Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 12:58 PM JST

PDB ID	:	5X9R
Title	:	Structural insights into the elevator-like mechanism of the sodium/citrate symporter CitS
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Deposited on	:	2017-03-08
Resolution	:	3.98 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 ⓘ 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 ⓘ) were used in the production of this report:

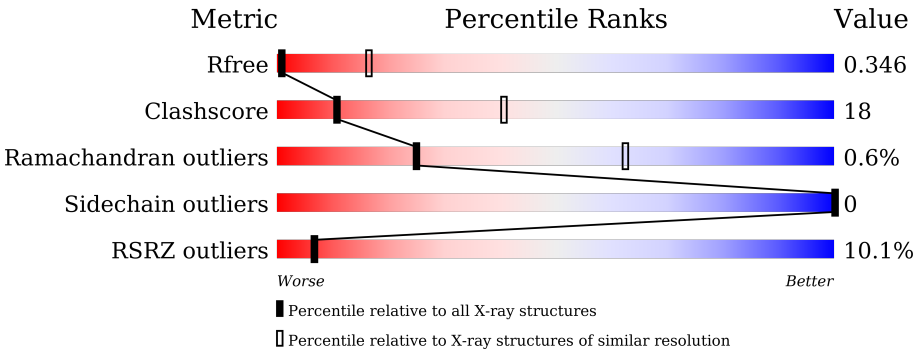
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.98 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	1039 (4.26-3.70)
Clashscore	141614	1099 (4.26-3.70)
Ramachandran outliers	138981	1061 (4.26-3.70)
Sidechain outliers	138945	1053 (4.26-3.70)
RSRZ outliers	127900	1021 (4.30-3.66)

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	438	9% 74% 21% 5%
1	B	438	10% 72% 21% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6233 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.

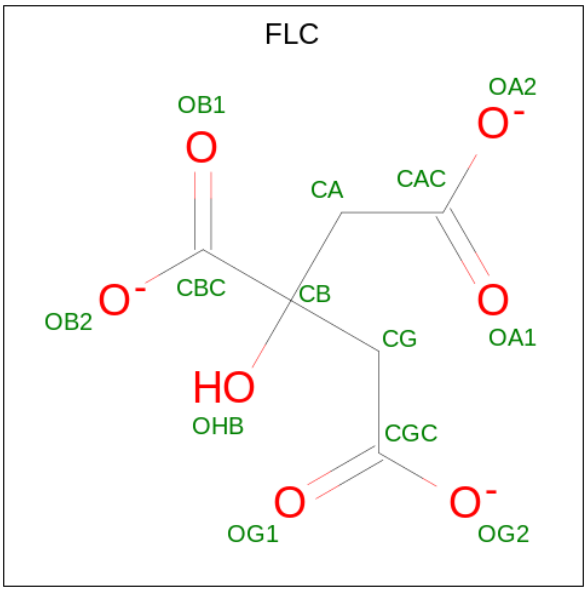
- Molecule 1 is a protein called Citrate-sodium symporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3120	2069	499	532	20			
1	B	409	Total	C	N	O	S	0	0	0
			3063	2036	487	521	19			

There are 8 discrepancies between the modelled and reference sequences:

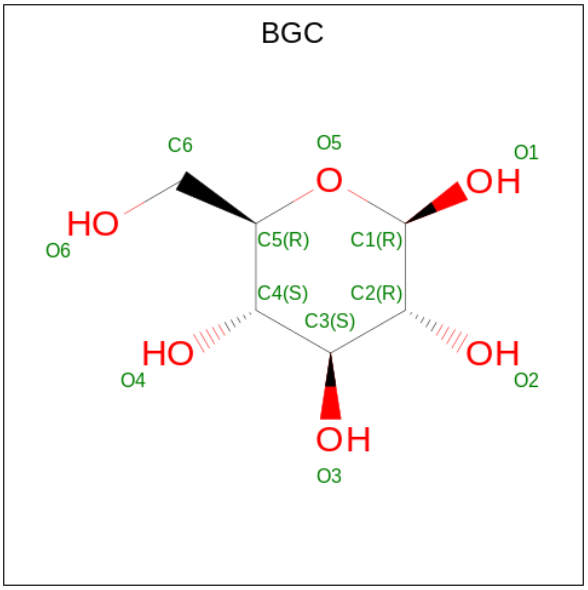
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLY	-	expression tag	UNP P31602
A	12	SER	-	expression tag	UNP P31602
A	447	PRO	-	expression tag	UNP P31602
A	448	ARG	-	expression tag	UNP P31602
B	11	GLY	-	expression tag	UNP P31602
B	12	SER	-	expression tag	UNP P31602
B	447	PRO	-	expression tag	UNP P31602
B	448	ARG	-	expression tag	UNP P31602

- 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 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0

- Molecule 3 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



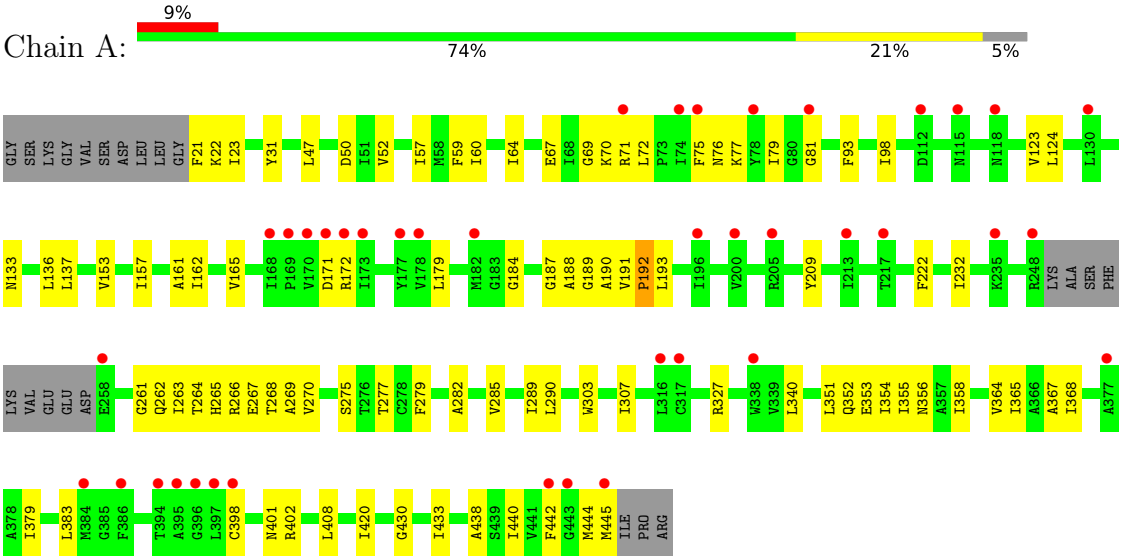
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	0
3	B	1	Total C O 12 6 6	0	0

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.

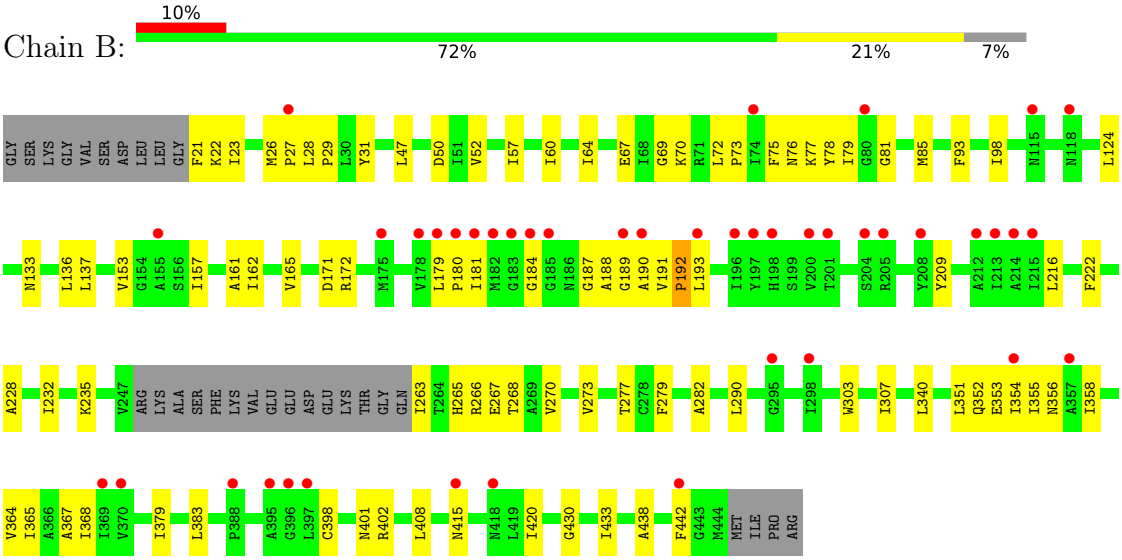
• Molecule 1: Citrate-sodium symporter

Chain A:



• Molecule 1: Citrate-sodium symporter

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	94.00Å 94.00Å 172.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.00 – 3.98 45.35 – 3.98	Depositor EDS
% Data completeness (in resolution range)	98.7 (94.00-3.98) 98.7 (45.35-3.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.273 , 0.323 0.287 , 0.346	Depositor DCC
R_{free} test set	596 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å^2)	196.9	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 239.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6233	wwPDB-VP
Average B, all atoms (Å^2)	271.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, BGC

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	0.42	0/3182	0.60	0/4317
1	B	0.42	0/3125	0.60	0/4243
All	All	0.42	0/6307	0.60	0/8560

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	3120	0	3290	108	0
1	B	3063	0	3231	131	0
2	A	13	0	5	1	0
2	B	13	0	5	1	0
3	A	12	0	12	0	0
3	B	12	0	12	0	0
All	All	6233	0	6555	234	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 18.

All (234) 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:78:TYR:CE2	1:B:232:ILE:CG1	1.88	1.57
1:B:78:TYR:CE2	1:B:232:ILE:HG12	1.02	1.52
1:B:180:PRO:C	1:B:216:LEU:HD21	1.38	1.39
1:B:75:PHE:CZ	1:B:85:MET:SD	2.27	1.27
1:B:438:ALA:O	1:B:442:PHE:HD1	1.15	1.26
1:B:78:TYR:HE2	1:B:232:ILE:CG1	1.32	1.25
1:B:438:ALA:O	1:B:442:PHE:CD1	1.90	1.25
1:B:78:TYR:CZ	1:B:232:ILE:HA	1.70	1.25
1:B:438:ALA:HB1	1:B:442:PHE:CE1	1.79	1.16
1:B:78:TYR:CD2	1:B:232:ILE:HG12	1.83	1.13
1:B:438:ALA:HB1	1:B:442:PHE:HE1	1.00	1.13
1:B:181:ILE:N	1:B:216:LEU:HD21	1.62	1.12
1:A:70:LYS:HA	1:A:76:ASN:HD22	1.13	1.12
1:B:181:ILE:HA	1:B:216:LEU:CD2	1.80	1.10
1:B:70:LYS:O	1:B:76:ASN:ND2	1.83	1.09
1:A:438:ALA:HB1	1:A:442:PHE:CE1	1.88	1.08
1:B:180:PRO:C	1:B:216:LEU:CD2	2.25	1.05
1:A:438:ALA:HB1	1:A:442:PHE:HE1	1.10	1.05
1:B:438:ALA:C	1:B:442:PHE:HD1	1.63	1.02
1:B:181:ILE:HA	1:B:216:LEU:HD22	1.39	1.01
1:B:438:ALA:CB	1:B:442:PHE:HE1	1.74	1.00
1:B:181:ILE:CA	1:B:216:LEU:CD2	2.41	0.97
1:B:181:ILE:N	1:B:216:LEU:CD2	2.27	0.96
1:A:72:LEU:HB2	1:A:75:PHE:HB2	1.46	0.96
1:B:263:ILE:HA	1:B:267:GLU:OE1	1.63	0.95
1:A:265:HIS:O	1:A:269:ALA:N	1.99	0.94
1:B:72:LEU:CB	1:B:75:PHE:HB3	2.01	0.91
1:A:70:LYS:CA	1:A:76:ASN:HD22	1.86	0.89
1:A:70:LYS:HA	1:A:76:ASN:ND2	1.87	0.88
1:A:438:ALA:CB	1:A:442:PHE:HE1	1.87	0.88
1:A:77:LYS:CD	1:A:232:ILE:HD11	2.04	0.87
1:B:78:TYR:CE2	1:B:232:ILE:CB	2.59	0.86
1:B:263:ILE:HG23	1:B:267:GLU:OE1	1.75	0.86
1:B:78:TYR:CD2	1:B:232:ILE:CG1	2.49	0.85
1:B:78:TYR:CZ	1:B:232:ILE:CA	2.58	0.85
1:B:180:PRO:O	1:B:216:LEU:CD2	2.24	0.84
1:B:180:PRO:O	1:B:216:LEU:HD21	1.78	0.82
1:B:77:LYS:HE3	1:B:228:ALA:HB1	1.60	0.82
1:B:438:ALA:C	1:B:442:PHE:CD1	2.45	0.81
1:A:188:ALA:O	1:A:192:PRO:HG3	1.80	0.81
1:B:78:TYR:OH	1:B:232:ILE:HG23	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ALA:O	1:B:192:PRO:HG3	1.80	0.81
1:A:438:ALA:O	1:A:442:PHE:HD1	1.65	0.80
1:A:77:LYS:HD3	1:A:232:ILE:HD11	1.64	0.79
1:B:72:LEU:HB2	1:B:75:PHE:HB3	1.63	0.79
1:B:72:LEU:HD12	1:B:75:PHE:CD1	2.20	0.76
1:B:263:ILE:CA	1:B:267:GLU:OE1	2.33	0.76
1:B:75:PHE:CE1	1:B:85:MET:SD	2.79	0.75
1:A:69:GLY:O	1:A:76:ASN:HB2	1.86	0.74
1:B:78:TYR:CE2	1:B:232:ILE:HA	2.21	0.74
1:B:72:LEU:HB3	1:B:75:PHE:HB3	1.69	0.74
1:B:78:TYR:OH	1:B:232:ILE:HA	1.88	0.74
1:B:181:ILE:CA	1:B:216:LEU:HD22	2.13	0.74
1:B:23:ILE:N	1:B:26:MET:O	2.21	0.74
1:A:77:LYS:HD2	1:A:232:ILE:HD11	1.69	0.73
1:B:78:TYR:CE2	1:B:232:ILE:HG13	2.19	0.72
1:A:72:LEU:HD13	1:A:75:PHE:CE2	2.25	0.72
1:B:124:LEU:HB3	1:B:420:ILE:HG21	1.72	0.72
1:A:21:PHE:CD2	1:A:22:LYS:HG3	2.25	0.71
1:A:354:ILE:HG22	1:A:358:ILE:HD11	1.72	0.71
1:A:188:ALA:O	1:A:192:PRO:CG	2.39	0.71
1:A:124:LEU:HB3	1:A:420:ILE:HG21	1.71	0.71
1:B:355:ILE:HD13	1:B:358:ILE:HD12	1.72	0.71
1:B:69:GLY:O	1:B:76:ASN:HB2	1.91	0.70
1:A:355:ILE:HD13	1:A:358:ILE:HD12	1.72	0.70
1:B:188:ALA:O	1:B:192:PRO:CG	2.39	0.70
1:B:354:ILE:HG22	1:B:358:ILE:HD11	1.72	0.70
1:A:438:ALA:C	1:A:442:PHE:HD1	1.94	0.70
1:B:72:LEU:HD12	1:B:75:PHE:CG	2.27	0.69
1:B:438:ALA:CB	1:B:442:PHE:CE1	2.60	0.69
1:A:438:ALA:O	1:A:442:PHE:CD1	2.44	0.69
1:B:181:ILE:HA	1:B:216:LEU:HD23	1.72	0.69
1:B:78:TYR:CE2	1:B:232:ILE:CA	2.78	0.67
1:A:440:ILE:O	1:A:444:MET:HG2	1.94	0.66
1:B:23:ILE:HG23	1:B:67:GLU:HG3	1.78	0.65
1:B:263:ILE:CG2	1:B:267:GLU:OE1	2.45	0.65
1:A:265:HIS:HA	1:A:268:THR:OG1	1.97	0.64
1:B:22:LYS:HE2	1:B:27:PRO:HG3	1.79	0.64
1:B:75:PHE:HZ	1:B:85:MET:SD	2.12	0.64
1:A:77:LYS:HD3	1:A:232:ILE:CD1	2.29	0.62
1:B:187:GLY:O	1:B:192:PRO:HD3	1.99	0.62
1:A:21:PHE:CE2	1:A:22:LYS:HG3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASN:CG	1:A:81:GLY:HA3	2.20	0.62
1:A:187:GLY:O	1:A:192:PRO:HD3	2.00	0.61
1:B:78:TYR:CD2	1:B:232:ILE:HG13	2.33	0.61
1:B:265:HIS:O	1:B:268:THR:N	2.34	0.60
1:A:264:THR:N	1:A:267:GLU:OE1	2.35	0.59
1:A:72:LEU:HD12	1:A:75:PHE:CD1	2.38	0.59
1:A:354:ILE:O	1:A:358:ILE:HG13	2.03	0.59
1:A:72:LEU:HD13	1:A:75:PHE:CD2	2.38	0.58
1:A:402:ARG:NE	2:A:501:FLC:OG2	2.36	0.58
1:B:187:GLY:O	1:B:191:VAL:HB	2.04	0.58
1:B:354:ILE:O	1:B:358:ILE:HG13	2.03	0.58
1:A:266:ARG:O	1:A:270:VAL:HG23	2.03	0.58
1:A:438:ALA:CB	1:A:442:PHE:CE1	2.72	0.58
1:B:402:ARG:NE	2:B:501:FLC:OG2	2.37	0.57
1:B:75:PHE:CE2	1:B:85:MET:SD	2.95	0.57
1:A:264:THR:OG1	1:A:267:GLU:N	2.33	0.57
1:B:78:TYR:OH	1:B:232:ILE:CA	2.51	0.57
1:A:187:GLY:O	1:A:191:VAL:HB	2.04	0.57
1:A:190:ALA:HB1	1:A:209:TYR:CD1	2.40	0.56
1:B:47:LEU:CD2	1:B:57:ILE:HD11	2.35	0.56
1:A:340:LEU:HD21	1:A:408:LEU:HD13	1.88	0.56
1:B:180:PRO:O	1:B:216:LEU:HD22	2.05	0.56
1:A:67:GLU:O	1:A:71:ARG:HG3	2.07	0.55
1:B:190:ALA:HB1	1:B:209:TYR:CD1	2.41	0.55
1:A:47:LEU:CD2	1:A:57:ILE:HD11	2.36	0.55
1:B:438:ALA:CA	1:B:442:PHE:CE1	2.89	0.55
1:B:190:ALA:HB1	1:B:209:TYR:CE1	2.42	0.55
1:B:340:LEU:HD21	1:B:408:LEU:HD13	1.88	0.55
1:A:438:ALA:C	1:A:442:PHE:CD1	2.80	0.54
1:B:77:LYS:HD2	1:B:232:ILE:HD11	1.89	0.54
1:B:77:LYS:HE3	1:B:228:ALA:CB	2.36	0.54
1:A:72:LEU:HD12	1:A:75:PHE:CG	2.43	0.54
1:A:261:GLY:O	1:A:262:GLN:HG3	2.08	0.54
1:A:190:ALA:HB1	1:A:209:TYR:CE1	2.42	0.53
1:B:184:GLY:O	1:B:188:ALA:HB3	2.08	0.53
1:B:266:ARG:O	1:B:270:VAL:HG23	2.09	0.53
1:A:179:LEU:HD13	1:A:442:PHE:CE1	2.44	0.53
1:B:47:LEU:HD21	1:B:57:ILE:HD11	1.90	0.53
1:B:23:ILE:O	1:B:26:MET:HB2	2.10	0.52
1:B:78:TYR:OH	1:B:232:ILE:CG2	2.54	0.52
1:A:184:GLY:O	1:A:188:ALA:HB3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:HD21	1:A:57:ILE:HD11	1.91	0.52
1:A:69:GLY:O	1:A:76:ASN:CB	2.55	0.52
1:A:60:ILE:HD11	1:B:277:THR:HG22	1.92	0.52
1:A:70:LYS:CB	1:A:76:ASN:HD22	2.22	0.52
1:A:264:THR:H	1:A:267:GLU:HB2	1.75	0.51
1:A:162:ILE:HD13	1:A:365:ILE:HA	1.92	0.51
1:B:21:PHE:CE2	1:B:22:LYS:O	2.64	0.51
1:A:70:LYS:HA	1:A:76:ASN:CB	2.40	0.51
1:B:179:LEU:HD13	1:B:442:PHE:CE1	2.45	0.51
1:A:72:LEU:HB2	1:A:75:PHE:CB	2.31	0.51
1:A:23:ILE:HD12	1:A:31:TYR:CD2	2.45	0.50
1:B:72:LEU:CD1	1:B:75:PHE:CG	2.93	0.50
1:B:354:ILE:HG22	1:B:358:ILE:CD1	2.41	0.50
1:A:133:ASN:HD22	1:A:136:LEU:HD13	1.76	0.50
1:B:133:ASN:HD22	1:B:136:LEU:HD13	1.76	0.50
1:B:162:ILE:HD13	1:B:365:ILE:HA	1.93	0.50
1:A:189:GLY:O	1:A:193:LEU:HB2	2.11	0.49
1:A:263:ILE:HD13	1:A:327:ARG:NH1	2.27	0.49
1:B:31:TYR:OH	1:B:64:ILE:HB	2.11	0.49
1:A:21:PHE:CZ	1:A:22:LYS:HE3	2.47	0.49
1:A:263:ILE:CD1	1:A:327:ARG:NH1	2.75	0.49
1:A:351:LEU:O	1:A:355:ILE:HG12	2.12	0.49
1:B:79:ILE:HB	1:B:415:ASN:HB2	1.94	0.49
1:A:31:TYR:OH	1:A:64:ILE:HB	2.12	0.49
1:A:93:PHE:HA	1:A:98:ILE:HD12	1.94	0.49
1:B:189:GLY:O	1:B:193:LEU:HB2	2.12	0.49
1:A:279:PHE:CD1	1:B:52:VAL:HG11	2.48	0.48
1:B:93:PHE:HA	1:B:98:ILE:HD12	1.95	0.48
1:B:263:ILE:CB	1:B:267:GLU:OE1	2.60	0.48
1:A:354:ILE:HG22	1:A:358:ILE:CD1	2.41	0.48
1:B:398:CYS:HA	1:B:401:ASN:ND2	2.28	0.48
1:A:282:ALA:HB2	1:A:307:ILE:HD12	1.93	0.48
1:A:353:GLU:HA	1:A:356:ASN:HD22	1.78	0.48
1:B:70:LYS:C	1:B:76:ASN:ND2	2.64	0.48
1:B:76:ASN:OD1	1:B:81:GLY:HA3	2.14	0.48
1:B:181:ILE:CA	1:B:216:LEU:HD23	2.36	0.48
1:B:282:ALA:HB2	1:B:307:ILE:HD12	1.95	0.48
1:A:161:ALA:O	1:A:165:VAL:HG23	2.14	0.48
1:A:398:CYS:HA	1:A:401:ASN:ND2	2.28	0.48
1:B:351:LEU:O	1:B:355:ILE:HG12	2.12	0.48
1:B:22:LYS:HG2	1:B:27:PRO:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ILE:HD11	1:B:364:VAL:HG12	1.96	0.47
1:B:77:LYS:CE	1:B:228:ALA:HB1	2.39	0.47
1:A:76:ASN:OD1	1:A:77:LYS:N	2.47	0.47
1:A:72:LEU:CD1	1:A:75:PHE:CD2	2.97	0.47
1:B:161:ALA:O	1:B:165:VAL:HG23	2.14	0.47
1:B:353:GLU:HA	1:B:356:ASN:HD22	1.79	0.47
1:A:379:ILE:O	1:A:383:LEU:HG	2.15	0.47
1:B:265:HIS:O	1:B:266:ARG:C	2.53	0.46
1:A:52:VAL:HG11	1:B:279:PHE:CD1	2.51	0.46
1:B:78:TYR:CZ	1:B:232:ILE:CB	2.96	0.46
1:A:162:ILE:HD11	1:A:364:VAL:HG12	1.96	0.46
1:B:222:PHE:CE2	1:B:367:ALA:HB2	2.51	0.46
1:A:72:LEU:CD1	1:A:75:PHE:CG	2.99	0.46
1:A:277:THR:HG22	1:B:60:ILE:HD11	1.97	0.46
1:B:180:PRO:O	1:B:216:LEU:CD1	2.64	0.46
1:B:379:ILE:O	1:B:383:LEU:HG	2.15	0.46
1:A:76:ASN:CB	1:A:81:GLY:HA3	2.47	0.45
1:A:222:PHE:CE2	1:A:367:ALA:HB2	2.52	0.45
1:A:442:PHE:O	1:A:445:MET:HG2	2.16	0.45
1:B:78:TYR:CD1	1:B:235:LYS:HD2	2.52	0.45
1:A:76:ASN:OD1	1:A:81:GLY:N	2.47	0.45
1:B:22:LYS:HG2	1:B:27:PRO:CA	2.47	0.45
1:B:171:ASP:OD1	1:B:172:ARG:N	2.50	0.45
1:A:171:ASP:OD1	1:A:172:ARG:N	2.50	0.45
1:A:355:ILE:HD13	1:A:358:ILE:CD1	2.45	0.45
1:A:162:ILE:HD12	1:A:368:ILE:HG13	1.98	0.44
1:B:352:GLN:HG2	1:B:353:GLU:N	2.32	0.44
1:A:352:GLN:HG2	1:A:353:GLU:N	2.32	0.44
1:B:162:ILE:HD12	1:B:368:ILE:HG13	1.97	0.44
1:B:93:PHE:O	1:B:98:ILE:N	2.51	0.43
1:A:76:ASN:OD1	1:A:81:GLY:HA3	2.19	0.43
1:A:189:GLY:O	1:A:193:LEU:N	2.40	0.43
1:A:77:LYS:CD	1:A:232:ILE:CD1	2.88	0.43
1:A:430:GLY:HA2	1:A:433:ILE:HD12	2.01	0.43
1:A:21:PHE:CE2	1:A:22:LYS:HE3	2.53	0.43
1:A:222:PHE:CZ	1:A:367:ALA:HB2	2.54	0.43
1:B:290:LEU:HD22	1:B:303:TRP:HZ2	1.84	0.43
1:A:290:LEU:HD22	1:A:303:TRP:HZ2	1.84	0.43
1:B:28:LEU:HB2	1:B:29:PRO:HD3	2.01	0.43
1:B:47:LEU:HD21	1:B:57:ILE:CD1	2.48	0.43
1:A:47:LEU:HD21	1:A:57:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:VAL:HB	1:A:192:PRO:HD3	2.01	0.42
1:B:133:ASN:HB2	1:B:136:LEU:HD13	2.02	0.42
1:A:133:ASN:HB2	1:A:136:LEU:HD13	2.02	0.42
1:A:264:THR:HG23	1:A:267:GLU:CD	2.40	0.42
1:A:261:GLY:C	1:A:262:GLN:HG3	2.40	0.42
1:B:222:PHE:CZ	1:B:367:ALA:HB2	2.54	0.42
1:A:264:THR:O	1:A:268:THR:N	2.44	0.42
1:B:191:VAL:HB	1:B:192:PRO:HD3	2.01	0.42
1:B:430:GLY:HA2	1:B:433:ILE:HD12	2.01	0.42
1:B:189:GLY:O	1:B:193:LEU:N	2.39	0.42
1:B:355:ILE:HD13	1:B:358:ILE:CD1	2.46	0.42
1:B:50:ASP:OD1	1:B:52:VAL:N	2.50	0.42
1:B:78:TYR:HH	1:B:232:ILE:HA	1.84	0.41
1:A:50:ASP:OD1	1:A:52:VAL:N	2.50	0.41
1:B:179:LEU:N	1:B:180:PRO:HD2	2.36	0.41
1:A:59:PHE:CG	1:B:273:VAL:HG22	2.55	0.41
1:B:77:LYS:CE	1:B:228:ALA:CB	2.99	0.41
1:B:153:VAL:O	1:B:157:ILE:HG12	2.21	0.41
1:A:123:VAL:HA	1:A:275:SER:OG	2.21	0.41
1:A:354:ILE:HG22	1:A:358:ILE:CG1	2.51	0.41
1:B:179:LEU:HD13	1:B:442:PHE:CZ	2.56	0.41
1:A:264:THR:O	1:A:267:GLU:N	2.55	0.40
1:A:285:VAL:HA	1:A:289:ILE:HB	2.02	0.40
1:A:153:VAL:O	1:A:157:ILE:HG12	2.21	0.40
1:B:28:LEU:O	1:B:29:PRO:C	2.59	0.40
1:A:72:LEU:HD13	1:A:75:PHE:CZ	2.56	0.40
1:A:79:ILE:HG22	1:A:79:ILE:O	2.22	0.40
1:A:93:PHE:O	1:A:98:ILE:N	2.52	0.40
1:B:351:LEU:HD23	1:B:354:ILE:HD12	2.03	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	412/438 (94%)	380 (92%)	30 (7%)	2 (0%)	29	66
1	B	405/438 (92%)	370 (91%)	32 (8%)	3 (1%)	22	60
All	All	817/876 (93%)	750 (92%)	62 (8%)	5 (1%)	25	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	B	137	LEU
1	A	192	PRO
1	B	192	PRO
1	B	73	PRO

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	325/343 (95%)	325 (100%)	0	100	100
1	B	319/343 (93%)	319 (100%)	0	100	100
All	All	644/686 (94%)	644 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	186	ASN
1	A	356	ASN
1	B	133	ASN
1	B	356	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 monosaccharides in this entry.

5.6 Ligand geometry

4 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	$\#\|Z\| > 2$
2	FLC	B	501	-	12,12,12	2.06	3 (25%)	17,17,17	4.68	9 (52%)
3	BGC	B	502	-	12,12,12	0.41	0	17,17,17	0.83	0
3	BGC	A	502	-	12,12,12	0.32	0	17,17,17	0.81	0
2	FLC	A	501	-	12,12,12	1.74	3 (25%)	17,17,17	4.68	8 (47%)

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	FLC	B	501	-	-	5/16/16/16	-
3	BGC	B	502	-	-	0/2/22/22	0/1/1/1
3	BGC	A	502	-	-	0/2/22/22	0/1/1/1
2	FLC	A	501	-	-	4/16/16/16	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FLC	CB-CBC	-5.19	1.48	1.53
2	A	501	FLC	CB-CBC	-3.82	1.49	1.53
2	B	501	FLC	CG-CB	-2.60	1.50	1.53
2	B	501	FLC	CA-CB	-2.36	1.50	1.53
2	A	501	FLC	OHB-CB	2.09	1.47	1.43
2	A	501	FLC	CA-CB	-2.02	1.51	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	FLC	OB1-CBC-CB	-8.71	109.92	122.25
2	A	501	FLC	OHB-CB-CBC	-8.56	96.84	108.86
2	B	501	FLC	OB2-CBC-CB	8.47	127.76	113.05
2	B	501	FLC	OHB-CB-CBC	-8.41	97.06	108.86
2	A	501	FLC	OB1-CBC-CB	-8.29	110.52	122.25
2	A	501	FLC	OB2-CBC-CB	7.99	126.93	113.05
2	A	501	FLC	OHB-CB-CA	-7.96	90.78	109.40
2	B	501	FLC	OHB-CB-CA	-7.69	91.41	109.40
2	A	501	FLC	CG-CB-CBC	5.84	122.66	110.11
2	B	501	FLC	CA-CB-CBC	5.67	122.29	110.11
2	B	501	FLC	CG-CB-CBC	5.48	121.88	110.11
2	A	501	FLC	CA-CB-CBC	5.38	121.67	110.11
2	A	501	FLC	OHB-CB-CG	-5.19	97.25	109.40
2	B	501	FLC	OHB-CB-CG	-3.76	100.60	109.40
2	B	501	FLC	CB-CA-CAC	2.83	120.68	113.81
2	A	501	FLC	CB-CA-CAC	2.47	119.79	113.81
2	B	501	FLC	CB-CG-CGC	-2.16	108.59	113.81

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FLC	CBC-CB-CG-CGC
2	B	501	FLC	CBC-CB-CG-CGC
2	A	501	FLC	OHB-CB-CG-CGC
2	B	501	FLC	CAC-CA-CB-CBC
2	B	501	FLC	CG-CB-CBC-OB2
2	A	501	FLC	CAC-CA-CB-CBC
2	B	501	FLC	OHB-CB-CG-CGC
2	A	501	FLC	CG-CB-CBC-OB2
2	B	501	FLC	CG-CB-CBC-OB1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FLC	1	0
2	A	501	FLC	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	416/438 (94%)	0.51	40 (9%)	8	7	159, 261, 342, 404	0
1	B	409/438 (93%)	0.52	43 (10%)	6	6	196, 272, 351, 410	0
All	All	825/876 (94%)	0.52	83 (10%)	7	7	159, 264, 346, 410	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	GLY	8.4
1	A	395	ALA	6.2
1	A	442	PHE	4.5
1	B	183	GLY	4.4
1	B	295	GLY	4.2
1	B	201	THR	4.2
1	B	415	ASN	4.1
1	B	182	MET	4.0
1	B	193	LEU	4.0
1	A	173	ILE	3.9
1	A	445	MET	3.9
1	B	178	VAL	3.8
1	A	396	GLY	3.8
1	A	177	TYR	3.8
1	A	71	ARG	3.6
1	A	397	LEU	3.6
1	A	171	ASP	3.4
1	A	235	LYS	3.3
1	B	205	ARG	3.2
1	B	418	ASN	3.2
1	B	196	ILE	3.1
1	B	208	TYR	3.1
1	A	112	ASP	3.1
1	B	179	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	338	TRP	3.0
1	B	185	GLY	3.0
1	A	78	TYR	2.9
1	A	115	ASN	2.9
1	B	115	ASN	2.9
1	B	212	ALA	2.9
1	A	172	ARG	2.8
1	B	189	GLY	2.8
1	B	395	ALA	2.8
1	A	317	CYS	2.8
1	B	388	PRO	2.7
1	A	394	THR	2.7
1	B	181	ILE	2.6
1	A	178	VAL	2.6
1	B	190	ALA	2.6
1	A	316	LEU	2.6
1	B	198	HIS	2.6
1	A	200	VAL	2.6
1	B	197	TYR	2.5
1	B	354	ILE	2.5
1	A	169	PRO	2.5
1	B	175	MET	2.5
1	A	168	ILE	2.5
1	B	118	ASN	2.5
1	A	118	ASN	2.5
1	A	182	MET	2.5
1	A	258	GLU	2.5
1	B	27	PRO	2.5
1	B	370	VAL	2.5
1	A	170	VAL	2.4
1	B	200	VAL	2.4
1	B	213	ILE	2.4
1	B	74	ILE	2.4
1	B	369	ILE	2.4
1	B	204	SER	2.4
1	B	215	ILE	2.3
1	B	442	PHE	2.4
1	B	180	PRO	2.3
1	B	214	ALA	2.3
1	A	248	ARG	2.3
1	B	357	ALA	2.2
1	A	386	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	443	GLY	2.2
1	A	384	MET	2.2
1	A	205	ARG	2.2
1	A	75	PHE	2.2
1	B	396	GLY	2.1
1	B	155	ALA	2.1
1	A	74	ILE	2.1
1	B	298	ILE	2.1
1	B	397	LEU	2.1
1	A	196	ILE	2.1
1	A	398	CYS	2.1
1	A	130	LEU	2.1
1	A	217	THR	2.0
1	B	80	GLY	2.0
1	A	213	ILE	2.0
1	A	377	ALA	2.0
1	A	81	GLY	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
3	BGC	A	502	12/12	0.79	0.27	218,246,269,274	0
2	FLC	A	501	13/13	0.81	0.42	229,257,267,269	0
3	BGC	B	502	12/12	0.87	0.37	260,278,281,281	0
2	FLC	B	501	13/13	0.89	0.19	231,248,253,259	0

6.5 Other polymers (i)

There are no such residues in this entry.