Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:25 PM GMT

PDB ID	:	1OYE
Title	:	Structural Basis of Multiple Binding Capacity of the AcrB multidrug Efflux Pump
Authors	:	Yu, E.W.; McDermott, G.; Zgurskaya, H.I.; Nikaido, H.; Koshland Jr., D.E.
Deposited on	:	2003-04-03
Resolution	:	3.48 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:

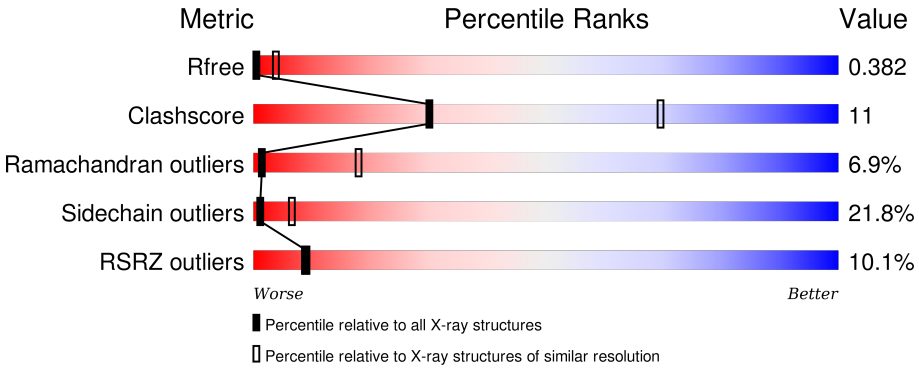
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.48 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	1173 (3.60-3.36)
Clashscore	102246	1010 (3.58-3.38)
Ramachandran outliers	100387	1245 (3.60-3.36)
Sidechain outliers	100360	1246 (3.60-3.36)
RSRZ outliers	91569	1180 (3.60-3.36)

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	1049	10% 56% 32% 7%

2 Entry composition

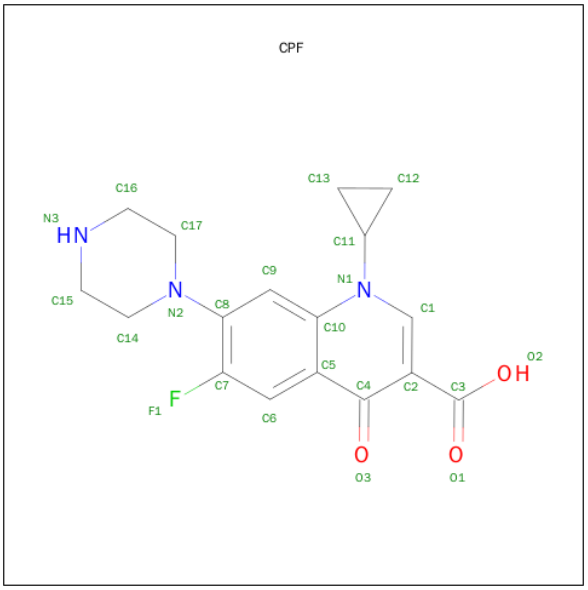
There are 2 unique types of molecules in this entry. The entry contains 7663 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1006	7639	4916	1262	1419	42	0	0	0

- Molecule 2 is 1-CYCLOPROPYL-6-FLUORO-4-OXO-7-PIPERAZIN-1-YL-1,4-DIHYDRO QUINOLINE-3-CARBOXYLIC ACID (three-letter code: CPF) (formula: $C_{17}H_{18}FN_3O_3$).



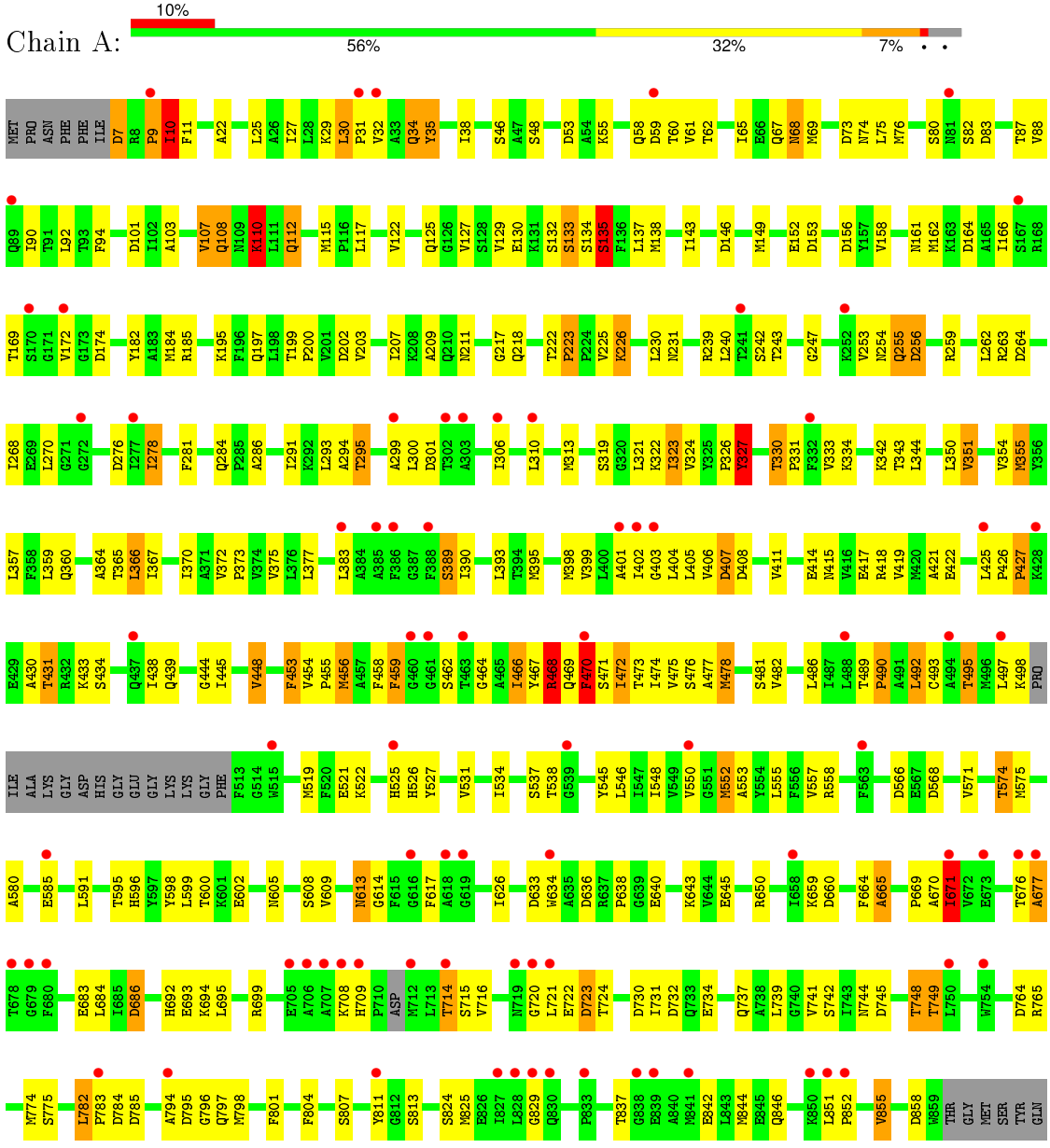
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	24	17	1	3	3	0	0

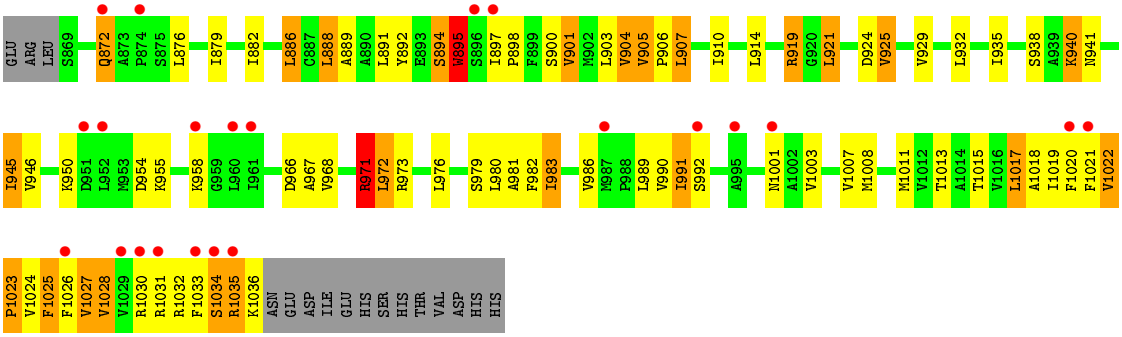
3 Residue-property plots (i)

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: Acriflavine resistance protein B

Chain A:




GLU ARG LEU S869 Q872 A873 P874 S875 L876 I879 I882 L886 C887 L888 A889 A890 L891 Y892 E893 S894 W895 S896 I897 P898 F899 S900 V901 N902 L903 V904 V905 P906 L907 I910 L914 R919 G920 L921 D924 V925 V929 L932 I935 S938 A939 K940 N941
I945 V946 K950 D951 L952 N953 D954 K955 K958 G959 L960 I961 D966 A967 V968 R971 I972 R973 L976 S979 I980 A981 F982 I983 V986 N987 F988 L989 V990 I991 S992 A995 N1001 A1002 V1003 V1007 M1008 M1011 V1012 T1013 A1014 T1015 V1016 L1017 A1018 I1019 F1020 F1021 V1022
P1023 V1024 F1025 F1026 V1027 V1028 V1029 R1030 R1031 R1032 F1033 S1034 R1035 K1036 ASN GLU ASP ILE GLU HIS SER HIS THR VAL ASP HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	145.11Å 145.11Å 517.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.60 – 3.48 45.05 – 3.48	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.60-3.48) 99.1 (45.05-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.257 , 0.323 0.382 , 0.382	Depositor DCC
R_{free} test set	1390 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	132.4	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 45.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 27189 reflections	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	7663	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: CPF

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	0.34	0/7779	0.70	34/10563 (0.3%)

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	1	0

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	407	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	795	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	470	PHE	N-CA-C	6.18	127.69	111.00
1	A	568	ASP	CB-CG-OD2	6.07	123.77	118.30
1	A	858	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	59	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	174	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	924	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	7	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	146	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	730	ASP	CB-CG-OD2	5.36	123.13	118.30
1	A	408	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	276	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	101	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	732	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	660	ASP	CB-CG-OD2	5.28	123.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	785	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	83	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	784	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	566	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	764	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	202	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	966	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	723	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	636	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	53	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	256	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	153	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	745	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	633	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	264	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	301	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	73	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	954	ASP	CB-CG-OD2	5.00	122.80	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	470	PHE	CA

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	7639	0	7800	172	1
2	A	24	0	17	0	0
All	All	7663	0	7817	172	1

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 (172) 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:613:ASN:HD22	1:A:613:ASN:C	1.76	0.89
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.63	0.79
1:A:1023:PRO:HA	1:A:1026:PHE:HB2	1.67	0.76
1:A:448:VAL:HG11	1:A:888:LEU:HD23	1.68	0.75
1:A:393:LEU:HD11	1:A:466:ILE:HA	1.75	0.69
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.75	0.69
1:A:354:VAL:HG13	1:A:980:LEU:HD23	1.76	0.68
1:A:910:ILE:HG23	1:A:1013:THR:HG21	1.75	0.68
1:A:596:HIS:O	1:A:600:THR:HG22	1.95	0.66
1:A:343:THR:HG21	1:A:989:LEU:HD21	1.79	0.65
1:A:1015:THR:O	1:A:1019:ILE:HG22	1.97	0.65
1:A:613:ASN:C	1:A:613:ASN:ND2	2.49	0.63
1:A:979:SER:O	1:A:983:ILE:HG13	1.99	0.62
1:A:670:ALA:O	1:A:671:ILE:O	2.16	0.62
1:A:370:ILE:O	1:A:370:ILE:HG22	2.00	0.62
1:A:1018:ALA:HB1	1:A:1024:VAL:HG21	1.82	0.61
1:A:888:LEU:HD11	1:A:901:VAL:HB	1.83	0.59
1:A:888:LEU:HD12	1:A:898:PRO:HA	1.84	0.59
1:A:982:PHE:CD2	1:A:1011:MET:HG3	2.37	0.59
1:A:367:ILE:HG23	1:A:492:LEU:HD13	1.84	0.59
1:A:403:GLY:HA3	1:A:982:PHE:CD1	2.37	0.59
1:A:466:ILE:H	1:A:466:ILE:HD12	1.66	0.59
1:A:351:VAL:HG23	1:A:981:ALA:HB1	1.84	0.59
1:A:454:VAL:N	1:A:455:PRO:HD2	2.18	0.59
1:A:475:VAL:HG22	1:A:478:MET:CE	2.32	0.59
1:A:968:VAL:HB	1:A:1025:PHE:HZ	1.67	0.58
1:A:575:MET:HB3	1:A:626:ILE:HD12	1.85	0.58
1:A:475:VAL:HG22	1:A:478:MET:HE1	1.85	0.58
1:A:218:GLN:HE21	1:A:231:ASN:HD21	1.51	0.58
1:A:112:GLN:HG2	1:A:112:GLN:O	2.03	0.57
1:A:390:ILE:HG23	1:A:395:MET:SD	2.44	0.57
1:A:291:ILE:HG21	1:A:306:ILE:HD11	1.86	0.56
1:A:613:ASN:HD22	1:A:614:GLY:N	2.03	0.56
1:A:359:LEU:HD13	1:A:364:ALA:HB1	1.86	0.56
1:A:372:VAL:N	1:A:373:PRO:HD2	2.21	0.56
1:A:399:VAL:HA	1:A:402:ILE:HD12	1.87	0.54
1:A:108:GLN:HB2	1:A:129:VAL:HG21	1.89	0.54
1:A:716:VAL:HG12	1:A:829:GLY:HA3	1.89	0.53
1:A:903:LEU:O	1:A:906:PRO:HD2	2.08	0.53
1:A:527:TYR:OH	1:A:1019:ILE:O	2.24	0.53
1:A:897:ILE:HG23	1:A:946:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1018:ALA:CB	1:A:1024:VAL:HG21	2.39	0.53
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	1.92	0.52
1:A:709:HIS:CG	1:A:709:HIS:O	2.62	0.52
1:A:403:GLY:HA3	1:A:982:PHE:CE1	2.45	0.52
1:A:30:LEU:HD23	1:A:390:ILE:HG13	1.91	0.52
1:A:468:ARG:O	1:A:472:ILE:HG22	2.09	0.52
1:A:684:LEU:HD11	1:A:855:VAL:HG13	1.92	0.52
1:A:9:PRO:C	1:A:10:ILE:HD13	2.31	0.52
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.92	0.51
1:A:343:THR:CG2	1:A:989:LEU:HD21	2.40	0.51
1:A:401:ALA:O	1:A:405:LEU:HG	2.11	0.51
1:A:489:THR:HB	1:A:490:PRO:HD3	1.93	0.51
1:A:546:LEU:O	1:A:550:VAL:HG23	2.10	0.51
1:A:721:LEU:HD22	1:A:825:MET:CE	2.41	0.50
1:A:326:PRO:O	1:A:327:TYR:C	2.48	0.50
1:A:172:VAL:HG13	1:A:291:ILE:HG23	1.94	0.50
1:A:525:HIS:O	1:A:527:TYR:N	2.43	0.50
1:A:695:LEU:HD22	1:A:825:MET:SD	2.51	0.50
1:A:402:ILE:HA	1:A:405:LEU:HD12	1.93	0.50
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.92	0.50
1:A:979:SER:HB2	1:A:1015:THR:HG21	1.94	0.49
1:A:468:ARG:HG2	1:A:469:GLN:N	2.27	0.49
1:A:373:PRO:O	1:A:377:LEU:HG	2.12	0.49
1:A:907:LEU:O	1:A:1013:THR:HG22	2.12	0.49
1:A:454:VAL:HG22	1:A:475:VAL:HG21	1.93	0.49
1:A:10:ILE:HG12	1:A:11:PHE:CD2	2.45	0.49
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.93	0.49
1:A:971:ARG:C	1:A:971:ARG:HD2	2.33	0.49
1:A:456:MET:HA	1:A:876:LEU:HB3	1.95	0.49
1:A:300:LEU:HD22	1:A:333:VAL:HG11	1.94	0.49
1:A:365:THR:O	1:A:365:THR:HG23	2.12	0.49
1:A:904:VAL:HG13	1:A:1024:VAL:HG22	1.95	0.49
1:A:294:ALA:O	1:A:295:THR:C	2.51	0.49
1:A:897:ILE:N	1:A:898:PRO:CD	2.76	0.49
1:A:466:ILE:HG23	1:A:925:VAL:HG21	1.94	0.49
1:A:401:ALA:HB2	1:A:474:ILE:HG12	1.95	0.48
1:A:407:ASP:O	1:A:411:VAL:HG23	2.13	0.48
1:A:211:ASN:HA	1:A:240:LEU:HD23	1.94	0.48
1:A:894:SER:O	1:A:895:TRP:HB2	2.14	0.48
1:A:595:THR:HG22	1:A:599:LEU:HD12	1.96	0.48
1:A:92:LEU:HD22	1:A:107:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.43	0.47
1:A:967:ALA:O	1:A:971:ARG:HG3	2.14	0.47
1:A:945:ILE:HA	1:A:971:ARG:NH1	2.29	0.47
1:A:426:PRO:N	1:A:427:PRO:HD2	2.29	0.47
1:A:1022:VAL:CG2	1:A:1023:PRO:HD2	2.39	0.47
1:A:425:LEU:C	1:A:427:PRO:HD2	2.35	0.47
1:A:482:VAL:O	1:A:486:LEU:HG	2.15	0.47
1:A:721:LEU:HD22	1:A:825:MET:HE2	1.95	0.47
1:A:664:PHE:O	1:A:665:ALA:HB2	2.15	0.47
1:A:90:ILE:HD12	1:A:90:ILE:N	2.29	0.47
1:A:905:VAL:HG13	1:A:935:ILE:HG12	1.96	0.46
1:A:744:ASN:O	1:A:748:THR:HG22	2.16	0.46
1:A:448:VAL:CG1	1:A:888:LEU:HD23	2.43	0.46
1:A:405:LEU:HD23	1:A:481:SER:HB3	1.96	0.46
1:A:434:SER:O	1:A:438:ILE:HG13	2.15	0.46
1:A:493:CYS:O	1:A:497:LEU:HB2	2.16	0.46
1:A:405:LEU:HD21	1:A:477:ALA:HB1	1.96	0.46
1:A:466:ILE:CG2	1:A:925:VAL:HG21	2.46	0.46
1:A:278:ILE:HG13	1:A:613:ASN:HB3	1.98	0.46
1:A:222:THR:HB	1:A:223:PRO:HD3	1.98	0.46
1:A:1024:VAL:O	1:A:1025:PHE:CG	2.69	0.46
1:A:851:LEU:HB3	1:A:852:PRO:CD	2.46	0.46
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.51	0.46
1:A:247:GLY:HA2	1:A:268:ILE:HD12	1.97	0.46
1:A:200:PRO:HD2	1:A:749:THR:HG23	1.98	0.46
1:A:892:TYR:HB3	1:A:897:ILE:HD13	1.98	0.45
1:A:472:ILE:HA	1:A:475:VAL:HB	1.97	0.45
1:A:907:LEU:HG	1:A:1017:LEU:HD23	1.98	0.45
1:A:1022:VAL:O	1:A:1023:PRO:O	2.34	0.45
1:A:453:PHE:HE2	1:A:474:ILE:HB	1.82	0.45
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.98	0.45
1:A:92:LEU:HD13	1:A:107:VAL:HG21	1.99	0.45
1:A:545:TYR:HA	1:A:548:ILE:HD12	1.99	0.45
1:A:855:VAL:O	1:A:855:VAL:HG12	2.17	0.44
1:A:403:GLY:HA3	1:A:982:PHE:HD1	1.81	0.44
1:A:68:ASN:HD22	1:A:110:LYS:HD2	1.82	0.44
1:A:972:LEU:HD13	1:A:972:LEU:C	2.38	0.44
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.99	0.44
1:A:30:LEU:CD2	1:A:390:ILE:HG13	2.48	0.44
1:A:851:LEU:HB3	1:A:852:PRO:HD2	2.00	0.44
1:A:879:ILE:HA	1:A:882:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:GLY:HA2	1:A:891:LEU:HD23	2.00	0.43
1:A:531:VAL:O	1:A:534:ILE:HG12	2.18	0.43
1:A:919:ARG:HB3	1:A:921:LEU:HD23	2.00	0.43
1:A:94:PHE:CE2	1:A:103:ALA:HB1	2.53	0.43
1:A:929:VAL:HA	1:A:932:LEU:HD12	2.00	0.43
1:A:1033:PHE:O	1:A:1035:ARG:N	2.52	0.43
1:A:986:VAL:HG12	1:A:990:VAL:CG2	2.49	0.43
1:A:456:MET:O	1:A:876:LEU:HD13	2.19	0.43
1:A:203:VAL:O	1:A:207:ILE:HG13	2.18	0.43
1:A:1033:PHE:O	1:A:1034:SER:C	2.57	0.43
1:A:310:LEU:HD21	1:A:323:ILE:HD12	2.00	0.43
1:A:330:THR:HB	1:A:331:PRO:HD3	2.01	0.43
1:A:62:THR:OG1	1:A:88:VAL:HG21	2.19	0.43
1:A:782:LEU:HB3	1:A:783:PRO:HD2	2.01	0.43
1:A:31:PRO:HG2	1:A:389:SER:HB3	2.01	0.42
1:A:1003:VAL:O	1:A:1007:VAL:HG23	2.20	0.42
1:A:886:LEU:N	1:A:886:LEU:HD23	2.34	0.42
1:A:892:TYR:HB3	1:A:897:ILE:HG21	2.00	0.42
1:A:351:VAL:CG2	1:A:981:ALA:HB1	2.47	0.42
1:A:34:GLN:HG2	1:A:333:VAL:HG22	2.01	0.42
1:A:419:VAL:HG12	1:A:430:ALA:HB1	2.02	0.42
1:A:553:ALA:O	1:A:557:VAL:HG23	2.19	0.42
1:A:158:VAL:HG22	1:A:162:MET:CE	2.50	0.42
1:A:941:ASN:HD21	1:A:1015:THR:HG22	1.85	0.42
1:A:458:PHE:O	1:A:459:PHE:O	2.37	0.42
1:A:1027:VAL:HG23	1:A:1028:VAL:H	1.85	0.41
1:A:990:VAL:O	1:A:1001:ASN:ND2	2.53	0.41
1:A:398:MET:O	1:A:402:ILE:HG13	2.20	0.41
1:A:686:ASP:HB2	1:A:695:LEU:HD12	2.02	0.41
1:A:470:PHE:CD1	1:A:929:VAL:HG11	2.55	0.41
1:A:133:SER:O	1:A:135:SER:N	2.54	0.41
1:A:466:ILE:HG22	1:A:467:TYR:N	2.36	0.41
1:A:108:GLN:HB3	1:A:129:VAL:HG11	2.02	0.41
1:A:383:LEU:HD11	1:A:473:THR:HG23	2.03	0.41
1:A:676:THR:O	1:A:677:ALA:HB3	2.21	0.41
1:A:419:VAL:CG1	1:A:430:ALA:HB1	2.51	0.41
1:A:254:ASN:O	1:A:256:ASP:N	2.54	0.41
1:A:574:THR:HG21	1:A:598:TYR:OH	2.21	0.41
1:A:65:ILE:O	1:A:69:MET:HB2	2.21	0.41
1:A:905:VAL:HB	1:A:906:PRO:CD	2.51	0.41
1:A:207:ILE:HG22	1:A:211:ASN:HD22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:O	1:A:370:ILE:CG2	2.69	0.40
1:A:709:HIS:CD2	1:A:709:HIS:O	2.75	0.40
1:A:968:VAL:HG22	1:A:972:LEU:HB2	2.03	0.40
1:A:390:ILE:O	1:A:390:ILE:HG22	2.21	0.40
1:A:580:ALA:HB1	1:A:724:THR:HG22	2.04	0.40
1:A:469:GLN:HA	1:A:472:ILE:HG23	2.02	0.40
1:A:355:MET:HA	1:A:355:MET:HE2	2.04	0.40
1:A:9:PRO:HB3	1:A:495:THR:OG1	2.21	0.40

All (1) 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)
1:A:226:LYS:O	1:A:596:HIS:NE2[12_455]	2.06	0.14

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	998/1049 (95%)	788 (79%)	141 (14%)	69 (7%)	1 18

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	255	GLN
1	A	459	PHE
1	A	466	ILE
1	A	526	HIS
1	A	665	ALA
1	A	671	ILE
1	A	714	THR

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Mol	Chain	Res	Type
1	A	794	ALA
1	A	901	VAL
1	A	1017	LEU
1	A	1021	PHE
1	A	1023	PRO
1	A	1025	PHE
1	A	1034	SER
1	A	9	PRO
1	A	134	SER
1	A	135	SER
1	A	152	GLU
1	A	161	ASN
1	A	169	THR
1	A	295	THR
1	A	327	TYR
1	A	427	PRO
1	A	431	THR
1	A	464	GLY
1	A	468	ARG
1	A	521	GLU
1	A	775	SER
1	A	872	GLN
1	A	894	SER
1	A	900	SER
1	A	940	LYS
1	A	955	LYS
1	A	1027	VAL
1	A	34	GLN
1	A	74	ASN
1	A	110	LYS
1	A	209	ALA
1	A	366	LEU
1	A	421	ALA
1	A	495	THR
1	A	720	GLY
1	A	889	ALA
1	A	895	TRP
1	A	22	ALA
1	A	184	MET
1	A	299	ALA
1	A	522	LYS
1	A	538	THR

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Mol	Chain	Res	Type
1	A	638	PRO
1	A	722	GLU
1	A	723	ASP
1	A	971	ARG
1	A	992	SER
1	A	35	TYR
1	A	133	SER
1	A	677	ALA
1	A	837	THR
1	A	197	GLN
1	A	552	MET
1	A	571	VAL
1	A	330	THR
1	A	223	PRO
1	A	490	PRO
1	A	669	PRO
1	A	796	GLY
1	A	217	GLY
1	A	991	ILE

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	818/855 (96%)	640 (78%)	178 (22%)	1 6

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	10	ILE
1	A	25	LEU
1	A	27	ILE
1	A	29	LYS
1	A	30	LEU
1	A	32	VAL

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Mol	Chain	Res	Type
1	A	35	TYR
1	A	38	ILE
1	A	46	SER
1	A	48	SER
1	A	55	LYS
1	A	58	GLN
1	A	67	GLN
1	A	68	ASN
1	A	75	LEU
1	A	76	MET
1	A	80	SER
1	A	82	SER
1	A	87	THR
1	A	107	VAL
1	A	108	GLN
1	A	110	LYS
1	A	112	GLN
1	A	115	MET
1	A	117	LEU
1	A	122	VAL
1	A	125	GLN
1	A	127	VAL
1	A	130	GLU
1	A	132	SER
1	A	135	SER
1	A	137	LEU
1	A	138	MET
1	A	149	MET
1	A	156	ASP
1	A	164	ASP
1	A	166	ILE
1	A	182	TYR
1	A	185	ARG
1	A	195	LYS
1	A	199	THR
1	A	225	VAL
1	A	226	LYS
1	A	230	LEU
1	A	239	ARG
1	A	242	SER
1	A	243	THR
1	A	253	VAL

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Mol	Chain	Res	Type
1	A	255	GLN
1	A	259	ARG
1	A	263	ARG
1	A	270	LEU
1	A	278	ILE
1	A	284	GLN
1	A	293	LEU
1	A	313	MET
1	A	319	SER
1	A	321	LEU
1	A	322	LYS
1	A	323	ILE
1	A	327	TYR
1	A	334	LYS
1	A	342	LYS
1	A	350	LEU
1	A	351	VAL
1	A	355	MET
1	A	357	LEU
1	A	360	GLN
1	A	366	LEU
1	A	389	SER
1	A	404	LEU
1	A	406	VAL
1	A	414	GLU
1	A	415	ASN
1	A	417	GLU
1	A	418	ARG
1	A	422	GLU
1	A	431	THR
1	A	433	LYS
1	A	439	GLN
1	A	445	ILE
1	A	448	VAL
1	A	453	PHE
1	A	456	MET
1	A	462	SER
1	A	468	ARG
1	A	470	PHE
1	A	471	SER
1	A	472	ILE
1	A	476	SER

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Mol	Chain	Res	Type
1	A	478	MET
1	A	492	LEU
1	A	498	LYS
1	A	519	MET
1	A	537	SER
1	A	552	MET
1	A	555	LEU
1	A	558	ARG
1	A	574	THR
1	A	585	GLU
1	A	591	LEU
1	A	602	GLU
1	A	605	ASN
1	A	608	SER
1	A	609	VAL
1	A	613	ASN
1	A	617	PHE
1	A	634	TRP
1	A	640	GLU
1	A	643	LYS
1	A	645	GLU
1	A	650	ARG
1	A	659	LYS
1	A	671	ILE
1	A	683	GLU
1	A	686	ASP
1	A	692	HIS
1	A	693	GLU
1	A	694	LYS
1	A	699	ARG
1	A	708	LYS
1	A	714	THR
1	A	715	SER
1	A	731	ILE
1	A	734	GLU
1	A	737	GLN
1	A	739	LEU
1	A	741	VAL
1	A	742	SER
1	A	748	THR
1	A	749	THR
1	A	765	ARG

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Mol	Chain	Res	Type
1	A	774	MET
1	A	782	LEU
1	A	797	GLN
1	A	798	MET
1	A	801	PHE
1	A	804	PHE
1	A	807	SER
1	A	811	TYR
1	A	813	SER
1	A	824	SER
1	A	842	GLU
1	A	844	MET
1	A	846	GLN
1	A	855	VAL
1	A	872	GLN
1	A	886	LEU
1	A	888	LEU
1	A	895	TRP
1	A	904	VAL
1	A	905	VAL
1	A	907	LEU
1	A	914	LEU
1	A	919	ARG
1	A	921	LEU
1	A	925	VAL
1	A	938	SER
1	A	940	LYS
1	A	945	ILE
1	A	950	LYS
1	A	958	LYS
1	A	971	ARG
1	A	972	LEU
1	A	973	ARG
1	A	976	LEU
1	A	983	ILE
1	A	991	ILE
1	A	1008	MET
1	A	1020	PHE
1	A	1022	VAL
1	A	1028	VAL
1	A	1030	ARG
1	A	1031	ARG

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Mol	Chain	Res	Type
1	A	1032	ARG
1	A	1035	ARG
1	A	1036	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	124	GLN
1	A	181	GLN
1	A	194	ASN
1	A	218	GLN
1	A	228	GLN
1	A	284	GLN
1	A	605	ASN
1	A	613	ASN
1	A	622	GLN
1	A	667	ASN
1	A	760	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

1 ligand is 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	CPF	A	5001	-	21,27,27	0.95	1 (4%)	28,40,40	1.15	2 (7%)

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	CPF	A	5001	-	-	0/4/22/22	0/3/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5001	CPF	C4-C5	3.40	1.45	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	5001	CPF	C2-C4-C5	-3.50	115.92	121.87
2	A	5001	CPF	C4-C5-C10	2.92	121.39	118.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1006/1049 (95%)	0.65	102 (10%)	9	9	74, 104, 116, 130	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	679	GLY	7.3
1	A	1021	PHE	6.9
1	A	676	THR	5.5
1	A	658	ILE	5.2
1	A	1033	PHE	4.9
1	A	252	LYS	4.8
1	A	303	ALA	4.7
1	A	494	ALA	4.2
1	A	461	GLY	4.1
1	A	709	HIS	4.1
1	A	829	GLY	3.9
1	A	299	ALA	3.9
1	A	951	ASP	3.9
1	A	680	PHE	3.8
1	A	960	LEU	3.8
1	A	677	ALA	3.7
1	A	706	ALA	3.7
1	A	167	SER	3.7
1	A	383	LEU	3.7
1	A	1001	ASN	3.7
1	A	678	THR	3.6
1	A	31	PRO	3.6
1	A	437	GLN	3.6
1	A	1030	ARG	3.5
1	A	838	GLY	3.4
1	A	241	THR	3.4
1	A	497	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	32	VAL	3.3
1	A	714	THR	3.2
1	A	1026	PHE	3.2
1	A	425	LEU	3.2
1	A	896	SER	3.2
1	A	9	PRO	3.1
1	A	851	LEU	3.1
1	A	310	LEU	3.1
1	A	402	ILE	3.1
1	A	720	GLY	3.0
1	A	401	ALA	3.0
1	A	992	SER	3.0
1	A	852	PRO	3.0
1	A	386	PHE	2.9
1	A	619	GLY	2.9
1	A	302	THR	2.9
1	A	403	GLY	2.9
1	A	833	PRO	2.9
1	A	306	ILE	2.8
1	A	616	GLY	2.8
1	A	618	ALA	2.8
1	A	1034	SER	2.8
1	A	961	ILE	2.7
1	A	850	LYS	2.7
1	A	952	LEU	2.7
1	A	719	ASN	2.7
1	A	872	GLN	2.7
1	A	515	TRP	2.6
1	A	89	GLN	2.6
1	A	811	TYR	2.6
1	A	1035	ARG	2.5
1	A	172	VAL	2.5
1	A	539	GLY	2.5
1	A	827	ILE	2.5
1	A	550	VAL	2.5
1	A	385	ALA	2.5
1	A	987	MET	2.5
1	A	712	MET	2.5
1	A	460	GLY	2.5
1	A	585	GLU	2.4
1	A	1020	PHE	2.4
1	A	170	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	470	PHE	2.4
1	A	707	ALA	2.4
1	A	828	LEU	2.4
1	A	332	PHE	2.3
1	A	1031	ARG	2.3
1	A	897	ILE	2.3
1	A	1029	VAL	2.3
1	A	463	THR	2.3
1	A	958	LYS	2.3
1	A	721	LEU	2.2
1	A	705	GLU	2.2
1	A	750	LEU	2.2
1	A	81	ASN	2.2
1	A	874	PRO	2.2
1	A	525	HIS	2.2
1	A	830	GLN	2.2
1	A	428	LYS	2.2
1	A	277	ILE	2.2
1	A	671	ILE	2.2
1	A	841	MET	2.1
1	A	488	LEU	2.1
1	A	563	PHE	2.1
1	A	634	TRP	2.1
1	A	708	LYS	2.1
1	A	839	GLU	2.1
1	A	272	GLY	2.1
1	A	673	GLU	2.1
1	A	388	PHE	2.1
1	A	783	PRO	2.1
1	A	995	ALA	2.1
1	A	754	TRP	2.0
1	A	794	ALA	2.0
1	A	59	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

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	CPF	A	5001	24/24	0.68	0.61	-	150,167,172,181	0

6.5 Other polymers

There are no such residues in this entry.