP
1	B	1	MET
1	B	2	ASN
1	B	42	PHE
1	B	44	ARG
1	B	70	ILE
1	B	110	SER
1	B	118	ASP
1	B	120	ILE
1	B	226	HIS
1	B	248	ASN
1	B	252	SER
1	B	254	LEU
1	B	273	ASN
1	B	294	ARG
1	B	295	VAL
1	B	326	GLN

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Mol	Chain	Res	Type
1	B	357	MET
1	B	377	ASP
1	B	387	VAL
1	B	393	SER
1	B	419	PHE
1	B	451	ASP
1	B	462	ILE
1	B	463	ARG
1	B	507	SER
1	B	510	THR
1	B	549	THR
1	B	576	TRP
1	B	582	ASP
1	B	600	ARG
1	B	613	ARG
1	B	616	ASN
1	B	621	LYS
1	B	682	ASP
1	B	712	MET
1	B	766	SER
1	B	791	GLN
1	B	807	GLU
1	B	827	VAL
1	B	836	GLN
1	B	839	ASN
1	B	842	GLN
1	B	851	ASP
1	B	927	GLU
1	B	937	ARG
1	B	940	LEU
1	B	942	ASP
1	B	967	GLU
1	B	981	LYS
1	B	982	VAL
1	B	997	THR
1	B	1025	LEU
1	B	1060	VAL
1	B	1067	ARG
1	B	1105	ILE
1	B	1107	GLU
1	B	1109	MET
1	B	1111	MET

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Mol	Chain	Res	Type
1	B	1113	THR
1	B	1119	PHE
1	B	1120	ASP
1	B	1129	SER
1	B	1130	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	68	ASN
1	A	82	HIS
1	A	112	HIS
1	A	223	ASN
1	A	292	ASN
1	A	312	GLN
1	A	333	GLN
1	A	383	GLN
1	A	415	ASN
1	A	479	ASN
1	A	746	ASN
1	A	797	GLN
1	A	821	ASN
1	A	830	HIS
1	B	43	HIS
1	B	68	ASN
1	B	82	HIS
1	B	112	HIS
1	B	223	ASN
1	B	292	ASN
1	B	312	GLN
1	B	333	GLN
1	B	383	GLN
1	B	415	ASN
1	B	479	ASN
1	B	616	ASN
1	B	746	ASN
1	B	797	GLN
1	B	821	ASN
1	B	830	HIS

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 6 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
2	2BA	A	2000	-	15,24,50	1.25	1 (6%)	16,35,78	2.21	3 (18%)
3	FLC	A	2001	-	3,12,12	1.51	1 (33%)	3,17,17	2.73	2 (66%)
2	2BA	B	1202	-	15,24,50	1.28	1 (6%)	16,35,78	2.37	3 (18%)
3	FLC	B	1203	-	3,12,12	1.25	0	3,17,17	1.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2BA	A	2000	-	-	0/3/25/62	0/3/3/7
3	FLC	A	2001	-	-	0/6/16/16	0/0/0/0
2	2BA	B	1202	-	-	0/3/25/62	0/3/3/7
3	FLC	B	1203	-	-	0/6/16/16	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	FLC	CG-CB	2.31	1.58	1.54
2	B	1202	2BA	C5-C4	2.62	1.46	1.40
2	A	2000	2BA	C5-C4	2.76	1.46	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1202	2BA	N3-C2-N1	-7.40	123.23	128.89
2	A	2000	2BA	N3-C2-N1	-6.85	123.65	128.89
2	B	1202	2BA	C1'-N9-C4	-4.57	120.05	126.94
3	A	2001	FLC	CB-CA-CAC	-3.37	109.56	114.96
2	A	2000	2BA	C4-C5-N7	-2.89	106.82	109.48
2	B	1202	2BA	C2'-C1'-N9	-2.32	110.75	114.29
3	A	2001	FLC	CG-CB-CA	3.28	117.66	109.81
2	A	2000	2BA	O5'-C5'-C4'	3.45	121.75	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2000	2BA	0	1
2	B	1202	2BA	0	1
3	B	1203	FLC	1	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, 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	1073/1147 (93%)	0.04	42 (3%)	43	43	47, 73, 115, 152	0
1	B	1073/1147 (93%)	-0.10	39 (3%)	46	46	34, 64, 104, 140	0
All	All	2146/2294 (93%)	-0.03	81 (3%)	44	44	34, 68, 109, 152	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	906	PHE	5.6
1	B	1120	ASP	4.9
1	A	904	ILE	4.6
1	B	135	PRO	4.5
1	A	903	THR	4.4
1	A	934	LEU	4.2
1	B	1123	VAL	4.1
1	B	1100	GLY	4.1
1	A	502	TYR	4.0
1	A	207	MET	3.9
1	A	1090	VAL	3.6
1	B	287	TYR	3.4
1	B	1096	SER	3.4
1	A	905	ASP	3.4
1	A	898	TYR	3.3
1	A	1102	PRO	3.3
1	B	207	MET	3.3
1	A	135	PRO	3.3
1	A	1100	GLY	3.2
1	B	1097	VAL	3.2
1	A	936	GLY	3.2
1	A	886	PHE	3.1
1	A	933	VAL	3.1
1	B	134	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	210	LYS	3.0
1	B	835	GLY	3.0
1	A	528	LYS	3.0
1	A	897	VAL	3.0
1	A	1120	ASP	2.9
1	B	1105	ILE	2.9
1	A	1118	PRO	2.9
1	B	1115	ILE	2.8
1	A	620	TYR	2.8
1	B	1113	THR	2.8
1	B	208	ASN	2.7
1	B	1066	ALA	2.7
1	B	1108	ALA	2.7
1	B	1141	ILE	2.6
1	A	902	ASP	2.6
1	B	288	PHE	2.5
1	B	368	SER	2.5
1	B	1143	VAL	2.5
1	A	503	GLY	2.5
1	B	1116	GLN	2.5
1	B	1142	GLU	2.5
1	A	1096	SER	2.5
1	B	1091	VAL	2.4
1	B	289	ILE	2.4
1	A	937	ARG	2.4
1	B	874	THR	2.4
1	A	368	SER	2.3
1	A	1119	PHE	2.3
1	B	502	TYR	2.3
1	A	287	TYR	2.3
1	B	280	LEU	2.3
1	B	1118	PRO	2.3
1	A	504	SER	2.3
1	B	1103	LEU	2.3
1	A	1092	LYS	2.2
1	A	773	THR	2.2
1	B	369	THR	2.2
1	B	1102	PRO	2.2
1	A	1097	VAL	2.2
1	B	1088	GLN	2.2
1	A	896	ASP	2.2
1	A	206	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	820	LEU	2.1
1	B	127	LEU	2.1
1	B	1090	VAL	2.1
1	B	1114	THR	2.1
1	B	1119	PHE	2.1
1	A	966	TYR	2.1
1	A	835	GLY	2.1
1	A	205	CYS	2.1
1	A	399	CYS	2.1
1	A	398	LEU	2.1
1	A	935	LYS	2.1
1	A	1101	ASP	2.1
1	A	505	GLN	2.0
1	B	123	LYS	2.0
1	B	1101	ASP	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
4	MN	A	2002	1/1	0.99	0.28	1.03	91,91,91,91	0
4	MN	B	1201	1/1	0.97	0.26	0.95	65,65,65,65	0
2	2BA	A	2000	22/44	0.97	0.12	-0.64	52,62,76,79	0
3	FLC	A	2001	13/13	0.92	0.13	-1.19	73,82,88,91	0
3	FLC	B	1203	13/13	0.93	0.13	-1.47	64,78,86,87	0
2	2BA	B	1202	22/44	0.98	0.10	-1.78	41,49,53,54	0

6.5 Other polymers (i)

There are no such residues in this entry.