Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 06:14 AM EDT

PDB ID	:	7TBV
Title	:	Crystal structure of the shikimate kinase + 3-dehydroquinate dehydratase + 3-dehydroshikimate dehydrogenase domains of Aro1 from Candida albicans
Authors	:	Stogios, P.J.; Evdokimova, E.; Michalska, K.; Di Leo, R.; Savchenko, A.; Joachimiak, A.; Satchell, K.J.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2021-12-22
Resolution	:	2.30 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

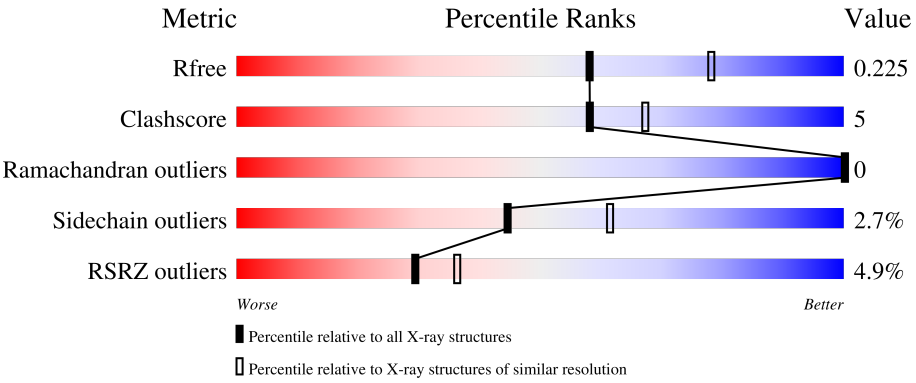
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	696	88% 9%
1	B	696	8% 84% 13%
1	C	696	9% 84% 12%
1	D	696	87% 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 23380 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 Pentafunctional AROM polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	682	Total	C	N	O	S	0	0	0
			5353	3421	903	1014	15			
1	B	679	Total	C	N	O	S	0	0	0
			5329	3409	900	1005	15			
1	C	678	Total	C	N	O	S	0	2	0
			5330	3409	899	1007	15			
1	D	680	Total	C	N	O	S	0	0	0
			5335	3412	901	1007	15			

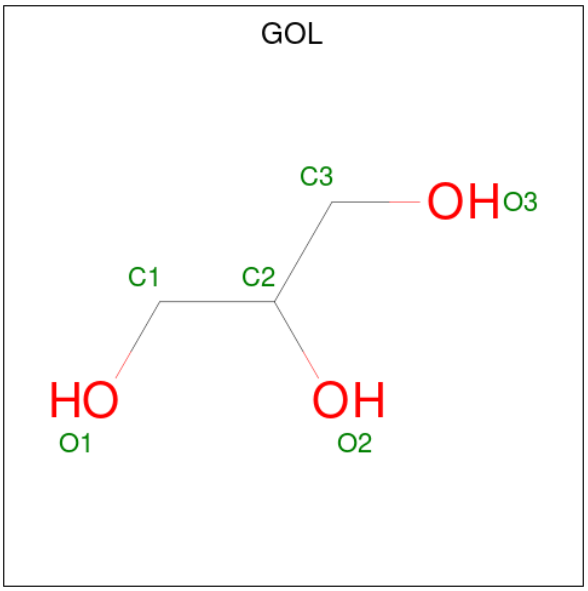
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

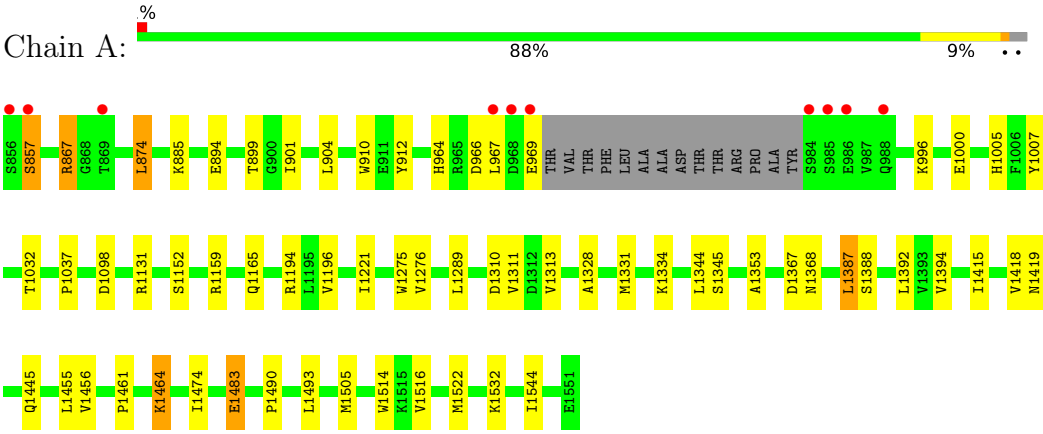
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	656	Total O 669 669	0	13
5	B	320	Total O 323 323	0	3
5	C	312	Total O 314 314	0	2
5	D	638	Total O 643 643	0	5

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

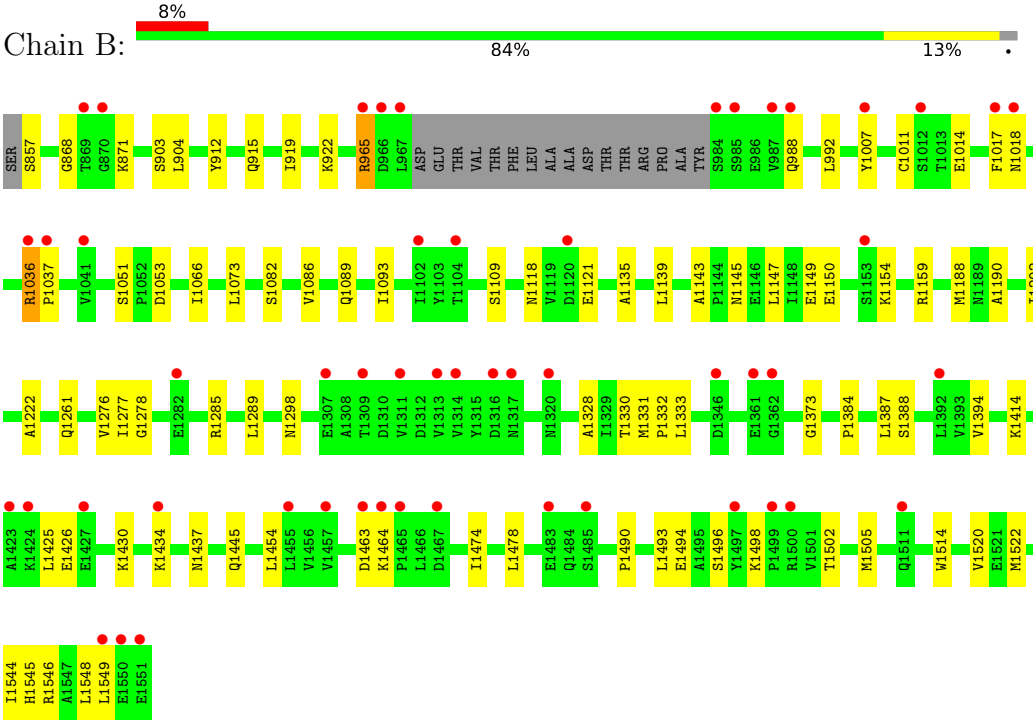
• Molecule 1: Pentafunctional AROM polypeptide

Chain A:

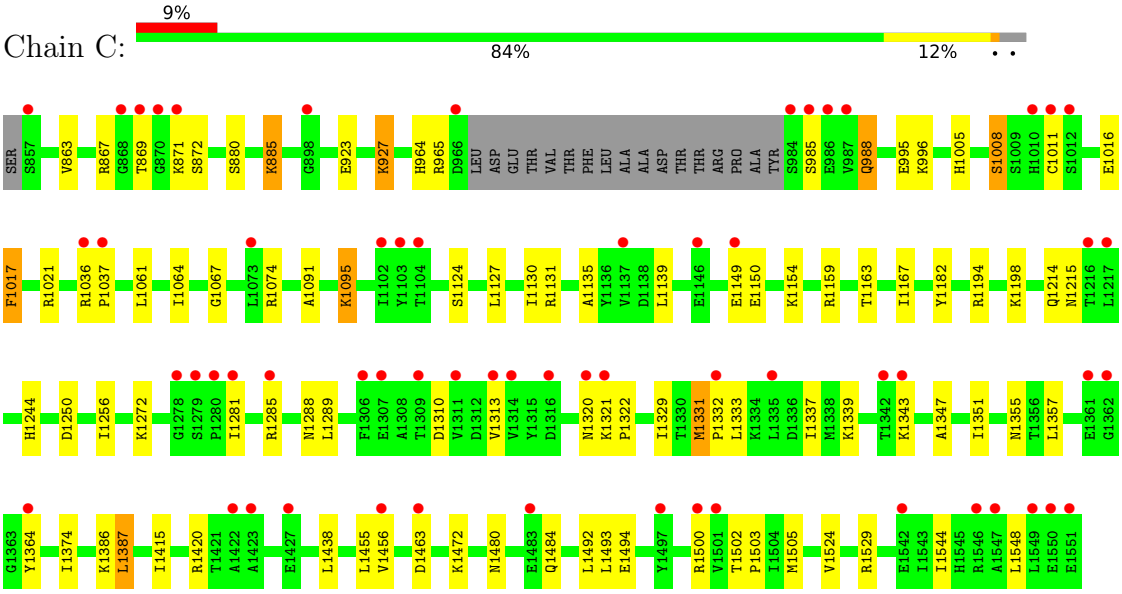


• Molecule 1: Pentafunctional AROM polypeptide

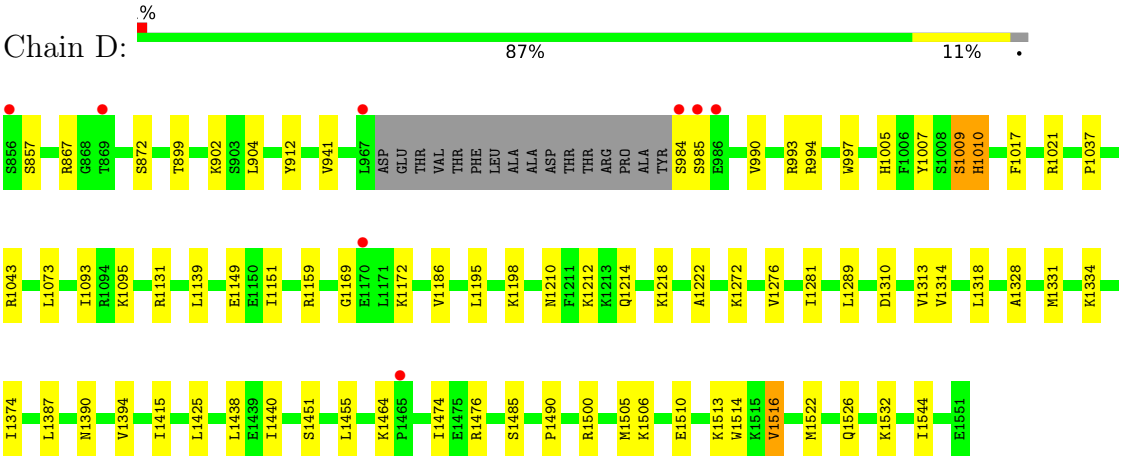
Chain B:



• Molecule 1: Pentafunctional AROM polypeptide



• Molecule 1: Pentafunctional AROM polypeptide



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.68Å 89.24Å 270.71Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	29.82 – 2.30 29.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.2 (29.82-2.30) 94.8 (29.82-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.178 , 0.226 0.178 , 0.225	Depositor DCC
R_{free} test set	1998 reflections (1.22%)	wwPDB-VP
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	23380	wwPDB-VP
Average B, all atoms (Å^2)	52.0	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 33.15 % 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 8.3804e-04. 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, 0.333 respectively for untwinned datasets, and 0.375, 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: CL, GOL, MG

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	0.31	0/5459	0.48	0/7381
1	B	0.26	0/5435	0.47	0/7350
1	C	0.27	0/5442	0.47	0/7359
1	D	0.27	0/5441	0.47	0/7358
All	All	0.28	0/21777	0.47	0/29448

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5353	0	5383	44	0
1	B	5329	0	5368	55	0
1	C	5330	0	5368	58	0
1	D	5335	0	5373	48	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	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	1	0
4	A	24	0	32	5	0
4	B	12	0	16	0	0
4	C	12	0	16	2	0
4	D	30	0	40	2	0
5	A	669	0	0	5	0
5	B	323	0	0	5	0
5	C	314	0	0	5	0
5	D	643	0	0	9	0
All	All	23380	0	21596	207	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (207) 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:1005:HIS:HE2	1:A:1007:TYR:HE1	1.15	0.91
1:D:1522:MET:O	1:D:1526:GLN:HG3	1.85	0.76
1:D:1506:LYS:NZ	1:D:1510:GLU:OE1	2.21	0.74
1:C:1011:CYS:HB3	1:C:1016:GLU:HB3	1.71	0.73
1:D:1374:ILE:HG12	1:D:1522:MET:HE2	1.71	0.72
1:D:1009:SER:HB3	1:D:1095:LYS:HD2	1.75	0.69
1:D:1043:ARG:O	4:D:1604:GOL:H2	1.94	0.67
1:C:1021:ARG:HG3	4:C:1603:GOL:H2	1.75	0.67
1:A:867:ARG:HD2	1:A:867:ARG:H	1.59	0.66
1:B:1373:GLY:HA3	1:B:1526:GLN:HG2	1.78	0.66
1:C:1036:ARG:HH11	1:C:1036:ARG:HG3	1.60	0.66
1:C:1272:LYS:NZ	5:C:1702:HOH:O	2.27	0.65
1:C:964:HIS:HB2	1:C:1005:HIS:HE1	1.62	0.64
1:D:1276:VAL:HG22	1:D:1281:ILE:HD11	1.79	0.64
1:A:1505:MET:HG2	1:A:1516:VAL:HG13	1.78	0.64
1:C:1037:PRO:HG2	1:C:1159:ARG:HD2	1.78	0.64
1:A:874:LEU:HD13	4:A:1604:GOL:H2	1.80	0.64
1:B:1289:LEU:HG	1:B:1544:ILE:HB	1.80	0.63
1:D:867:ARG:HH22	1:D:994:ARG:HH22	1.47	0.63
1:B:1394:VAL:HG11	1:B:1474:ILE:HD11	1.81	0.63
1:B:1414:LYS:HG2	1:B:1437:ASN:HB3	1.81	0.62
1:C:1331:MET:HG3	1:C:1332:PRO:HA	1.81	0.62
1:A:1493:LEU:HD21	1:A:1522:MET:HE2	1.82	0.61
1:C:1502:THR:HG22	1:C:1505:MET:SD	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1074:ARG:HD3	4:C:1602:GOL:H32	1.82	0.61
1:B:1278:GLY:HA2	1:B:1333:LEU:HD23	1.82	0.61
1:C:1285:ARG:HB3	1:C:1548:LEU:HD11	1.84	0.60
1:B:1014:GLU:HA	1:B:1017:PHE:HB2	1.83	0.60
1:D:1037:PRO:O	1:D:1159:ARG:NE	2.34	0.59
1:C:1524:VAL:HG22	1:C:1548:LEU:HD23	1.83	0.59
1:A:969:GLU:OE1	1:A:969:GLU:N	2.31	0.59
1:D:1212:LYS:HE2	1:D:1222:ALA:HB3	1.85	0.58
1:B:922:LYS:NZ	5:B:1705:HOH:O	2.36	0.58
1:C:1329:ILE:HD13	1:C:1337:ILE:HG21	1.84	0.58
1:B:915:GLN:O	1:B:919:ILE:HG12	2.04	0.58
1:B:1522:MET:O	1:B:1526:GLN:HG3	2.04	0.57
1:C:1037:PRO:HG3	1:C:1135:ALA:HB1	1.86	0.57
1:C:863:VAL:HG12	1:C:871:LYS:HE3	1.87	0.57
1:D:1425:LEU:HD23	1:D:1440:ILE:HG23	1.87	0.57
1:C:1339:LYS:NZ	5:C:1701:HOH:O	2.29	0.57
1:C:1387:LEU:HD21	1:C:1455:LEU:HD11	1.87	0.56
1:C:1480:ASN:O	1:C:1484:GLN:NE2	2.37	0.56
1:B:868:GLY:HA3	1:B:965:ARG:HH21	1.70	0.56
1:C:1415:ILE:HB	1:C:1438:LEU:HD23	1.88	0.56
1:B:1037:PRO:HG3	1:B:1135:ALA:HB1	1.88	0.56
1:D:1186:VAL:HG22	1:D:1218:LYS:HD2	1.88	0.56
1:C:1289:LEU:HG	1:C:1544:ILE:HB	1.88	0.55
1:B:1493:LEU:HD21	1:B:1522:MET:HE2	1.89	0.55
1:B:1053:ASP:OD1	1:B:1089:GLN:NE2	2.40	0.55
1:C:1150:GLU:HG3	1:C:1154:LYS:HE3	1.90	0.54
1:D:1425:LEU:HB3	1:D:1440:ILE:HD13	1.90	0.53
1:B:1036:ARG:NH2	5:B:1701:HOH:O	2.40	0.53
1:A:964:HIS:HB2	1:A:1005:HIS:CE1	2.43	0.53
1:B:1422:ALA:O	1:B:1426:GLU:N	2.38	0.53
1:D:1415:ILE:HB	1:D:1438:LEU:HD23	1.89	0.53
1:B:857:SER:N	5:B:1712:HOH:O	2.41	0.53
1:B:1285:ARG:NH2	5:B:1709:HOH:O	2.41	0.53
1:D:1005:HIS:CE1	1:D:1007:TYR:HE1	2.27	0.53
1:D:1394:VAL:HG11	1:D:1474:ILE:HD11	1.90	0.53
1:A:1289:LEU:HG	1:A:1544:ILE:HB	1.90	0.53
1:D:1289:LEU:HG	1:D:1544:ILE:HB	1.90	0.52
1:D:1314:VAL:HG13	1:D:1318:LEU:HD12	1.90	0.52
1:D:1131:ARG:NH1	5:D:1703:HOH:O	2.29	0.52
1:B:1212:LYS:HE2	1:B:1222:ALA:HB3	1.92	0.51
1:A:1387:LEU:HD21	1:A:1455:LEU:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1143:ALA:HB1	1:B:1147:LEU:HD23	1.91	0.51
1:A:1005:HIS:NE2	1:A:1007:TYR:HE1	1.97	0.51
1:D:904:LEU:HD11	1:D:912:TYR:HE2	1.75	0.51
1:A:1394:VAL:HG11	1:A:1474:ILE:HD11	1.92	0.51
1:B:1066:ILE:HG12	1:B:1540:PRO:HB3	1.93	0.51
1:C:1285:ARG:HB3	1:C:1548:LEU:CD1	2.41	0.51
1:C:1067:GLY:HA3	1:C:1256:ILE:HG12	1.93	0.50
1:A:1021:ARG:NH2	5:A:1711:HOH:O	2.36	0.50
1:A:1415:ILE:HB	1:A:1438:LEU:HD23	1.94	0.50
1:B:1490:PRO:HB2	1:B:1514:TRP:CD2	2.45	0.50
1:D:867:ARG:NH1	5:D:1717:HOH:O	2.44	0.50
1:A:1037:PRO:O	1:A:1159:ARG:NE	2.42	0.49
1:A:1275:TRP:CZ2	4:A:1606:GOL:H31	2.48	0.49
1:A:1461:PRO:HB2	1:A:1464:LYS:HE3	1.94	0.49
1:D:1490:PRO:HB2	1:D:1514:TRP:CD2	2.48	0.49
1:C:1036:ARG:HG3	1:C:1036:ARG:NH1	2.26	0.49
1:C:1494:GLU:OE1	1:C:1502:THR:HG21	2.13	0.48
1:A:867:ARG:NH2	5:A:1728:HOH:O	2.46	0.48
1:B:1331:MET:SD	1:B:1332:PRO:HA	2.53	0.48
1:D:1505:MET:HG2	1:D:1516:VAL:HG13	1.95	0.48
1:B:1419:ASN:HB3	1:B:1425:LEU:HD12	1.95	0.48
1:C:1502:THR:OG1	1:C:1503:PRO:HD2	2.12	0.48
1:B:1502:THR:OG1	1:B:1505:MET:HG3	2.14	0.48
1:B:1188:MET:HE2	1:B:1190:ALA:HB2	1.96	0.48
1:B:1082:SER:O	1:B:1086:VAL:HG23	2.14	0.47
1:A:1334:LYS:HB2	3:A:1602:CL:CL	2.51	0.47
1:D:1310:ASP:OD2	1:D:1313:VAL:HG23	2.14	0.47
1:B:988:GLN:O	1:B:992:LEU:HG	2.14	0.47
1:D:1272:LYS:NZ	5:D:1725:HOH:O	2.48	0.47
1:A:857:SER:HB2	1:A:1032:THR:O	2.15	0.47
1:A:996:LYS:O	1:A:1000:GLU:HG3	2.14	0.47
1:B:1276:VAL:HA	1:B:1328:ALA:O	2.15	0.47
1:B:1545:HIS:HD2	1:B:1546:ARG:HD2	1.80	0.47
1:A:1005:HIS:NE2	1:A:1007:TYR:CE1	2.77	0.47
1:C:1529:ARG:NH2	5:C:1728:HOH:O	2.48	0.47
1:A:1490:PRO:HB2	1:A:1514:TRP:CD2	2.51	0.46
1:B:1454:LEU:HD23	1:B:1490:PRO:HB3	1.97	0.46
1:B:1331:MET:CG	1:B:1332:PRO:HA	2.45	0.46
1:D:1149:GLU:HG3	5:D:2234:HOH:O	2.15	0.46
1:C:927:LYS:N	1:C:927:LYS:HD3	2.29	0.46
1:B:1036:ARG:H	1:B:1036:ARG:HG2	1.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1281:ILE:HD12	1:C:1281:ILE:HA	1.84	0.46
1:D:1169:GLY:HA3	1:D:1198:LYS:HB3	1.97	0.46
1:A:1276:VAL:HA	1:A:1328:ALA:O	2.16	0.46
1:A:1483:GLU:O	1:A:1483:GLU:HG2	2.16	0.46
1:C:995:GLU:HG3	1:C:996:LYS:N	2.30	0.46
1:C:1347:ALA:O	1:C:1351:ILE:HG13	2.16	0.46
1:A:867:ARG:H	1:A:867:ARG:CD	2.27	0.46
1:A:966:ASP:HB3	1:A:969:GLU:OE1	2.16	0.46
1:C:1061:LEU:HA	1:C:1061:LEU:HD23	1.83	0.46
1:C:1548:LEU:HD12	1:C:1548:LEU:HA	1.67	0.46
1:C:1036:ARG:HB3	1:C:1159:ARG:HE	1.81	0.46
1:B:1285:ARG:HA	1:B:1285:ARG:HD2	1.70	0.45
1:C:1017:PHE:HB3	1:C:1021:ARG:NH1	2.32	0.45
1:C:1472:LYS:HA	1:C:1472:LYS:HD3	1.80	0.45
1:A:1331:MET:SD	1:A:1331:MET:N	2.88	0.45
1:B:1073:LEU:HD13	1:B:1093:ILE:HD11	1.99	0.45
1:D:990:VAL:HG22	1:D:993:ARG:HH22	1.82	0.45
1:B:1150:GLU:HG2	1:B:1154:LYS:HD2	1.98	0.45
1:D:1139:LEU:HD21	1:D:1151:ILE:HG21	1.98	0.45
1:D:1010:HIS:O	1:D:1095:LYS:HE3	2.17	0.45
1:A:874:LEU:CD1	4:A:1604:GOL:H2	2.47	0.44
1:C:985:SER:HA	1:C:988:GLN:HG3	1.99	0.44
1:A:904:LEU:HD11	1:A:912:TYR:HE2	1.82	0.44
1:A:910:TRP:CZ2	4:A:1605:GOL:H32	2.53	0.44
1:A:964:HIS:HB2	1:A:1005:HIS:HE1	1.82	0.44
1:B:1018:ASN:O	1:B:1022:ARG:HG3	2.17	0.44
1:B:1021:ARG:NH2	5:B:1710:HOH:O	2.50	0.44
1:C:1289:LEU:HD12	1:C:1548:LEU:HD22	1.98	0.44
1:C:1357:LEU:HD11	1:C:1364:TYR:HB3	2.00	0.44
1:A:1131:ARG:NH1	5:A:1726:HOH:O	2.45	0.44
1:C:1131:ARG:HD3	5:C:1920:HOH:O	2.16	0.44
1:C:1492:LEU:HD22	1:C:1493:LEU:N	2.33	0.44
1:B:1430:LYS:HA	1:B:1434:LYS:NZ	2.32	0.44
1:C:885:LYS:HD2	1:C:885:LYS:HA	1.38	0.44
1:D:1017:PHE:HB3	1:D:1021:ARG:CZ	2.48	0.44
1:B:1118:ASN:HB3	1:B:1121:GLU:HB2	1.99	0.44
1:D:1073:LEU:HD13	1:D:1093:ILE:HD11	1.98	0.44
1:A:1419:ASN:HB2	1:A:1425:LEU:HD21	2.00	0.44
1:C:1374:ILE:HG23	1:C:1493:LEU:HD23	1.99	0.44
1:C:1500:ARG:HD3	1:C:1500:ARG:HA	1.79	0.44
1:C:1456:VAL:HB	1:C:1492:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:871:LYS:HB2	1:B:965:ARG:NH1	2.33	0.43
1:A:1310:ASP:HB3	1:A:1313:VAL:HG12	1.99	0.43
1:B:1139:LEU:HD23	1:B:1188:MET:HE3	2.01	0.43
1:B:1285:ARG:HB3	1:B:1548:LEU:HG	2.00	0.43
1:B:1520:VAL:HG11	1:B:1549:LEU:HD21	1.99	0.43
1:D:1390:ASN:ND2	1:D:1451:SER:O	2.42	0.43
1:C:1163:THR:HG23	1:C:1194:ARG:HG2	1.99	0.43
1:D:1334:LYS:HB2	3:D:1602:CL:CL	2.55	0.43
1:D:1387:LEU:HD21	1:D:1455:LEU:HD11	2.00	0.43
1:A:894:GLU:HG3	1:A:901:ILE:HG13	2.00	0.43
1:B:1331:MET:HG3	1:B:1332:PRO:HA	2.00	0.43
1:B:1430:LYS:H	1:B:1430:LYS:HG2	1.67	0.43
1:D:1172:LYS:NZ	5:D:1733:HOH:O	2.50	0.43
1:A:1392:LEU:HB3	1:A:1456:VAL:HG22	2.00	0.43
1:C:1320:ASN:O	1:C:1321:LYS:HD2	2.18	0.43
1:C:1502:THR:HG23	1:C:1505:MET:H	1.83	0.43
1:B:1036:ARG:HG3	1:B:1159:ARG:HH21	1.84	0.43
1:C:1329:ILE:HB	1:C:1355:ASN:HA	2.01	0.43
1:D:902:LYS:HA	1:D:902:LYS:HD2	1.77	0.43
1:D:990:VAL:HG22	1:D:993:ARG:NH2	2.34	0.43
1:D:1210:ASN:O	1:D:1214:GLN:HG3	2.18	0.43
1:A:1334:LYS:HB3	1:A:1353:ALA:HB1	2.01	0.43
1:C:1182:TYR:CE2	1:C:1215:ASN:HB3	2.54	0.43
1:A:1392:LEU:HD11	1:A:1418:VAL:HG23	2.01	0.43
1:D:1331:MET:N	1:D:1331:MET:SD	2.91	0.42
1:D:1513:LYS:HA	1:D:1513:LYS:HD2	1.60	0.42
1:D:904:LEU:HD11	1:D:912:TYR:CE2	2.53	0.42
1:B:1430:LYS:HB3	1:B:1430:LYS:HE2	1.77	0.42
1:B:1277:ILE:O	1:B:1330:THR:HG22	2.19	0.42
1:C:1310:ASP:HB3	1:C:1313:VAL:HG12	2.01	0.42
1:D:1276:VAL:HA	1:D:1328:ALA:O	2.20	0.42
4:D:1603:GOL:H2	5:D:1860:HOH:O	2.20	0.42
1:C:1091:ALA:O	1:C:1095:LYS:HG2	2.20	0.42
1:A:1017:PHE:HB3	1:A:1021:ARG:NH1	2.33	0.42
1:A:1194:ARG:HA	1:A:1221:ILE:O	2.20	0.42
1:B:1474:ILE:O	1:B:1478:LEU:HG	2.20	0.42
1:B:1030:LEU:HD12	1:B:1037:PRO:HD3	2.01	0.41
1:C:1167:ILE:O	1:C:1198:LYS:NZ	2.38	0.41
1:D:941:VAL:HB	1:D:997:TRP:HB3	2.02	0.41
1:C:1127:LEU:HA	1:C:1130:ILE:HD12	2.02	0.41
1:D:984:SER:OG	1:D:985:SER:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1344:LEU:HD23	1:A:1344:LEU:HA	1.79	0.41
1:B:904:LEU:HD11	1:B:912:TYR:HE2	1.85	0.41
1:C:880:SER:O	1:C:1387:LEU:HA	2.20	0.41
1:C:1214:GLN:NE2	5:C:1738:HOH:O	2.53	0.41
1:D:867:ARG:NH2	5:D:1719:HOH:O	2.44	0.41
1:B:1011:CYS:HB2	1:B:1017:PHE:CE1	2.56	0.41
1:B:1384:PRO:HG2	1:B:1387:LEU:CD2	2.50	0.41
1:C:1008:SER:O	1:C:1008:SER:OG	2.31	0.41
1:A:1532:LYS:HE2	5:A:2235:HOH:O	2.20	0.41
4:A:1603:GOL:H2	5:A:1926:HOH:O	2.21	0.41
1:C:1064:ILE:HA	1:C:1244:HIS:CD2	2.56	0.41
1:D:1198:LYS:NZ	5:D:1747:HOH:O	2.54	0.41
1:A:1367:ASP:OD1	1:A:1368:ASN:N	2.51	0.41
1:D:1500:ARG:HD2	5:D:2160:HOH:O	2.21	0.41
1:B:1494:GLU:HG3	1:B:1496:SER:H	1.85	0.40
1:A:1165:GLN:HG2	1:A:1196:VAL:HB	2.03	0.40
1:B:1261:GLN:HB2	1:B:1298:ASN:ND2	2.36	0.40
1:C:1331:MET:HA	1:C:1333:LEU:H	1.87	0.40
1:D:1195:LEU:O	1:D:1222:ALA:HA	2.22	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	678/696 (97%)	664 (98%)	14 (2%)	0	100	100
1	B	675/696 (97%)	658 (98%)	17 (2%)	0	100	100
1	C	676/696 (97%)	650 (96%)	26 (4%)	0	100	100
1	D	676/696 (97%)	662 (98%)	14 (2%)	0	100	100
All	All	2705/2784 (97%)	2634 (97%)	71 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	582/593 (98%)	567 (97%)	15 (3%)	46	63
1	B	579/593 (98%)	564 (97%)	15 (3%)	46	63
1	C	580/593 (98%)	556 (96%)	24 (4%)	30	43
1	D	580/593 (98%)	570 (98%)	10 (2%)	60	76
All	All	2321/2372 (98%)	2257 (97%)	64 (3%)	44	60

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	857	SER
1	A	867	ARG
1	A	874	LEU
1	A	885	LYS
1	A	899	THR
1	A	967	LEU
1	A	1098	ASP
1	A	1152	SER
1	A	1311	VAL
1	A	1345	SER
1	A	1387	LEU
1	A	1388	SER
1	A	1445	GLN
1	A	1464	LYS
1	A	1483	GLU
1	B	903	SER
1	B	965	ARG
1	B	1007	TYR
1	B	1021	ARG
1	B	1036	ARG
1	B	1051	SER
1	B	1109	SER

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Mol	Chain	Res	Type
1	B	1145	ASN
1	B	1149	GLU
1	B	1202	ILE
1	B	1388	SER
1	B	1445	GLN
1	B	1463	ASP
1	B	1464	LYS
1	B	1498	LYS
1	C	867	ARG
1	C	869	THR
1	C	872[A]	SER
1	C	872[B]	SER
1	C	885	LYS
1	C	923	GLU
1	C	927	LYS
1	C	965	ARG
1	C	988	GLN
1	C	1008	SER
1	C	1017	PHE
1	C	1095	LYS
1	C	1124	SER
1	C	1139	LEU
1	C	1149	GLU
1	C	1250	ASP
1	C	1288	ASN
1	C	1322	PRO
1	C	1331	MET
1	C	1343	LYS
1	C	1386	LYS
1	C	1387	LEU
1	C	1420	ARG
1	C	1463	ASP
1	D	857	SER
1	D	872	SER
1	D	899	THR
1	D	1009	SER
1	D	1010	HIS
1	D	1464	LYS
1	D	1476	ARG
1	D	1485	SER
1	D	1516	VAL
1	D	1532	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
4	GOL	A	1603	-	5,5,5	1.03	0	5,5,5	1.01	0
4	GOL	A	1606	-	5,5,5	0.27	0	5,5,5	0.56	0
4	GOL	D	1606	-	5,5,5	0.94	0	5,5,5	0.99	0
4	GOL	D	1604	-	5,5,5	0.96	0	5,5,5	1.02	0
4	GOL	A	1605	-	5,5,5	0.89	0	5,5,5	1.02	0
4	GOL	D	1605	-	5,5,5	0.87	0	5,5,5	1.01	0
4	GOL	C	1603	-	5,5,5	0.91	0	5,5,5	0.98	0
4	GOL	A	1604	-	5,5,5	0.87	0	5,5,5	0.95	0
4	GOL	B	1603	-	5,5,5	0.84	0	5,5,5	0.98	0
4	GOL	B	1602	-	5,5,5	0.84	0	5,5,5	1.07	0
4	GOL	C	1602	-	5,5,5	0.88	0	5,5,5	0.96	0
4	GOL	D	1607	-	5,5,5	0.91	0	5,5,5	0.96	0
4	GOL	D	1603	-	5,5,5	1.04	1 (20%)	5,5,5	0.93	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
4	GOL	A	1603	-	-	2/4/4/4	-
4	GOL	A	1606	-	-	2/4/4/4	-
4	GOL	D	1606	-	-	0/4/4/4	-
4	GOL	D	1604	-	-	1/4/4/4	-
4	GOL	A	1605	-	-	2/4/4/4	-
4	GOL	D	1605	-	-	2/4/4/4	-
4	GOL	C	1603	-	-	2/4/4/4	-
4	GOL	A	1604	-	-	2/4/4/4	-
4	GOL	B	1603	-	-	2/4/4/4	-
4	GOL	B	1602	-	-	2/4/4/4	-
4	GOL	C	1602	-	-	2/4/4/4	-
4	GOL	D	1607	-	-	4/4/4/4	-
4	GOL	D	1603	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1603	GOL	O2-C2	-2.02	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1603	GOL	O1-C1-C2-C3
4	A	1604	GOL	O1-C1-C2-C3
4	A	1606	GOL	C1-C2-C3-O3
4	B	1602	GOL	O1-C1-C2-C3
4	B	1603	GOL	C1-C2-C3-O3
4	C	1603	GOL	O1-C1-C2-C3
4	D	1603	GOL	C1-C2-C3-O3
4	D	1605	GOL	O1-C1-C2-C3
4	A	1603	GOL	O1-C1-C2-O2
4	A	1604	GOL	O1-C1-C2-O2
4	A	1606	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	C	1603	GOL	O1-C1-C2-O2
4	C	1602	GOL	O1-C1-C2-C3
4	D	1604	GOL	O1-C1-C2-C3
4	D	1607	GOL	O1-C1-C2-C3
4	D	1607	GOL	C1-C2-C3-O3
4	B	1602	GOL	O1-C1-C2-O2
4	D	1605	GOL	O1-C1-C2-O2
4	D	1607	GOL	O2-C2-C3-O3
4	B	1603	GOL	O2-C2-C3-O3
4	D	1603	GOL	O2-C2-C3-O3
4	A	1605	GOL	O1-C1-C2-O2
4	C	1602	GOL	O1-C1-C2-O2
4	D	1607	GOL	O1-C1-C2-O2
4	A	1605	GOL	O1-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1603	GOL	1	0
4	A	1606	GOL	1	0
4	D	1604	GOL	1	0
4	A	1605	GOL	1	0
4	C	1603	GOL	1	0
4	A	1604	GOL	2	0
4	C	1602	GOL	1	0
4	D	1603	GOL	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	682/696 (97%)	-0.24	10 (1%) 73 79	15, 36, 66, 119	0
1	B	679/696 (97%)	0.17	55 (8%) 12 16	21, 59, 109, 167	0
1	C	678/696 (97%)	0.29	61 (8%) 9 12	28, 62, 113, 142	0
1	D	680/696 (97%)	-0.19	8 (1%) 79 83	19, 40, 75, 132	0
All	All	2719/2784 (97%)	0.01	134 (4%) 29 36	15, 49, 99, 167	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	967	LEU	8.2
1	B	984	SER	8.1
1	D	984	SER	7.6
1	A	856	SER	7.1
1	C	984	SER	6.6
1	B	1423	ALA	6.3
1	C	1422	ALA	6.1
1	B	1037	PRO	6.0
1	C	869	THR	5.8
1	A	969	GLU	5.3
1	C	1362	GLY	5.3
1	A	984	SER	5.0
1	C	870	GLY	4.8
1	C	985	SER	4.8
1	C	1306	PHE	4.6
1	C	1314	VAL	4.6
1	A	968	ASP	4.5
1	C	1551	GLU	4.3
1	D	985	SER	4.3
1	C	1316	ASP	4.1
1	C	1279	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	966	ASP	4.1
1	C	868	GLY	4.1
1	D	856	SER	4.1
1	C	1423	ALA	4.0
1	B	1551	GLU	3.9
1	B	1549	LEU	3.8
1	C	1010	HIS	3.7
1	B	1311	VAL	3.7
1	C	1011	CYS	3.7
1	B	1313	VAL	3.7
1	B	869	THR	3.6
1	D	986	GLU	3.6
1	B	1012	SER	3.5
1	C	1547	ALA	3.5
1	B	1464	LYS	3.4
1	C	1332	PRO	3.4
1	B	967	LEU	3.4
1	B	1483	GLU	3.3
1	C	1280	PRO	3.3
1	C	1037	PRO	3.3
1	C	871	LYS	3.2
1	B	1427	GLU	3.2
1	B	1036	ARG	3.2
1	C	1550	GLU	3.2
1	C	1309	THR	3.1
1	B	1018	ASN	3.1
1	C	1549	LEU	3.1
1	A	985	SER	3.1
1	A	869	THR	3.0
1	C	987	VAL	3.0
1	B	1307	GLU	3.0
1	B	987	VAL	3.0
1	B	1422	ALA	2.9
1	C	1307	GLU	2.9
1	B	985	SER	2.9
1	B	1467	ASP	2.9
1	B	988	GLN	2.9
1	B	1361	GLU	2.9
1	A	857	SER	2.9
1	B	1550	GLU	2.9
1	C	1012	SER	2.8
1	C	1500	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	967	LEU	2.8
1	C	1146	GLU	2.7
1	B	1017	PHE	2.7
1	C	1104	THR	2.7
1	B	1362	GLY	2.7
1	C	1343	LYS	2.7
1	B	1497	TYR	2.7
1	D	1465	PRO	2.7
1	D	869	THR	2.6
1	B	870	GLY	2.6
1	B	1463	ASP	2.6
1	C	966	ASP	2.6
1	C	1073	LEU	2.6
1	B	1041	VAL	2.6
1	C	1311	VAL	2.6
1	B	965	ARG	2.6
1	C	986	GLU	2.6
1	B	1434	LYS	2.6
1	C	1497	TYR	2.6
1	C	1281	ILE	2.6
1	C	1278	GLY	2.5
1	C	1102	ILE	2.5
1	C	1335	LEU	2.5
1	C	857	SER	2.5
1	C	1427	GLU	2.5
1	C	1313	VAL	2.5
1	C	1103	TYR	2.5
1	C	1216	THR	2.5
1	D	1170	GLU	2.4
1	B	1424	LYS	2.4
1	B	1217	LEU	2.4
1	C	898	GLY	2.4
1	C	1342	THR	2.4
1	B	1455	LEU	2.4
1	C	1361	GLU	2.4
1	C	1546	ARG	2.4
1	C	1456	VAL	2.3
1	C	1149	GLU	2.3
1	C	1364	TYR	2.3
1	C	1463	ASP	2.3
1	A	988	GLN	2.3
1	A	986	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1317	ASN	2.2
1	B	1316	ASP	2.2
1	C	1285	ARG	2.2
1	B	1485	SER	2.2
1	B	1007	TYR	2.1
1	B	1457	VAL	2.1
1	B	1511	GLN	2.1
1	B	1320	ASN	2.1
1	B	1392	LEU	2.1
1	B	1500	ARG	2.1
1	C	1321	LYS	2.1
1	B	1465	PRO	2.1
1	C	1483	GLU	2.1
1	B	1309	THR	2.1
1	C	1501	VAL	2.1
1	B	1102	ILE	2.1
1	C	1217	LEU	2.1
1	B	1346	ASP	2.1
1	B	1282	GLU	2.1
1	C	1036	ARG	2.1
1	C	1320	ASN	2.1
1	C	1137	VAL	2.1
1	B	1499	PRO	2.1
1	B	1120	ASP	2.1
1	B	1420	ARG	2.1
1	B	1153	SER	2.0
1	C	1542	GLU	2.0
1	B	1314	VAL	2.0
1	B	1104	THR	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
4	GOL	A	1606	6/6	0.70	0.22	76,85,90,103	0
4	GOL	B	1603	6/6	0.79	0.14	64,67,76,80	0
4	GOL	D	1606	6/6	0.80	0.22	80,84,85,89	0
4	GOL	D	1604	6/6	0.81	0.17	50,54,58,61	0
4	GOL	A	1604	6/6	0.83	0.23	53,59,67,71	0
4	GOL	C	1603	6/6	0.85	0.17	75,75,88,91	0
4	GOL	D	1605	6/6	0.87	0.39	58,63,74,79	0
4	GOL	A	1605	6/6	0.88	0.19	50,59,66,78	0
4	GOL	D	1607	6/6	0.90	0.30	57,60,69,87	0
4	GOL	C	1602	6/6	0.92	0.24	50,52,60,61	0
4	GOL	B	1602	6/6	0.93	0.31	46,51,55,59	0
2	MG	C	1601	1/1	0.94	0.21	68,68,68,68	0
3	CL	D	1602	1/1	0.95	0.09	68,68,68,68	0
3	CL	A	1602	1/1	0.95	0.07	63,63,63,63	0
2	MG	D	1601	1/1	0.96	0.08	52,52,52,52	0
4	GOL	A	1603	6/6	0.96	0.28	27,32,40,45	0
2	MG	A	1601	1/1	0.96	0.12	42,42,42,42	0
4	GOL	D	1603	6/6	0.96	0.25	30,33,35,41	0
2	MG	B	1601	1/1	0.99	0.14	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.