Full wwPDB X-ray Structure Validation Report (i)

May 18, 2020 – 08:54 pm BST

PDB ID	:	3C2H
Title	:	Crystal Structure of SYS-1 at 2.6A resolution
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Deposited on	:	2008-01-25
Resolution	:	2.60 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 following versions of software and data (see references (1)) were used in the production of this report:

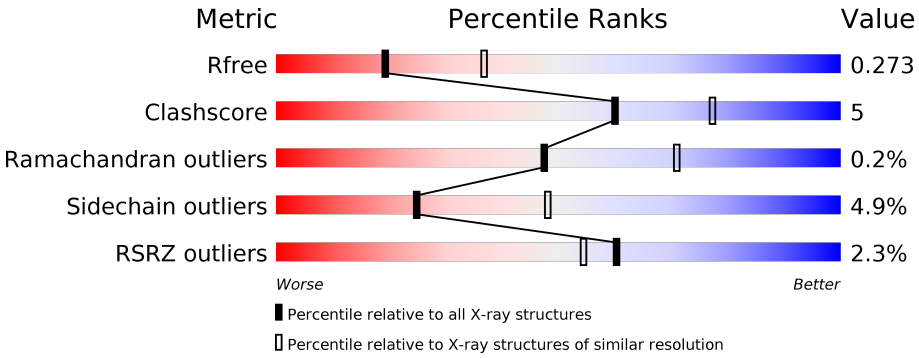
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	619	2% 85% 13%
1	B	619	2% 86% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FLC	A	1	-	-	-	X
3	GOL	B	4	-	-	-	X

2 Entry composition

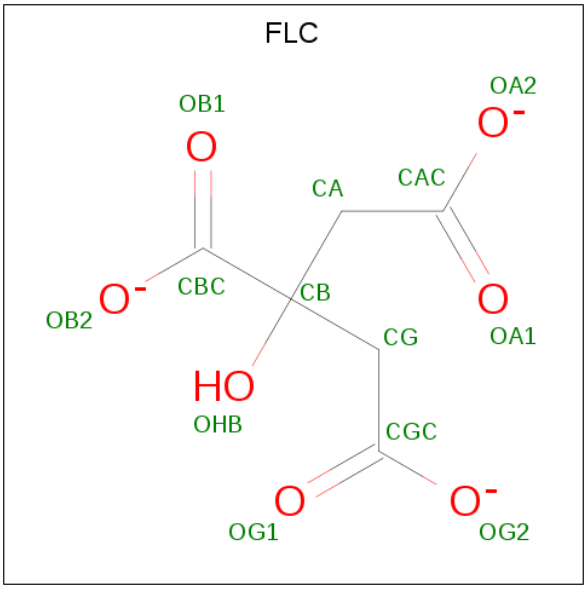
There are 4 unique types of molecules in this entry. The entry contains 9846 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sys-1 protein.

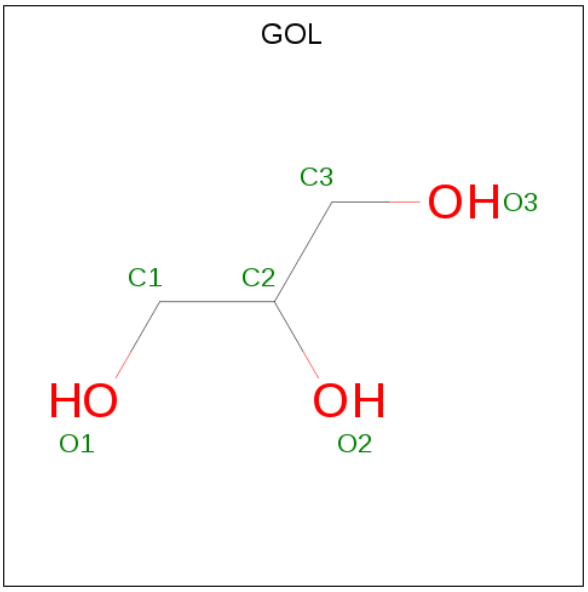
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	617	Total	C	N	O	S	0	0	0
			4876	3138	845	861	32			
1	B	618	Total	C	N	O	S	0	0	0
			4894	3150	852	861	31			

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

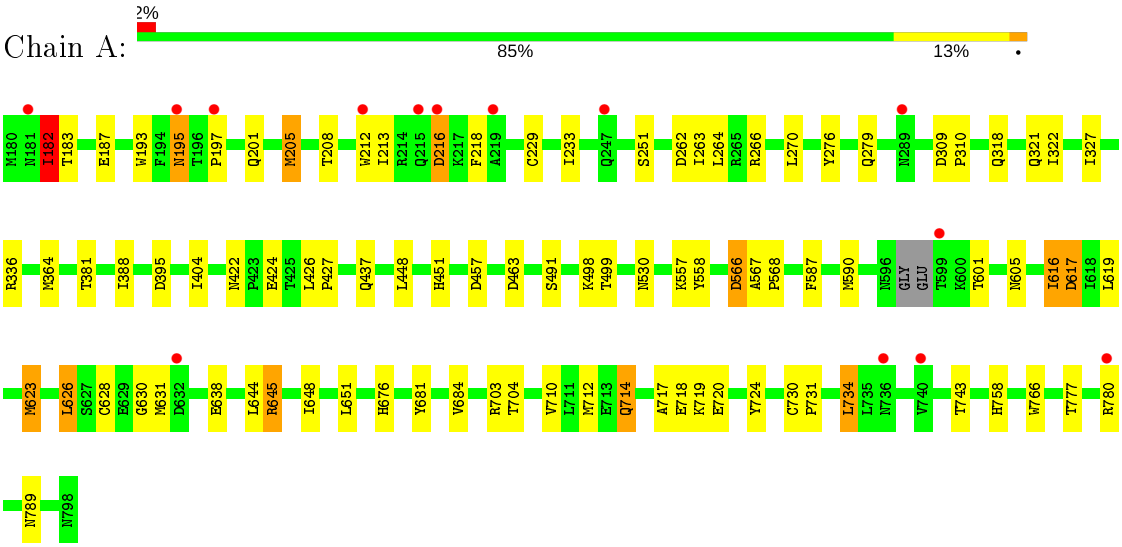
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	24	Total O 24 24	0	0
4	B	15	Total O 15 15	0	0

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 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.

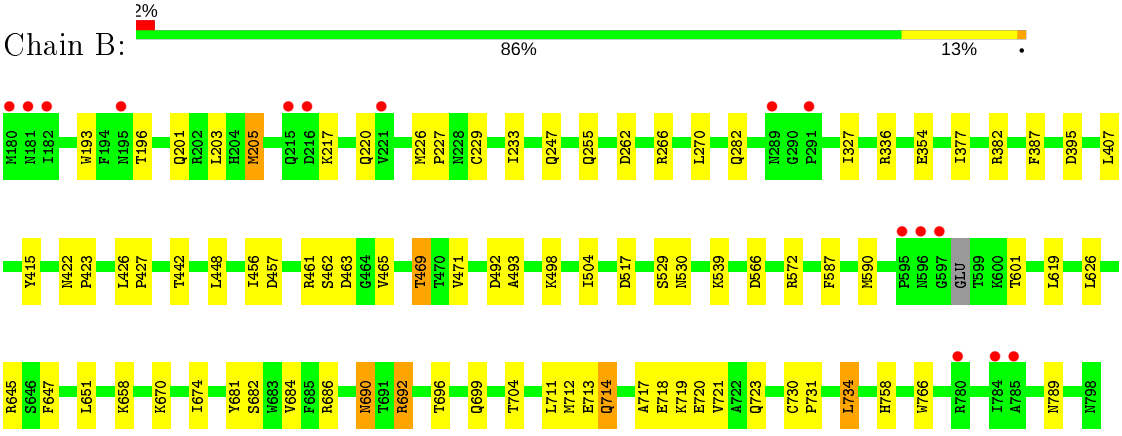
- Molecule 1: Sys-1 protein

Chain A:



- Molecule 1: Sys-1 protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	203.50Å 95.05Å 149.39Å 90.00° 124.71° 90.00°	Depositor
Resolution (Å)	49.57 – 2.60 49.56 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.57-2.60) 97.1 (49.56-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.245 , 0.286 0.233 , 0.273	Depositor DCC
R_{free} test set	3574 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	58.4	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9846	wwPDB-VP
Average B, all atoms (Å^2)	61.0	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 53.96 % 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 3.9133e-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, 0.333 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: GOL, FLC

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	0.43	0/4988	0.56	0/6794
1	B	0.43	0/5006	0.55	0/6815
All	All	0.43	0/9994	0.55	0/13609

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	4876	0	4911	46	0
1	B	4894	0	4951	44	0
2	A	13	0	5	0	0
3	A	12	0	16	1	0
3	B	12	0	16	1	0
4	A	24	0	0	0	0
4	B	15	0	0	0	0
All	All	9846	0	9899	90	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 (90) 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:539:LYS:HD3	1:B:590:MET:HE1	1.36	1.06
1:B:539:LYS:HD3	1:B:590:MET:CE	2.01	0.89
1:A:623:MET:HG2	1:A:676:HIS:CD2	2.18	0.79
1:A:587:PHE:O	1:A:590:MET:HG2	1.84	0.76
1:B:719:LYS:HG2	1:B:758:HIS:CD2	2.25	0.70
1:B:203:LEU:HD11	1:B:255:GLN:HG2	1.74	0.70
1:A:651:LEU:O	1:A:714:GLN:HG2	1.92	0.69
1:A:437:GLN:HG2	3:A:3:GOL:O2	1.92	0.69
1:B:651:LEU:O	1:B:658:LYS:HE2	1.96	0.66
1:A:213:ILE:HD13	1:A:263:ILE:HG23	1.77	0.65
1:A:628:CYS:C	1:A:630:GLY:H	2.01	0.64
1:B:601:THR:HG23	3:B:2:GOL:H2	1.80	0.62
1:A:730:CYS:HB2	1:A:766:TRP:CG	2.35	0.61
1:B:201:GLN:O	1:B:205:MET:HB2	1.99	0.61
1:A:182:ILE:HD12	1:A:183:THR:H	1.66	0.61
1:B:465:VAL:O	1:B:469:THR:HG23	2.01	0.60
1:A:318:GLN:HA	1:A:321:GLN:HE21	1.66	0.60
1:B:469:THR:HG21	1:B:504:ILE:HG23	1.83	0.60
1:A:719:LYS:HG2	1:A:758:HIS:CD2	2.37	0.59
1:B:587:PHE:O	1:B:590:MET:HG2	2.04	0.58
1:A:731:PRO:O	1:A:734:LEU:HB2	2.04	0.58
1:A:777:THR:HG23	1:A:789:ASN:HB3	1.86	0.57
1:A:712:MET:HG2	1:A:718:GLU:HA	1.88	0.55
1:A:327:ILE:O	1:A:336:ARG:NH2	2.41	0.53
1:B:712:MET:HG2	1:B:718:GLU:HA	1.90	0.53
1:B:731:PRO:O	1:B:734:LEU:HB2	2.08	0.53
1:A:645:ARG:HG3	1:A:703:ARG:CZ	2.38	0.53
1:B:713:GLU:OE1	1:B:714:GLN:NE2	2.42	0.53
1:A:193:TRP:CE3	1:A:205:MET:HE3	2.44	0.52
1:B:226:MET:HB2	1:B:227:PRO:HD3	1.91	0.52
1:A:262:ASP:OD2	1:A:266:ARG:NH1	2.40	0.52
1:A:229:CYS:O	1:A:233:ILE:HG12	2.10	0.52
1:A:623:MET:HG2	1:A:676:HIS:CG	2.45	0.52
1:B:229:CYS:O	1:B:233:ILE:HG12	2.09	0.52
1:A:213:ILE:HG12	1:A:218:PHE:HE2	1.76	0.50
1:A:567:ALA:HB3	1:A:568:PRO:HD3	1.94	0.50
1:A:264:LEU:HD23	1:A:322:ILE:HD13	1.94	0.50
1:A:212:TRP:O	1:A:216:ASP:HB2	2.11	0.50
1:A:266:ARG:O	1:A:270:LEU:HB2	2.12	0.49
1:A:201:GLN:O	1:A:205:MET:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:LEU:HB3	1:B:427:PRO:HD3	1.93	0.49
1:B:415:TYR:HB2	1:B:471:VAL:HG22	1.95	0.48
1:A:557:LYS:HE2	1:A:558:TYR:CZ	2.48	0.48
1:B:492:ASP:HB3	1:B:530:ASN:HB3	1.94	0.48
1:B:719:LYS:O	1:B:723:GLN:HG2	2.13	0.48
1:B:462:SER:O	1:B:463:ASP:HB2	2.14	0.47
1:A:422:ASN:ND2	1:A:424:GLU:HB2	2.29	0.47
1:B:681:TYR:CD1	1:B:704:THR:HG21	2.49	0.47
1:A:195:ASN:O	1:A:197:PRO:HD3	2.14	0.46
1:B:262:ASP:OD2	1:B:266:ARG:NH1	2.47	0.46
1:B:717:ALA:HA	1:B:720:GLU:OE1	2.15	0.46
1:B:690:ASN:HD22	1:B:692:ARG:HB2	1.80	0.46
1:B:456:ILE:HG22	1:B:493:ALA:HB2	1.98	0.46
1:A:717:ALA:HB1	1:A:720:GLU:HG2	1.96	0.46
1:B:719:LYS:HE2	1:B:758:HIS:HD2	1.81	0.46
1:A:710:VAL:O	1:A:714:GLN:HB2	2.17	0.45
1:A:309:ASP:HA	1:A:310:PRO:HD3	1.89	0.44
1:A:720:GLU:O	1:A:724:TYR:HD2	2.00	0.44
1:B:193:TRP:HA	1:B:205:MET:HE3	1.99	0.44
1:B:377:ILE:HD11	1:B:387:PHE:CD2	2.53	0.44
1:B:674:ILE:HD13	1:B:711:LEU:HD13	2.00	0.44
1:A:426:LEU:HB3	1:A:427:PRO:HD3	2.00	0.44
1:A:619:LEU:O	1:A:623:MET:HB2	2.19	0.43
1:B:266:ARG:O	1:B:270:LEU:HB2	2.18	0.43
1:B:674:ILE:CD1	1:B:721:VAL:HG22	2.49	0.43
1:A:628:CYS:C	1:A:630:GLY:N	2.70	0.43
1:B:696:THR:HA	1:B:699:GLN:HG2	2.00	0.43
1:A:422:ASN:HD21	1:A:424:GLU:HB2	1.84	0.43
1:A:644:LEU:O	1:A:648:ILE:HG13	2.19	0.42
1:A:566:ASP:OD2	1:A:568:PRO:HD2	2.20	0.42
1:B:457:ASP:O	1:B:461:ARG:HG3	2.20	0.42
1:A:388:ILE:HG23	1:A:404:ILE:HD12	2.00	0.42
1:B:465:VAL:HG12	1:B:504:ILE:HD13	2.01	0.42
1:A:681:TYR:CD1	1:A:704:THR:HG21	2.54	0.42
1:B:682:SER:HB3	1:B:686:ARG:HH12	1.85	0.42
1:A:213:ILE:HG12	1:A:218:PHE:CE2	2.55	0.41
1:B:539:LYS:CD	1:B:590:MET:HE1	2.27	0.41
1:B:730:CYS:HB2	1:B:766:TRP:CG	2.55	0.41
1:A:381:THR:HG23	1:A:451:HIS:CE1	2.55	0.41
1:B:327:ILE:O	1:B:336:ARG:NH2	2.54	0.41
1:A:616:ILE:HG13	1:A:617:ASP:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:LEU:HD12	1:A:626:LEU:HA	1.95	0.41
1:B:674:ILE:HD12	1:B:721:VAL:HG22	2.03	0.41
1:A:276:TYR:O	1:A:279:GLN:HB2	2.21	0.40
1:B:619:LEU:CD2	1:B:647:PHE:HE1	2.35	0.40
1:B:682:SER:HB3	1:B:686:ARG:NH1	2.35	0.40
1:B:651:LEU:O	1:B:714:GLN:HG2	2.22	0.40
1:A:491:SER:HB2	1:A:530:ASN:HB2	2.03	0.40
1:B:422:ASN:HA	1:B:423:PRO:HD2	1.91	0.40
1:B:407:LEU:HD22	1:B:442:THR:HG23	2.02	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	613/619 (99%)	593 (97%)	19 (3%)	1 (0%)	47 71
1	B	614/619 (99%)	583 (95%)	30 (5%)	1 (0%)	47 71
All	All	1227/1238 (99%)	1176 (96%)	49 (4%)	2 (0%)	47 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	ILE
1	B	690	ASN

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	539/563 (96%)	510 (95%)	29 (5%)	22 44
1	B	542/563 (96%)	518 (96%)	24 (4%)	28 53
All	All	1081/1126 (96%)	1028 (95%)	53 (5%)	25 48

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	ILE
1	A	187	GLU
1	A	195	ASN
1	A	205	MET
1	A	208	THR
1	A	216	ASP
1	A	251	SER
1	A	364	MET
1	A	395	ASP
1	A	448	LEU
1	A	457	ASP
1	A	463	ASP
1	A	498	LYS
1	A	499	THR
1	A	566	ASP
1	A	601	THR
1	A	605	ASN
1	A	616	ILE
1	A	617	ASP
1	A	623	MET
1	A	626	LEU
1	A	631	MET
1	A	638	GLU
1	A	645	ARG
1	A	684	VAL
1	A	714	GLN
1	A	734	LEU
1	A	743	THR
1	A	780	ARG
1	B	196	THR
1	B	205	MET
1	B	217	LYS
1	B	220	GLN

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Mol	Chain	Res	Type
1	B	247	GLN
1	B	282	GLN
1	B	354	GLU
1	B	382	ARG
1	B	395	ASP
1	B	448	LEU
1	B	469	THR
1	B	498	LYS
1	B	517	ASP
1	B	529	SER
1	B	566	ASP
1	B	572	ARG
1	B	626	LEU
1	B	645	ARG
1	B	670	LYS
1	B	684	VAL
1	B	692	ARG
1	B	714	GLN
1	B	734	LEU
1	B	789	ASN

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	247	GLN
1	A	321	GLN
1	A	390	ASN
1	A	515	HIS
1	A	733	ASN
1	A	758	HIS
1	A	789	ASN
1	B	223	GLN
1	B	247	GLN
1	B	390	ASN
1	B	746	HIS
1	B	758	HIS

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)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	B	2	-	5,5,5	0.38	0	5,5,5	0.29	0
3	GOL	A	3	-	5,5,5	0.41	0	5,5,5	0.18	0
3	GOL	B	4	-	5,5,5	0.35	0	5,5,5	0.45	0
2	FLC	A	1	-	3,12,12	0.74	0	3,17,17	1.01	0
3	GOL	A	799	-	5,5,5	0.38	0	5,5,5	0.30	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
3	GOL	B	2	-	-	2/4/4/4	-
3	GOL	A	3	-	-	2/4/4/4	-
3	GOL	B	4	-	-	0/4/4/4	-
2	FLC	A	1	-	-	1/6/16/16	-
3	GOL	A	799	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3	GOL	O1-C1-C2-C3
3	B	2	GOL	O1-C1-C2-C3
3	A	799	GOL	O1-C1-C2-C3
3	A	3	GOL	O1-C1-C2-O2
3	A	799	GOL	O1-C1-C2-O2
2	A	1	FLC	CBC-CB-CG-CGC
3	B	2	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2	GOL	1	0
3	A	3	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	617/619 (99%)	-0.01	14 (2%)	60	54	36, 59, 93, 112	21 (3%)
1	B	618/619 (99%)	-0.05	15 (2%)	59	53	37, 59, 91, 111	16 (2%)
All	All	1235/1238 (99%)	-0.03	29 (2%)	60	54	36, 59, 92, 112	37 (2%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	780	ARG	4.2
1	A	247	GLN	3.8
1	B	595	PRO	3.6
1	B	289	ASN	3.5
1	A	632	ASP	3.4
1	B	785	ALA	3.4
1	A	216	ASP	3.3
1	A	289	ASN	3.1
1	B	182	ILE	3.1
1	B	596	ASN	3.1
1	B	195	ASN	2.9
1	B	215	GLN	2.8
1	A	599	THR	2.7
1	B	780	ARG	2.5
1	B	291	PRO	2.5
1	A	212	TRP	2.5
1	A	215	GLN	2.3
1	B	180	MET	2.3
1	A	740	VAL	2.3
1	B	181	ASN	2.3
1	A	181	ASN	2.3
1	A	197	PRO	2.2
1	B	216	ASP	2.2
1	B	597	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	221	VAL	2.1
1	B	784	ILE	2.1
1	A	195	ASN	2.1
1	A	736	ASN	2.1
1	A	219	ALA	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. 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
3	GOL	A	799	6/6	0.66	0.24	70,79,79,80	0
3	GOL	B	4	6/6	0.72	0.47	137,138,138,139	0
2	FLC	A	1	13/13	0.73	0.47	129,129,130,130	0
3	GOL	A	3	6/6	0.76	0.19	75,79,79,79	0
3	GOL	B	2	6/6	0.81	0.21	89,92,92,92	0

6.5 Other polymers (i)

There are no such residues in this entry.