Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2023 – 02:25 PM EDT

PDB ID	:	4RLF
Title	:	Crystal structure of a benzoate coenzyme A ligase with p-Toluic acid and o-Toluic acid
Authors	:	Strom, S.; Nosrati, M.; Thornburg, C.; Walker, K.; Geiger, J.H.
Deposited on	:	2014-10-16
Resolution	:	1.73 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:

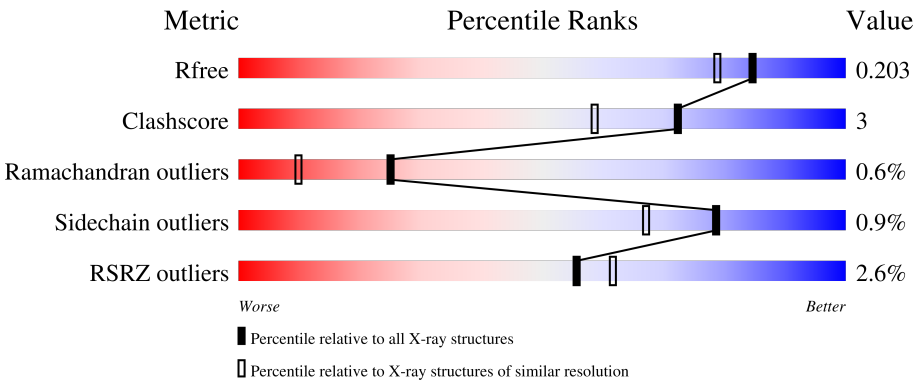
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.73 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	519	2% 92% 7% •
1	B	519	3% 91% 8% •

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
4	GOL	B	1007	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8442 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.

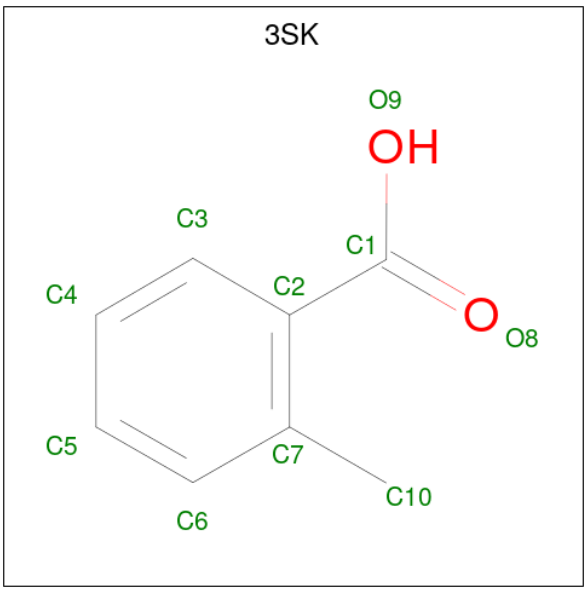
- Molecule 1 is a protein called Benzoate-coenzyme A ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	516	3906	2502	674	720	10	0	1	0
1	B	519	3904	2499	674	720	11	0	3	0

There are 6 discrepancies between the modelled and reference sequences:

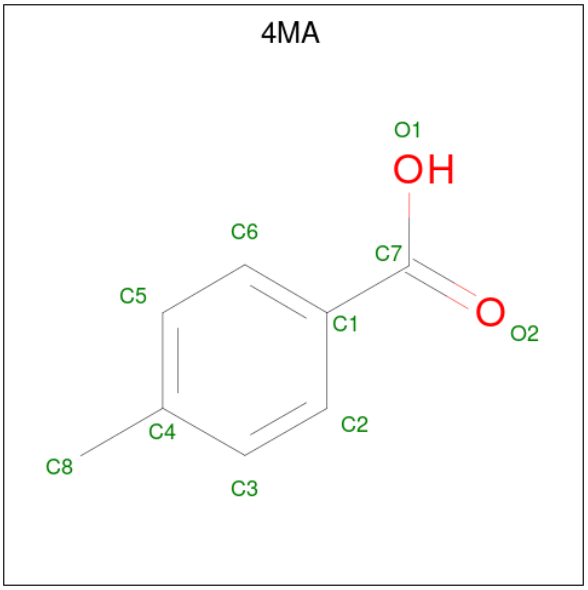
Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ALA	THR	conflict	UNP Q93TK0
A	341	ASP	GLY	conflict	UNP Q93TK0
A	524	GLY	-	expression tag	UNP Q93TK0
B	83	ALA	THR	conflict	UNP Q93TK0
B	341	ASP	GLY	conflict	UNP Q93TK0
B	524	GLY	-	expression tag	UNP Q93TK0

- Molecule 2 is 2-methylbenzoic acid (three-letter code: 3SK) (formula: $C_8H_8O_2$).



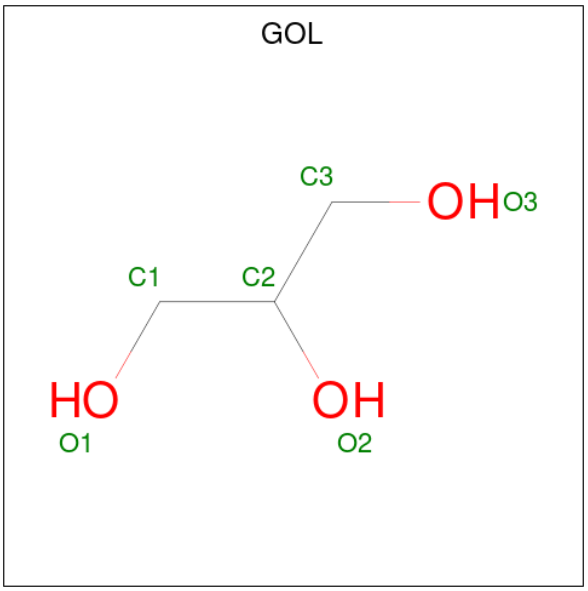
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			10	8	2			
2	B	1	Total	C	O		0	0
			10	8	2			

- Molecule 3 is 4-METHYLBENZOIC ACID (three-letter code: 4MA) (formula: $C_8H_8O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			10	8	2			
3	B	1	Total	C	O		0	0
			10	8	2			

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



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

- Molecule 5 is water.

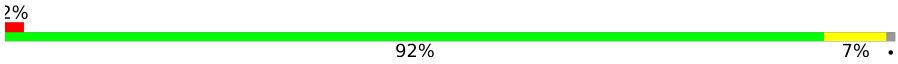
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	282	282	282	0	0
			Total	O		
5	B	262	262	262	0	0

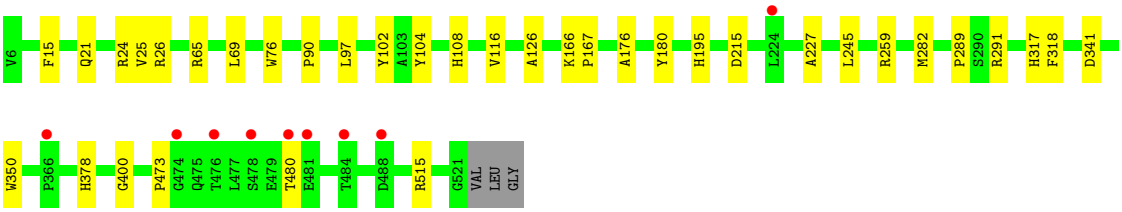
3 Residue-property plots (i)

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: Benzoate-coenzyme A ligase

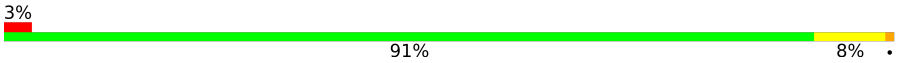
Chain A:

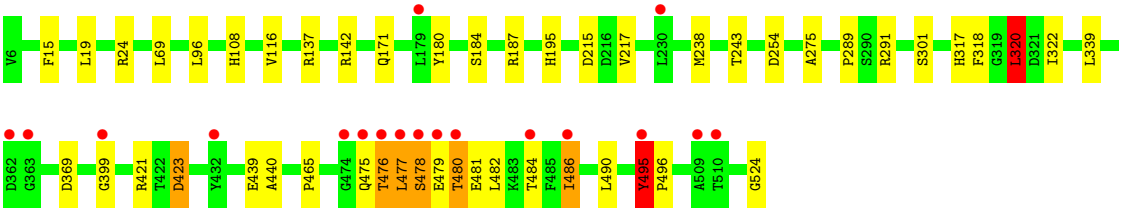




• Molecule 1: Benzoate-coenzyme A ligase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.72Å 95.37Å 95.78Å 90.00° 104.69° 90.00°	Depositor
Resolution (Å)	32.23 – 1.73 32.23 – 1.73	Depositor EDS
% Data completeness (in resolution range)	95.7 (32.23-1.73) 95.7 (32.23-1.73)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.159 , 0.195 0.172 , 0.203	Depositor DCC
R_{free} test set	5121 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	19.4	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 51.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8442	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 4MA, 3SK

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	0.98	1/4014 (0.0%)	0.98	6/5478 (0.1%)
1	B	0.98	2/4016 (0.0%)	1.01	16/5482 (0.3%)
All	All	0.98	3/8030 (0.0%)	0.99	22/10960 (0.2%)

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	B	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	439	GLU	CB-CG	-6.08	1.40	1.52
1	B	184	SER	CB-OG	-5.75	1.34	1.42
1	A	350	TRP	CG-CD1	5.29	1.44	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	215	ASP	CB-CG-OD1	8.91	126.32	118.30
1	B	137	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	B	187	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	A	65	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	B	423	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	B	423	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	104	TYR	CB-CG-CD1	-6.20	117.28	121.00
1	B	187	ARG	NE-CZ-NH1	6.20	123.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	495	TYR	C-N-CD	-5.73	108.00	120.60
1	A	215	ASP	CB-CG-OD1	5.72	123.44	118.30
1	B	137	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	369	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	320	LEU	CB-CG-CD1	5.43	120.23	111.00
1	B	24	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	439	GLU	CB-CA-C	-5.38	99.64	110.40
1	A	341	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	104	TYR	CB-CG-CD2	5.18	124.11	121.00
1	B	320	LEU	CA-CB-CG	5.14	127.13	115.30
1	B	254	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	215	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	B	524	GLY	CA-C-O	-5.08	111.45	120.60
1	A	26	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	476	THR	Peptide
1	B	478	SER	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	3906	0	3827	19	0
1	B	3904	0	3812	33	0
2	A	10	0	7	3	0
2	B	10	0	7	0	0
3	A	10	0	7	1	0
3	B	10	0	7	0	0
4	A	12	0	16	0	0
4	B	36	0	47	5	0
5	A	282	0	0	5	0
5	B	262	0	0	3	0
All	All	8442	0	7730	53	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 3.

All (53) 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:421:ARG:NH2	1:B:423:ASP:OD2	2.04	0.91
1:A:15:PHE:H	1:A:195:HIS:HD2	1.22	0.87
1:B:15:PHE:H	1:B:195:HIS:HD2	1.21	0.86
1:A:25:VAL:HG13	5:A:1307:HOH:O	1.77	0.83
1:B:495:TYR:HA	5:B:1356:HOH:O	1.81	0.81
1:B:486:ILE:HD13	1:B:490:LEU:HD12	1.64	0.80
1:B:495:TYR:CB	1:B:496:PRO:CA	2.62	0.76
2:A:1000:3SK:C10	5:A:1340:HOH:O	2.39	0.71
1:B:495:TYR:CB	1:B:496:PRO:HA	2.25	0.66
1:B:486:ILE:CD1	1:B:490:LEU:HD12	2.26	0.65
1:B:289:PRO:O	1:B:317:HIS:HE1	1.78	0.65
1:A:289:PRO:O	1:A:317:HIS:HE1	1.81	0.63
1:B:108:HIS:HD2	1:B:180:TYR:OH	1.82	0.63
2:A:1000:3SK:H6	5:A:1340:HOH:O	2.00	0.62
1:B:465:PRO:HG2	1:B:495:TYR:CB	2.30	0.61
1:A:15:PHE:H	1:A:195:HIS:CD2	2.12	0.61
1:B:15:PHE:H	1:B:195:HIS:CD2	2.10	0.61
1:B:421:ARG:HH21	1:B:423:ASP:CG	2.05	0.58
1:A:378:HIS:HD2	1:A:400:GLY:O	1.86	0.57
1:A:227:ALA:HB3	2:A:1000:3SK:H5	1.86	0.57
1:A:291:ARG:HG2	1:A:318:PHE:HA	1.88	0.56
1:B:291:ARG:HG2	1:B:318:PHE:HA	1.88	0.56
1:B:479:GLU:CG	1:B:480:THR:H	2.20	0.55
1:A:515:ARG:HD3	5:A:1299:HOH:O	2.09	0.53
1:B:479:GLU:HG2	1:B:480:THR:H	1.74	0.52
1:A:195:HIS:HE1	5:A:1346:HOH:O	1.92	0.52
1:B:96:LEU:HG	4:B:1007:GOL:H12	1.91	0.51
1:A:21:GLN:HE21	1:A:24:ARG:HH11	1.59	0.50
1:A:166:LYS:HB2	1:A:167:PRO:HD2	1.96	0.48
1:B:96:LEU:CG	4:B:1007:GOL:H12	2.44	0.48
1:B:195:HIS:HE1	5:B:1217:HOH:O	1.97	0.47
1:B:479:GLU:HG2	1:B:480:THR:N	2.29	0.47
1:A:108:HIS:HD2	1:A:180:TYR:OH	1.98	0.46
1:B:320:LEU:HD12	4:B:1004:GOL:H11	1.97	0.46
1:B:476:THR:HA	1:B:477:LEU:CB	2.46	0.46
1:A:97:LEU:HB2	1:A:102:TYR:CZ	2.50	0.46
1:A:90:PRO:HD2	1:A:176:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:TYR:CA	5:B:1356:HOH:O	2.53	0.45
1:B:275:ALA:HB2	4:B:1002:GOL:H2	1.98	0.45
1:A:126:ALA:HA	1:B:440:ALA:HB1	1.98	0.45
1:B:482:LEU:O	1:B:486:ILE:HG23	2.16	0.44
1:A:21:GLN:NE2	1:A:24:ARG:HH11	2.14	0.44
1:B:19:LEU:HB3	1:B:238[A]:MET:HE1	2.00	0.44
1:B:142:ARG:HD2	4:B:1005:GOL:H2	1.99	0.44
1:B:339:LEU:HD22	1:B:339:LEU:N	2.35	0.42
1:B:479:GLU:C	1:B:481:GLU:H	2.23	0.42
1:A:282:MET:HG3	3:A:1001:4MA:H82	2.02	0.42
1:B:217:VAL:HA	1:B:243:THR:O	2.20	0.42
1:B:301[B]:SER:HB2	1:B:322:ILE:CG2	2.51	0.41
1:A:69:LEU:O	1:A:116:VAL:HA	2.21	0.41
1:B:69:LEU:O	1:B:116:VAL:HA	2.19	0.41
1:B:479:GLU:CG	1:B:480:THR:N	2.84	0.40
1:A:245:LEU:HD21	1:A:259:ARG:HG2	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	515/519 (99%)	501 (97%)	14 (3%)	0	100 100
1	B	520/519 (100%)	502 (96%)	12 (2%)	6 (1%)	13 3
All	All	1035/1038 (100%)	1003 (97%)	26 (2%)	6 (1%)	25 10

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	475	GLN
1	B	495	TYR

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Mol	Chain	Res	Type
1	B	399	GLY
1	B	480	THR
1	B	477	LEU
1	B	478	SER

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	397/412 (96%)	394 (99%)	3 (1%)	81	72
1	B	394/412 (96%)	390 (99%)	4 (1%)	76	63
All	All	791/824 (96%)	784 (99%)	7 (1%)	78	67

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	TRP
1	A	473	PRO
1	A	480	THR
1	B	171	GLN
1	B	320	LEU
1	B	484	THR
1	B	486	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	50	GLN
1	A	108	HIS
1	A	112	GLN
1	A	195	HIS
1	A	317	HIS
1	A	378	HIS

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Mol	Chain	Res	Type
1	A	411	ASN
1	B	108	HIS
1	B	112	GLN
1	B	195	HIS
1	B	317	HIS
1	B	378	HIS
1	B	411	ASN

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)

12 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	$\#\|Z\| > 2$
4	GOL	A	1002	-	5,5,5	0.39	0	5,5,5	0.88	0
4	GOL	A	1003	-	5,5,5	0.69	0	5,5,5	0.83	0
4	GOL	B	1006	-	5,5,5	0.73	0	5,5,5	1.57	1 (20%)
4	GOL	B	1007	-	5,5,5	1.46	2 (40%)	5,5,5	3.65	3 (60%)
2	3SK	A	1000	-	10,10,10	1.98	2 (20%)	13,13,13	1.66	3 (23%)
2	3SK	B	1000	-	10,10,10	2.22	2 (20%)	13,13,13	2.06	3 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	4MA	B	1001	-	10,10,10	1.53	2 (20%)	13,13,13	1.57	3 (23%)
3	4MA	A	1001	-	10,10,10	0.91	0	13,13,13	1.09	1 (7%)
4	GOL	B	1005	-	5,5,5	0.68	0	5,5,5	0.97	0
4	GOL	B	1004	-	5,5,5	0.92	0	5,5,5	1.75	2 (40%)
4	GOL	B	1002	-	5,5,5	0.52	0	5,5,5	1.49	1 (20%)
4	GOL	B	1003	-	5,5,5	0.85	0	5,5,5	0.50	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	1002	-	-	0/4/4/4	-
4	GOL	A	1003	-	-	0/4/4/4	-
4	GOL	B	1006	-	-	1/4/4/4	-
4	GOL	B	1007	-	-	4/4/4/4	-
2	3SK	A	1000	-	-	2/4/4/4	0/1/1/1
2	3SK	B	1000	-	-	0/4/4/4	0/1/1/1
3	4MA	B	1001	-	-	0/4/4/4	0/1/1/1
3	4MA	A	1001	-	-	0/4/4/4	0/1/1/1
4	GOL	B	1005	-	-	0/4/4/4	-
4	GOL	B	1004	-	-	2/4/4/4	-
4	GOL	B	1002	-	-	2/4/4/4	-
4	GOL	B	1003	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	3SK	C2-C7	5.20	1.49	1.40
2	A	1000	3SK	C2-C7	3.76	1.46	1.40
2	A	1000	3SK	O8-C1	3.48	1.33	1.22
2	B	1000	3SK	C3-C2	-3.48	1.34	1.39
3	B	1001	4MA	O2-C7	2.67	1.30	1.22
4	B	1007	GOL	O1-C1	-2.39	1.32	1.42
4	B	1007	GOL	C1-C2	-2.07	1.43	1.51
3	B	1001	4MA	C6-C5	2.02	1.42	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1000	3SK	C7-C2-C1	-6.03	115.74	122.78
4	B	1007	GOL	O1-C1-C2	-5.02	86.14	110.20
4	B	1007	GOL	O2-C2-C3	4.76	130.09	109.12
4	B	1007	GOL	C3-C2-C1	-4.11	95.72	111.70
2	A	1000	3SK	C10-C7-C6	-3.28	113.91	120.31
3	B	1001	4MA	O1-C7-C1	3.04	122.72	114.85
4	B	1006	GOL	O2-C2-C1	-2.98	95.99	109.12
3	B	1001	4MA	C6-C5-C4	-2.71	117.75	121.38
2	B	1000	3SK	C3-C2-C1	2.64	124.71	118.63
2	B	1000	3SK	C10-C7-C2	-2.44	119.00	122.79
4	B	1004	GOL	O2-C2-C1	2.42	119.77	109.12
4	B	1002	GOL	O3-C3-C2	2.26	121.02	110.20
2	A	1000	3SK	C5-C4-C3	2.21	123.56	120.19
3	A	1001	4MA	C2-C3-C4	-2.20	118.43	121.38
2	A	1000	3SK	C6-C7-C2	2.19	120.50	117.72
4	B	1004	GOL	C3-C2-C1	2.08	119.81	111.70
3	B	1001	4MA	O1-C7-O2	-2.00	118.91	123.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1002	GOL	C1-C2-C3-O3
4	B	1007	GOL	O1-C1-C2-C3
4	B	1007	GOL	C1-C2-C3-O3
4	B	1007	GOL	O1-C1-C2-O2
4	B	1007	GOL	O2-C2-C3-O3
4	B	1006	GOL	C1-C2-C3-O3
4	B	1002	GOL	O2-C2-C3-O3
4	B	1004	GOL	O2-C2-C3-O3
4	B	1004	GOL	O1-C1-C2-O2
2	A	1000	3SK	O9-C1-C2-C3
2	A	1000	3SK	O8-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1007	GOL	2	0
2	A	1000	3SK	3	0
3	A	1001	4MA	1	0
4	B	1005	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1004	GOL	1	0
4	B	1002	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	516/519 (99%)	-0.30	9 (1%)	70	76	11, 20, 37, 51	0
1	B	519/519 (100%)	-0.15	18 (3%)	44	49	11, 21, 38, 71	0
All	All	1035/1038 (99%)	-0.23	27 (2%)	56	61	11, 20, 38, 71	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	474	GLY	7.0
1	B	477	LEU	5.6
1	A	474	GLY	3.9
1	B	362	ASP	3.8
1	A	476	THR	3.7
1	A	478	SER	3.5
1	B	476	THR	3.4
1	B	495	TYR	3.3
1	A	480	THR	3.3
1	B	399	GLY	3.3
1	B	475	GLN	3.1
1	B	363	GLY	3.1
1	B	486	ILE	3.0
1	A	488	ASP	2.8
1	B	509	ALA	2.7
1	B	478	SER	2.7
1	B	484	THR	2.7
1	B	510	THR	2.5
1	A	484	THR	2.5
1	B	230	LEU	2.4
1	B	179	LEU	2.3
1	A	366	PRO	2.3
1	B	432	TYR	2.3
1	A	481	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	480	THR	2.1
1	B	479	GLU	2.1
1	A	224	LEU	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, 95th 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
2	3SK	A	1000	10/10	0.88	0.10	21,22,26,27	0
4	GOL	B	1006	6/6	0.90	0.10	27,32,38,44	0
2	3SK	B	1000	10/10	0.92	0.13	20,22,29,29	0
4	GOL	B	1002	6/6	0.93	0.14	27,28,31,32	0
4	GOL	B	1003	6/6	0.94	0.08	19,22,23,26	0
3	4MA	A	1001	10/10	0.95	0.06	20,22,24,24	0
3	4MA	B	1001	10/10	0.95	0.08	18,20,21,23	0
4	GOL	B	1005	6/6	0.95	0.07	22,33,35,36	0
4	GOL	A	1002	6/6	0.95	0.12	25,27,28,31	0
4	GOL	A	1003	6/6	0.96	0.08	17,23,26,30	0
4	GOL	B	1004	6/6	0.96	0.08	17,25,26,37	0
4	GOL	B	1007	6/6	0.96	0.10	20,27,31,33	0

6.5 Other polymers (i)

There are no such residues in this entry.