Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 09:29 PM GMT

PDB ID	:	5A1S
Title	:	Crystal structure of the sodium-dependent citrate symporter SeCitS form Salmonella enterica.
Authors	:	Woehlert, D.; Groetzinger, M.J.; Kuhlbrandt, W.; Yildiz, O.
Deposited on	:	2015-05-05
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

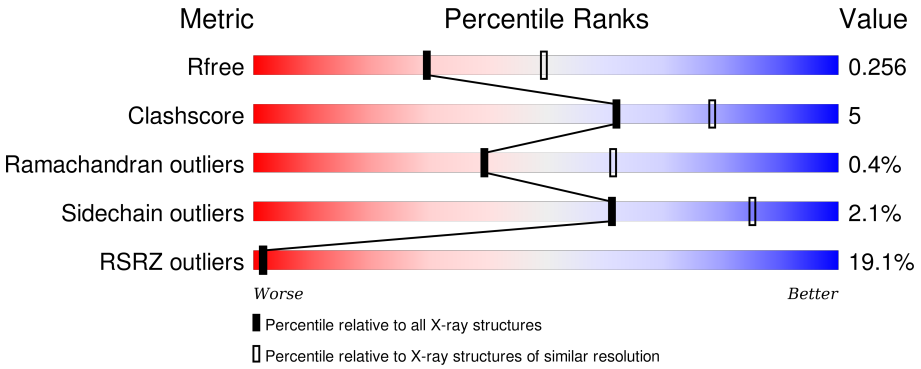
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	448	16% 85% 12% •
1	B	448	23% 80% 15% 5%
1	C	448	20% 79% 16% • •
1	D	448	15% 82% 14% • •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLC	B	1449	-	-	-	X
4	BOG	A	1456	-	-	-	X
5	UND	D	1450	-	-	-	X
7	PTY	A	1455	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13270 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	433	Total	C	N	O	S	0	0	0
			3256	2151	516	567	22			
1	B	426	Total	C	N	O	S	0	0	0
			3201	2117	508	554	22			
1	C	428	Total	C	N	O	S	0	0	0
			3206	2118	511	555	22			
1	D	434	Total	C	N	O	S	0	0	0
			3253	2147	517	567	22			

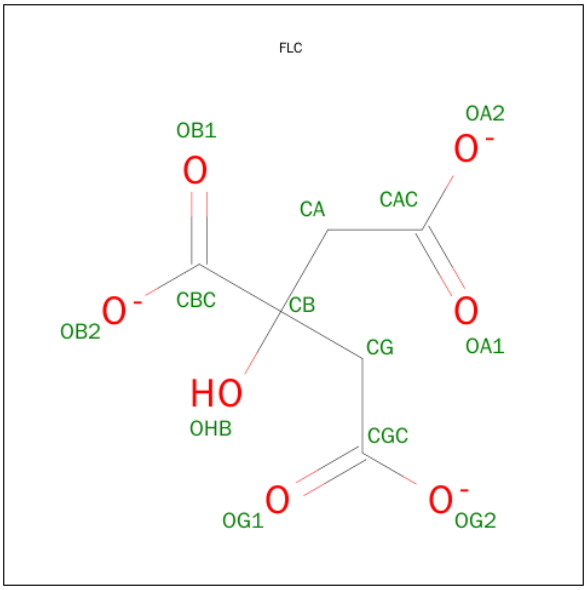
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	LEU	-	EXPRESSION TAG	UNP G4BX92
A	448	GLU	-	EXPRESSION TAG	UNP G4BX92
B	447	LEU	-	EXPRESSION TAG	UNP G4BX92
B	448	GLU	-	EXPRESSION TAG	UNP G4BX92
C	447	LEU	-	EXPRESSION TAG	UNP G4BX92
C	448	GLU	-	EXPRESSION TAG	UNP G4BX92
D	447	LEU	-	EXPRESSION TAG	UNP G4BX92
D	448	GLU	-	EXPRESSION TAG	UNP G4BX92

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

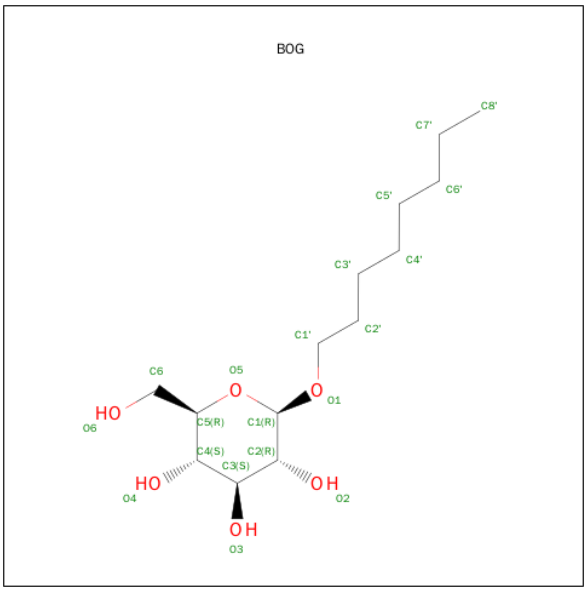
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	2	Total	Na	0	0
			2	2		
2	D	2	Total	Na	0	0
			2	2		
2	C	2	Total	Na	0	0
			2	2		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



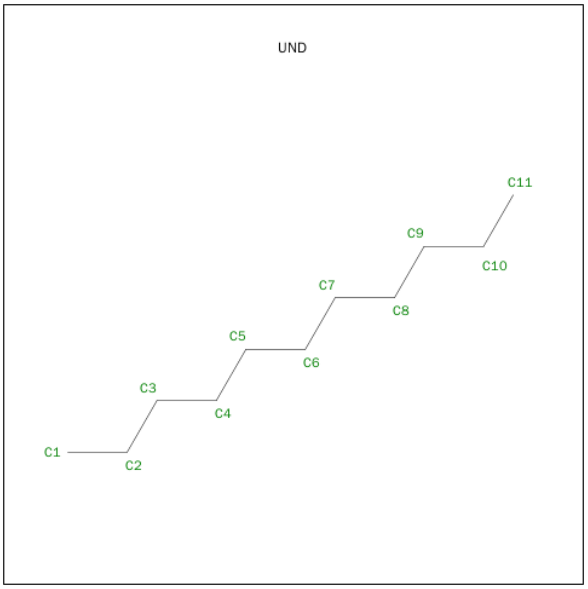
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	A	1	Total C O 13 6 7	0	0
3	A	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0
3	C	1	Total C O 13 6 7	0	0
3	D	1	Total C O 13 6 7	0	0

- Molecule 4 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 14 6	0	0
4	A	1	Total C O 20 14 6	0	0
4	C	1	Total C O 20 14 6	0	0
4	C	1	Total C O 20 14 6	0	0
4	D	1	Total C O 20 14 6	0	0

- Molecule 5 is UNDECANE (three-letter code: UND) (formula: $C_{11}H_{24}$).

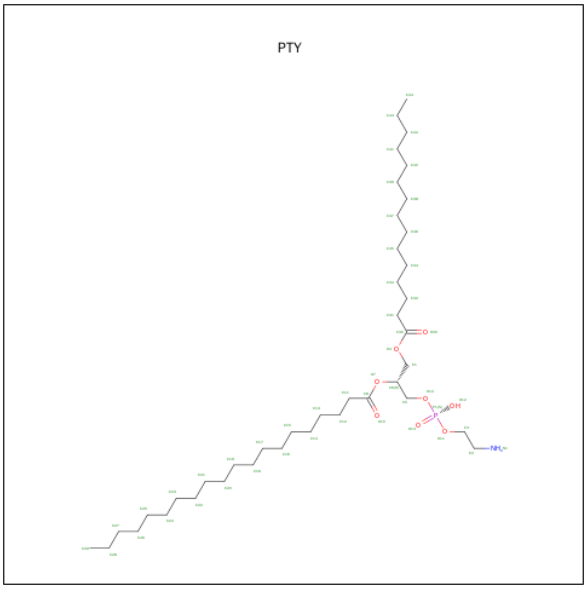


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 11 11	0	0
5	D	1	Total C 11 11	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

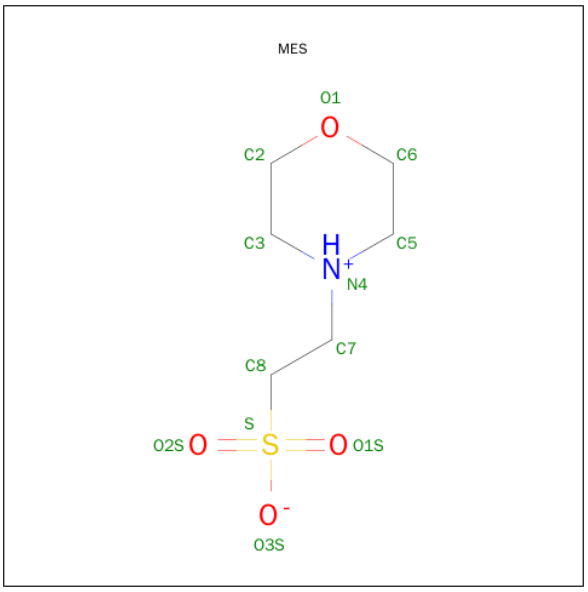
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	D	2	Total Cl 2 2	0	0

- Molecule 7 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O P 50 40 1 8 1	0	0

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 9 is water.

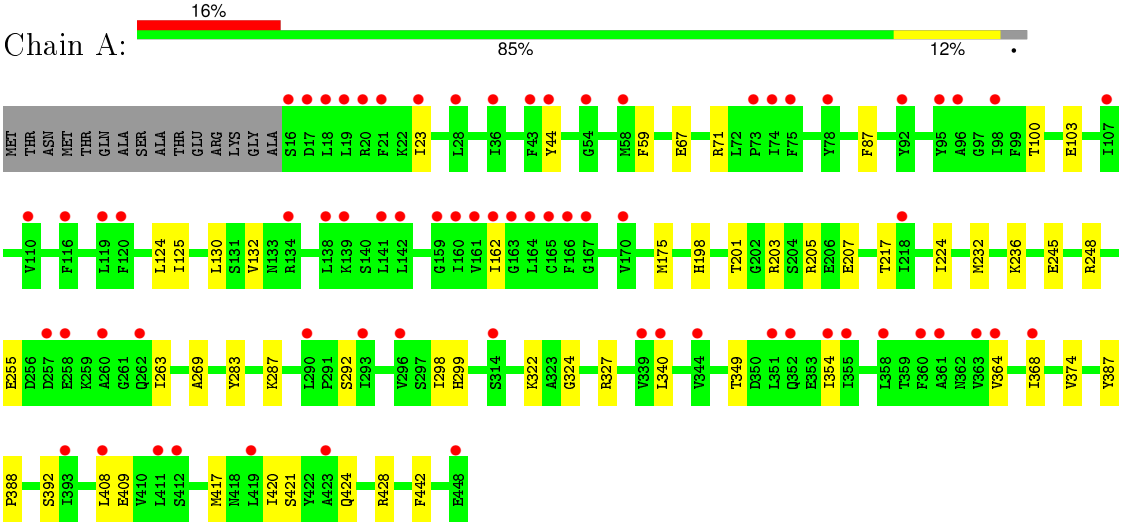
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	24	Total O 24 24	0	0
9	B	14	Total O 14 14	0	0
9	C	13	Total O 13 13	0	0
9	D	18	Total O 18 18	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

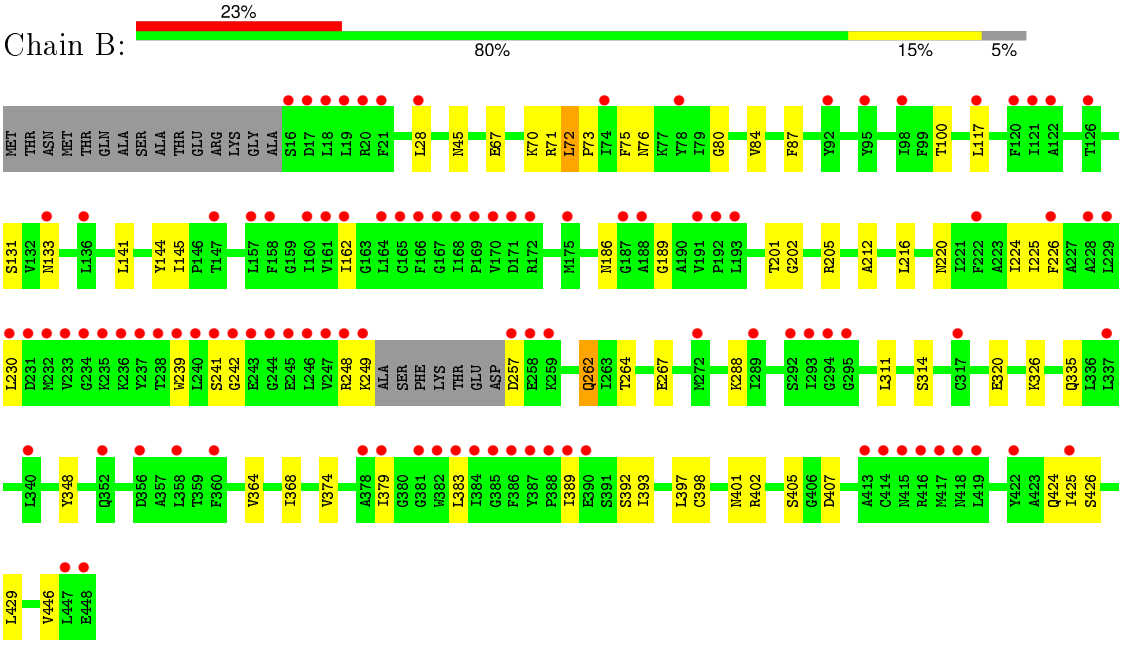
- Molecule 1: CITRATE-SODIUM SYMPORTER

Chain A:



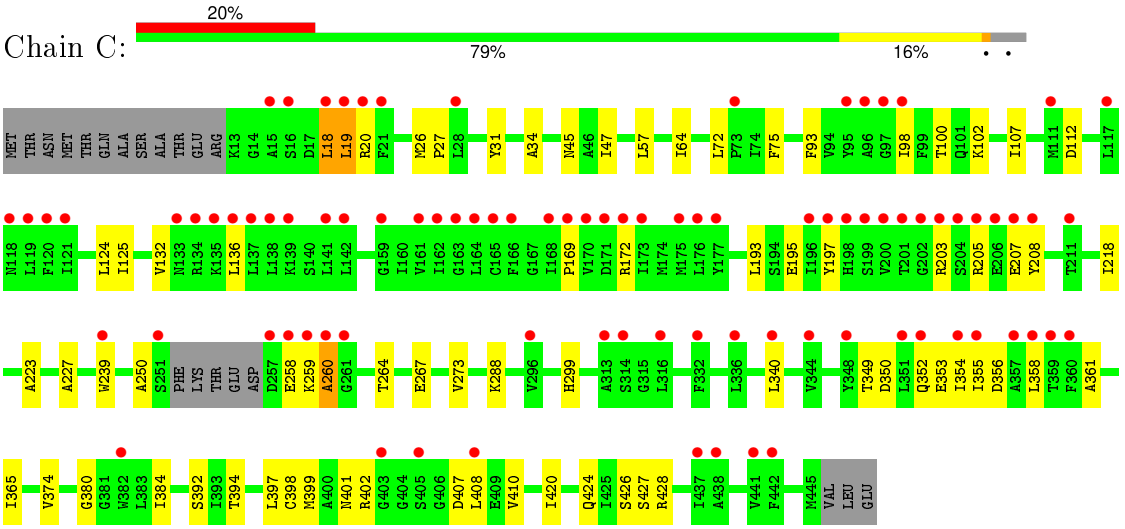
- Molecule 1: CITRATE-SODIUM SYMPORTER

Chain B:



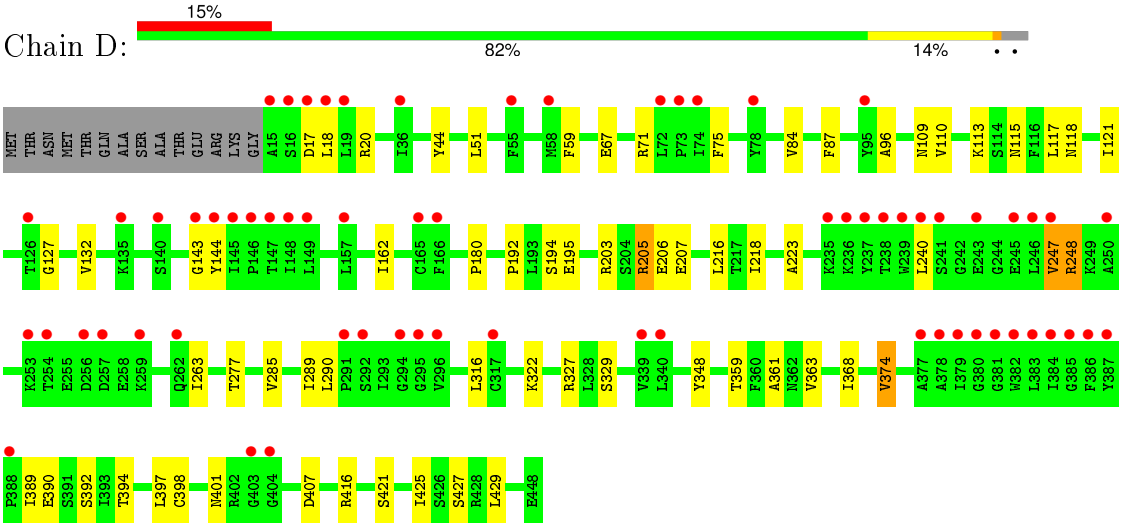
- Molecule 1: CITRATE-SODIUM SYMPORTER

Chain C:



- Molecule 1: CITRATE-SODIUM SYMPORTER

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	86.38Å 89.94Å 91.84Å 90.44° 113.79° 99.55°	Depositor
Resolution (Å)	47.98 – 2.50 47.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.98-2.50) 96.3 (47.98-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.208 , 0.246 0.218 , 0.256	Depositor DCC
R_{free} test set	4200 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	62.4	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 63.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 84850 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13270	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTY, CL, NA, UND, MES, FLC, BOG

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	0.23	0/3320	0.40	0/4503
1	B	0.23	0/3263	0.41	0/4425
1	C	0.23	0/3268	0.41	0/4430
1	D	0.23	0/3316	0.40	0/4498
All	All	0.23	0/13167	0.40	0/17856

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	3256	0	3414	34	0
1	B	3201	0	3365	36	0
1	C	3206	0	3369	39	0
1	D	3253	0	3407	34	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	39	0	15	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	0	10	2	0
3	C	13	0	5	0	0
3	D	13	0	5	1	0
4	A	40	0	56	2	0
4	C	40	0	56	0	0
4	D	20	0	28	1	0
5	A	11	0	24	0	0
5	D	11	0	24	0	0
6	A	1	0	0	0	0
6	D	2	0	0	0	0
7	A	50	0	79	4	0
8	D	12	0	13	2	0
9	A	24	0	0	3	0
9	B	14	0	0	0	0
9	C	13	0	0	0	0
9	D	18	0	0	0	0
All	All	13270	0	13870	145	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 (145) 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:C:136:LEU:HD21	1:C:250:ALA:HB1	1.65	0.78
1:A:340:LEU:HD21	1:A:408:LEU:HD13	1.66	0.77
1:C:340:LEU:HD21	1:C:408:LEU:HD13	1.71	0.73
1:A:67:GLU:HB3	1:A:71:ARG:HH21	1.55	0.72
1:C:288:LYS:NZ	1:D:44:TYR:O	2.26	0.69
1:D:285:VAL:HA	1:D:289:ILE:HB	1.76	0.68
1:B:424:GLN:OE1	3:B:1450:FLC:OHB	2.12	0.68
1:B:241:SER:HB2	1:B:389:ILE:HD12	1.77	0.65
1:C:124:LEU:HB3	1:C:420:ILE:HG21	1.80	0.64
1:C:72:LEU:HB3	1:C:75:PHE:HB3	1.81	0.63
1:B:401:ASN:ND2	1:B:407:ASP:OD1	2.32	0.63
1:C:18:LEU:H	1:C:18:LEU:HD13	1.63	0.63
1:A:236:LYS:NZ	9:A:2017:HOH:O	2.30	0.63
1:A:205:ARG:NH1	9:A:2013:HOH:O	2.33	0.62
1:C:352:GLN:NE2	1:C:356:ASP:OD1	2.30	0.61
1:B:262:GLN:NE2	1:B:262:GLN:O	2.33	0.61
1:A:67:GLU:OE1	1:A:71:ARG:NH2	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:ARG:NH1	1:D:207:GLU:OE1	2.33	0.61
1:C:195:GLU:OE1	1:C:205:ARG:NH1	2.35	0.59
1:A:125:ILE:HD11	1:A:424:GLN:HG3	1.84	0.59
1:A:263:ILE:HD11	1:A:324:GLY:HA2	1.85	0.59
1:D:194:SER:HB3	1:D:205:ARG:HB2	1.85	0.58
3:D:1449:FLC:OA1	3:D:1449:FLC:OHB	2.21	0.57
1:D:359:THR:HG22	1:D:361:ALA:H	1.68	0.57
1:A:162:ILE:HD12	1:A:368:ILE:HG13	1.86	0.56
1:D:206:GLU:HG2	8:D:1453:MES:H22	1.87	0.56
1:D:127:GLY:HA3	1:D:329:SER:HB2	1.86	0.55
1:A:299:HIS:HB3	1:A:428:ARG:HB3	1.89	0.55
1:C:125:ILE:HD11	1:C:424:GLN:HG3	1.89	0.55
1:B:141:LEU:HD23	1:B:145:ILE:HD12	1.88	0.55
1:C:399:MET:HG2	1:C:426:SER:HB3	1.90	0.54
1:B:425:ILE:HG23	1:B:429:LEU:HD12	1.90	0.54
1:A:203:ARG:NH2	9:A:2012:HOH:O	2.36	0.53
1:D:109:ASN:HA	1:D:113:LYS:HB3	1.91	0.53
1:C:361:ALA:O	1:C:365:ILE:HG12	2.09	0.53
1:B:67:GLU:O	1:B:71:ARG:HG2	2.09	0.53
1:C:218:ILE:HG12	1:C:354:ILE:HG23	1.91	0.53
1:A:245:GLU:OE2	4:A:1450:BOG:O4	2.16	0.52
1:D:425:ILE:HG23	1:D:429:LEU:HD12	1.91	0.52
1:C:374:VAL:HG13	1:C:392:SER:HB2	1.91	0.52
1:D:195:GLU:OE2	1:D:348:TYR:OH	2.17	0.52
1:D:374:VAL:HB	1:D:392:SER:HB2	1.92	0.51
1:A:87:PHE:CZ	1:A:349:THR:HG21	2.45	0.51
1:B:374:VAL:HG13	1:B:392:SER:HB3	1.91	0.51
1:C:169:PRO:HG2	1:C:172:ARG:HG3	1.93	0.51
1:A:374:VAL:HG13	1:A:392:SER:HB3	1.93	0.50
1:C:34:ALA:HA	1:D:277:THR:HG21	1.92	0.50
1:B:70:LYS:O	1:B:76:ASN:ND2	2.37	0.50
1:B:248:ARG:HG3	1:B:249:LYS:HG2	1.94	0.49
1:B:162:ILE:HG12	1:B:368:ILE:HG13	1.95	0.49
1:A:203:ARG:NH1	1:A:207:GLU:OE1	2.45	0.49
1:D:51:LEU:HD23	1:D:110:VAL:HG22	1.95	0.49
1:B:267:GLU:HG2	1:B:320:GLU:HB3	1.94	0.49
1:C:57:LEU:HD22	1:C:107:ILE:HD11	1.94	0.49
1:B:84:VAL:HA	1:B:87:PHE:CE2	2.48	0.49
1:B:241:SER:OG	1:B:242:GLY:O	2.27	0.48
1:A:292:SER:HA	1:A:298:ILE:HG12	1.95	0.48
1:A:23:ILE:HG23	1:A:67:GLU:HG3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:TYR:OH	1:D:394:THR:OG1	2.21	0.48
1:D:115:ASN:ND2	1:D:118:ASN:OD1	2.48	0.47
1:B:398:CYS:HA	1:B:401:ASN:ND2	2.29	0.47
1:A:248:ARG:HG2	1:A:387:TYR:CZ	2.50	0.47
7:A:1455:PTY:H201	7:A:1455:PTY:H231	1.75	0.47
1:B:144:TYR:OH	1:B:426:SER:OG	2.28	0.47
1:D:162:ILE:HG12	1:D:368:ILE:HD12	1.97	0.47
1:B:212:ALA:O	1:B:216:LEU:HB2	2.14	0.47
1:D:240:LEU:HB3	1:D:389:ILE:HG12	1.96	0.47
1:C:197:TYR:OH	1:C:207:GLU:OE2	2.21	0.47
1:A:263:ILE:HD13	1:A:327:ARG:HD2	1.97	0.46
1:B:364:VAL:O	1:B:368:ILE:HG12	2.15	0.46
1:D:180:PRO:O	1:D:216:LEU:HD21	2.15	0.46
1:D:390:GLU:O	1:D:394:THR:HG22	2.15	0.46
1:A:255:GLU:N	1:A:255:GLU:OE1	2.39	0.46
1:B:402:ARG:NH1	1:B:405:SER:OG	2.48	0.46
1:C:47:ILE:HG22	1:C:102:LYS:HG3	1.98	0.45
1:D:247:VAL:HG12	1:D:248:ARG:H	1.81	0.45
1:B:389:ILE:O	1:B:393:ILE:HG12	2.17	0.45
7:A:1455:PTY:H351	7:A:1455:PTY:H381	1.55	0.45
1:C:193:LEU:HB3	1:C:208:TYR:CE1	2.52	0.45
1:D:223:ALA:HA	1:D:397:LEU:HD22	1.98	0.45
1:C:380:GLY:O	1:C:384:ILE:HG12	2.16	0.45
1:B:72:LEU:HB3	1:B:75:PHE:HB3	1.98	0.45
1:A:175:MET:HG2	1:A:442:PHE:CE1	2.52	0.45
1:C:193:LEU:HB3	1:C:208:TYR:HE1	1.82	0.45
1:C:398:CYS:HA	1:C:401:ASN:ND2	2.32	0.45
1:D:84:VAL:HA	1:D:87:PHE:CE2	2.52	0.45
1:C:355:ILE:HA	1:C:358:LEU:HB2	1.99	0.45
1:C:299:HIS:HB3	1:C:428:ARG:HB3	1.99	0.45
1:C:407:ASP:OD2	1:C:427:SER:OG	2.34	0.45
3:B:1449:FLC:OHB	3:B:1449:FLC:OG1	2.33	0.45
1:C:264:THR:OG1	1:C:267:GLU:OE2	2.34	0.44
1:B:379:ILE:O	1:B:383:LEU:HG	2.17	0.44
1:D:390:GLU:OE2	1:D:416:ARG:NE	2.41	0.44
1:A:283:TYR:O	1:A:287:LYS:HB2	2.17	0.44
1:A:87:PHE:HZ	1:A:349:THR:HG21	1.82	0.44
1:C:203:ARG:NH1	1:C:207:GLU:OE1	2.51	0.44
1:B:311:LEU:O	1:B:314:SER:OG	2.26	0.44
1:A:44:TYR:HB3	1:B:288:LYS:HG3	1.98	0.44
1:C:349:THR:OG1	1:C:350:ASP:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:THR:OG1	1:B:202:GLY:N	2.51	0.43
1:D:218:ILE:HG21	1:D:363:VAL:HA	1.99	0.43
1:A:217:THR:HG22	1:A:354:ILE:HD11	1.99	0.43
1:C:223:ALA:HA	1:C:397:LEU:HD22	2.00	0.43
1:A:364:VAL:O	1:A:368:ILE:HG12	2.19	0.43
1:A:387:TYR:HA	1:A:388:PRO:HD3	1.90	0.43
1:C:273:VAL:HG22	1:D:59:PHE:CG	2.54	0.43
1:A:130:LEU:O	1:A:322:LYS:HE3	2.19	0.43
1:A:100:THR:HG23	1:A:103:GLU:H	1.83	0.43
1:B:133:ASN:HD21	1:B:257:ASP:HB3	1.84	0.43
1:C:258:GLU:O	1:C:260:ALA:N	2.53	0.42
1:A:201:THR:HG22	1:A:203:ARG:HG3	1.99	0.42
8:D:1453:MES:H82	8:D:1453:MES:H31	1.81	0.42
1:C:93:PHE:CD1	1:C:98:ILE:HD12	2.53	0.42
1:B:220:ASN:O	1:B:224:ILE:HG23	2.19	0.42
1:C:26:MET:HA	1:C:27:PRO:HD2	1.91	0.42
1:D:203:ARG:HD3	1:D:207:GLU:OE2	2.20	0.42
1:A:124:LEU:HB3	1:A:420:ILE:HG21	2.02	0.42
7:A:1455:PTY:H322	7:A:1455:PTY:H352	1.68	0.42
1:B:224:ILE:HG13	1:B:225:ILE:N	2.34	0.42
1:C:227:ALA:HB2	1:C:410:VAL:HG13	2.02	0.42
1:D:398:CYS:HA	1:D:401:ASN:ND2	2.34	0.42
1:C:19:LEU:HD23	1:C:20:ARG:H	1.84	0.41
1:B:162:ILE:HG12	1:B:368:ILE:HG21	2.03	0.41
1:B:201:THR:HG22	1:B:446:VAL:HG21	2.03	0.41
1:D:407:ASP:OD2	1:D:427:SER:OG	2.39	0.41
1:D:121:ILE:HD13	1:D:192:PRO:HB3	2.02	0.41
1:A:224:ILE:HD11	1:A:409:GLU:OE1	2.21	0.41
1:D:67:GLU:HG3	1:D:71:ARG:HH21	1.86	0.41
1:D:96:ALA:HA	4:D:1454:BOG:H61	2.03	0.41
1:D:17:ASP:OD1	1:D:20:ARG:NH2	2.54	0.41
1:A:198:HIS:ND1	1:A:203:ARG:O	2.54	0.41
1:B:45:ASN:OD1	1:B:100:THR:HG21	2.21	0.41
1:A:269:ALA:HB2	1:B:335:GLN:HB3	2.03	0.41
7:A:1455:PTY:H251	7:A:1455:PTY:H222	1.78	0.40
1:B:205:ARG:HD2	1:B:348:TYR:CE2	2.56	0.40
1:D:132:VAL:O	1:D:322:LYS:NZ	2.55	0.40
1:D:421:SER:O	1:D:425:ILE:HG12	2.22	0.40
1:C:394:THR:O	1:C:398:CYS:HB2	2.21	0.40
1:C:31:TYR:OH	1:C:64:ILE:HB	2.21	0.40
1:C:45:ASN:OD1	1:C:100:THR:HG21	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:PHE:O	1:B:230:LEU:HG	2.22	0.40
1:B:131:SER:HB3	1:B:326:LYS:HD3	2.03	0.40
1:C:424:GLN:O	1:C:428:ARG:HG2	2.22	0.40
1:A:132:VAL:HG11	4:A:1450:BOG:H1	2.04	0.40
1:B:80:GLY:HA2	1:B:402:ARG:CZ	2.51	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	431/448 (96%)	412 (96%)	19 (4%)	0	100	100
1	B	422/448 (94%)	395 (94%)	24 (6%)	3 (1%)	26	46
1	C	424/448 (95%)	402 (95%)	20 (5%)	2 (0%)	34	55
1	D	432/448 (96%)	409 (95%)	22 (5%)	1 (0%)	52	75
All	All	1709/1792 (95%)	1618 (95%)	85 (5%)	6 (0%)	39	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	259	LYS
1	B	73	PRO
1	D	143	GLY
1	B	186	ASN
1	C	260	ALA
1	B	189	GLY

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	343/354 (97%)	339 (99%)	4 (1%)	78 93
1	B	337/354 (95%)	330 (98%)	7 (2%)	61 85
1	C	336/354 (95%)	329 (98%)	7 (2%)	61 85
1	D	341/354 (96%)	330 (97%)	11 (3%)	46 74
All	All	1357/1416 (96%)	1328 (98%)	29 (2%)	61 85

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	PHE
1	A	232	MET
1	A	417	MET
1	A	421	SER
1	B	28	LEU
1	B	72	LEU
1	B	117	LEU
1	B	239	TRP
1	B	262	GLN
1	B	264	THR
1	B	397	LEU
1	C	18	LEU
1	C	19	LEU
1	C	112	ASP
1	C	132	VAL
1	C	239	TRP
1	C	353	GLU
1	C	402	ARG
1	D	18	LEU
1	D	75	PHE
1	D	117	LEU
1	D	205	ARG
1	D	247	VAL
1	D	248	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	263	ILE
1	D	290	LEU
1	D	316	LEU
1	D	327	ARG
1	D	374	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	262	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
3	FLC	A	1449	-	3,12,12	1.70	0	3,17,17	1.65	1 (33%)
4	BOG	A	1450	-	20,20,20	0.55	0	25,25,25	1.02	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	UND	A	1451	-	10,10,10	0.10	0	9,9,9	0.80	0
3	FLC	A	1453	-	3,12,12	1.57	0	3,17,17	2.10	2 (66%)
3	FLC	A	1454	-	3,12,12	1.75	1 (33%)	3,17,17	2.85	2 (66%)
7	PTY	A	1455	-	48,49,49	1.01	3 (6%)	49,54,54	1.12	3 (6%)
4	BOG	A	1456	-	20,20,20	0.46	0	25,25,25	1.08	2 (8%)
3	FLC	B	1449	-	3,12,12	1.66	0	3,17,17	1.29	1 (33%)
3	FLC	B	1450	-	3,12,12	1.67	0	3,17,17	2.51	2 (66%)
3	FLC	C	1446	-	3,12,12	1.67	0	3,17,17	2.02	2 (66%)
4	BOG	C	1447	-	20,20,20	0.52	0	25,25,25	0.89	1 (4%)
4	BOG	C	1448	-	20,20,20	0.49	0	25,25,25	0.91	1 (4%)
3	FLC	D	1449	-	3,12,12	1.67	0	3,17,17	2.14	2 (66%)
5	UND	D	1450	-	10,10,10	0.10	0	9,9,9	0.81	0
8	MES	D	1453	-	12,12,12	1.29	2 (16%)	15,16,16	2.76	4 (26%)
4	BOG	D	1454	-	20,20,20	0.41	0	25,25,25	1.37	2 (8%)

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	FLC	A	1449	-	-	0/6/16/16	0/0/0/0
4	BOG	A	1450	-	-	0/11/31/31	0/1/1/1
5	UND	A	1451	-	-	0/8/8/8	0/0/0/0
3	FLC	A	1453	-	-	0/6/16/16	0/0/0/0
3	FLC	A	1454	-	-	0/6/16/16	0/0/0/0
7	PTY	A	1455	-	-	0/53/53/53	0/0/0/0
4	BOG	A	1456	-	-	0/11/31/31	0/1/1/1
3	FLC	B	1449	-	-	0/6/16/16	0/0/0/0
3	FLC	B	1450	-	-	0/6/16/16	0/0/0/0
3	FLC	C	1446	-	-	0/6/16/16	0/0/0/0
4	BOG	C	1447	-	-	0/11/31/31	0/1/1/1
4	BOG	C	1448	-	-	0/11/31/31	0/1/1/1
3	FLC	D	1449	-	-	0/6/16/16	0/0/0/0
5	UND	D	1450	-	-	0/8/8/8	0/0/0/0
8	MES	D	1453	-	-	0/6/14/14	0/1/1/1
4	BOG	D	1454	-	-	0/11/31/31	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1455	PTY	O7-C6	-2.07	1.41	1.46
3	A	1454	FLC	CA-CB	-2.02	1.51	1.54
8	D	1453	MES	O1S-S	2.02	1.51	1.45
8	D	1453	MES	O2S-S	2.39	1.52	1.45
7	A	1455	PTY	O7-C8	3.08	1.43	1.34
7	A	1455	PTY	O4-C30	3.54	1.43	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	1453	MES	O3S-S-O2S	-4.76	100.72	111.26
3	A	1454	FLC	CB-CA-CAC	-3.69	109.18	114.95
3	B	1450	FLC	CB-CG-CGC	-3.41	109.62	114.95
4	A	1450	BOG	C1-O5-C5	-3.41	107.05	113.74
3	A	1454	FLC	CB-CG-CGC	-3.27	109.84	114.95
4	A	1456	BOG	C1-O5-C5	-3.24	107.39	113.74
4	C	1448	BOG	C1-O5-C5	-2.96	107.93	113.74
3	A	1453	FLC	CB-CA-CAC	-2.95	110.34	114.95
4	C	1447	BOG	C1-O5-C5	-2.91	108.03	113.74
3	D	1449	FLC	CB-CA-CAC	-2.83	110.53	114.95
3	C	1446	FLC	CB-CG-CGC	-2.78	110.61	114.95
3	B	1450	FLC	CB-CA-CAC	-2.68	110.77	114.95
3	A	1449	FLC	CB-CG-CGC	-2.63	110.84	114.95
3	D	1449	FLC	CB-CG-CGC	-2.38	111.24	114.95
7	A	1455	PTY	O4-C30-O30	-2.26	117.59	123.51
3	C	1446	FLC	CB-CA-CAC	-2.10	111.67	114.95
3	A	1453	FLC	CB-CG-CGC	-2.10	111.67	114.95
3	B	1449	FLC	CB-CG-CGC	-2.03	111.78	114.95
7	A	1455	PTY	O4-C30-C31	2.19	118.60	111.85
4	A	1456	BOG	O1-C1-C2	2.50	111.08	108.00
8	D	1453	MES	O3S-S-C8	2.67	110.53	104.99
4	D	1454	BOG	C3-C4-C5	3.48	116.44	110.23
4	D	1454	BOG	O5-C5-C4	4.10	117.49	109.67
7	A	1455	PTY	O7-C8-C11	4.24	120.46	111.53
8	D	1453	MES	O1S-S-C8	5.83	110.98	106.87
8	D	1453	MES	O2S-S-C8	6.67	111.58	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1450	BOG	2	0
7	A	1455	PTY	4	0
3	B	1449	FLC	1	0
3	B	1450	FLC	1	0
3	D	1449	FLC	1	0
8	D	1453	MES	2	0
4	D	1454	BOG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	433/448 (96%)	0.83	70 (16%) 3 2	34, 56, 99, 136	0
1	B	426/448 (95%)	1.32	103 (24%) 1 1	46, 80, 120, 132	0
1	C	428/448 (95%)	1.09	89 (20%) 1 1	38, 62, 109, 143	0
1	D	434/448 (96%)	0.85	66 (15%) 3 3	38, 59, 101, 142	0
All	All	1721/1792 (96%)	1.02	328 (19%) 2 1	34, 63, 110, 143	0

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	LEU	14.0
1	B	244	GLY	13.2
1	B	236	LYS	9.6
1	B	241	SER	9.4
1	B	387	TYR	9.4
1	B	239	TRP	8.9
1	B	237	TYR	8.9
1	C	19	LEU	8.8
1	B	18	LEU	8.8
1	B	17	ASP	8.8
1	C	442	PHE	8.7
1	C	197	TYR	8.4
1	A	360	PHE	8.4
1	B	16	SER	8.2
1	C	21	PHE	8.1
1	B	166	PHE	8.0
1	C	20	ARG	7.8
1	B	389	ILE	7.7
1	B	238	THR	7.6
1	C	168	ILE	7.5
1	C	172	ARG	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	382	TRP	7.3
1	B	243	GLU	7.2
1	D	384	ILE	7.2
1	B	388	PRO	7.1
1	A	21	PHE	7.1
1	B	232	MET	7.1
1	D	237	TYR	7.0
1	C	358	LEU	7.0
1	C	201	THR	6.8
1	D	239	TRP	6.8
1	C	257	ASP	6.7
1	B	235	LYS	6.7
1	C	138	LEU	6.6
1	B	386	PHE	6.4
1	B	171	ASP	6.4
1	A	354	ILE	6.4
1	D	18	LEU	6.3
1	B	246	LEU	6.3
1	D	382	TRP	6.2
1	C	134	ARG	6.1
1	B	233	VAL	6.0
1	B	167	GLY	6.0
1	C	355	ILE	5.8
1	A	138	LEU	5.8
1	C	441	VAL	5.8
1	C	173	ILE	5.8
1	B	245	GLU	5.7
1	D	236	LYS	5.7
1	C	203	ARG	5.7
1	C	135	LYS	5.7
1	B	247	VAL	5.6
1	C	137	LEU	5.6
1	C	28	LEU	5.6
1	C	198	HIS	5.6
1	C	175	MET	5.5
1	A	165	CYS	5.5
1	A	18	LEU	5.5
1	B	259	LYS	5.3
1	C	360	PHE	5.3
1	C	18	LEU	5.3
1	D	383	LEU	5.3
1	C	170	VAL	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	95	TYR	5.2
1	A	296	VAL	5.1
1	A	162	ILE	5.0
1	D	74	ILE	5.0
1	B	294	GLY	5.0
1	C	258	GLU	4.9
1	B	19	LEU	4.9
1	A	166	PHE	4.8
1	C	357	ALA	4.8
1	D	256	ASP	4.8
1	B	157	LEU	4.8
1	D	381	GLY	4.8
1	A	78	TYR	4.7
1	D	149	LEU	4.7
1	B	165	CYS	4.7
1	D	240	LEU	4.7
1	D	379	ILE	4.7
1	C	176	LEU	4.6
1	C	141	LEU	4.6
1	B	74	ILE	4.6
1	C	142	LEU	4.6
1	C	200	VAL	4.5
1	A	43	PHE	4.5
1	D	253	LYS	4.5
1	C	171	ASP	4.5
1	C	166	PHE	4.4
1	A	293	ILE	4.4
1	D	147	THR	4.4
1	A	358	LEU	4.4
1	C	139	LYS	4.4
1	B	258	GLU	4.3
1	B	383	LEU	4.3
1	D	385	GLY	4.3
1	B	242	GLY	4.3
1	A	92	TYR	4.2
1	C	204	SER	4.2
1	C	177	TYR	4.2
1	C	15	ALA	4.2
1	B	419	LEU	4.1
1	D	377	ALA	4.1
1	B	164	LEU	4.1
1	B	98	ILE	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	20	ARG	4.1
1	C	296	VAL	4.0
1	A	74	ILE	4.0
1	A	352	GLN	4.0
1	A	96	ALA	4.0
1	B	168	ILE	4.0
1	C	207	GLU	4.0
1	A	139	LYS	4.0
1	C	161	VAL	4.0
1	D	241	SER	4.0
1	B	229	LEU	3.9
1	C	117	LEU	3.9
1	B	418	ASN	3.9
1	B	293	ILE	3.9
1	B	228	ALA	3.9
1	B	248	ARG	3.9
1	B	447	LEU	3.9
1	B	95	TYR	3.9
1	B	20	ARG	3.8
1	B	230	LEU	3.8
1	C	313	ALA	3.7
1	A	164	LEU	3.7
1	C	260	ALA	3.7
1	C	196	ILE	3.7
1	A	142	LEU	3.7
1	B	417	MET	3.7
1	C	251	SER	3.7
1	B	121	ILE	3.7
1	A	141	LEU	3.7
1	B	78	TYR	3.6
1	B	21	PHE	3.6
1	D	295	GLY	3.6
1	C	159	GLY	3.6
1	C	259	LYS	3.6
1	C	206	GLU	3.6
1	D	148	ILE	3.6
1	A	258	GLU	3.5
1	B	415	ASN	3.5
1	D	387	TYR	3.5
1	A	257	ASP	3.5
1	C	352	GLN	3.5
1	D	386	PHE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	16	SER	3.5
1	C	133	ASN	3.5
1	B	231	ASP	3.5
1	C	136	LEU	3.4
1	B	295	GLY	3.4
1	C	96	ALA	3.4
1	C	16	SER	3.4
1	C	169	PRO	3.4
1	A	134	ARG	3.4
1	D	78	TYR	3.3
1	A	163	GLY	3.3
1	B	249	LYS	3.3
1	D	16	SER	3.3
1	B	358	LEU	3.2
1	C	354	ILE	3.2
1	C	95	TYR	3.2
1	B	390	GLU	3.2
1	D	250	ALA	3.2
1	C	121	ILE	3.2
1	A	44	TYR	3.2
1	C	119	LEU	3.2
1	D	262	GLN	3.2
1	A	355	ILE	3.2
1	B	292	SER	3.2
1	A	351	LEU	3.2
1	C	164	LEU	3.1
1	D	317	CYS	3.1
1	B	234	GLY	3.1
1	C	73	PRO	3.1
1	B	136	LEU	3.1
1	D	247	VAL	3.0
1	D	143	GLY	3.0
1	A	408	LEU	3.0
1	B	117	LEU	3.0
1	A	364	VAL	3.0
1	B	381	GLY	3.0
1	D	404	GLY	3.0
1	C	98	ILE	3.0
1	D	146	PRO	3.0
1	D	19	LEU	3.0
1	C	202	GLY	2.9
1	A	17	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	289	ILE	2.9
1	D	95	TYR	2.9
1	B	356	ASP	2.9
1	C	351	LEU	2.9
1	D	15	ALA	2.9
1	B	172	ARG	2.9
1	D	254	THR	2.9
1	B	422	TYR	2.9
1	D	292	SER	2.8
1	D	245	GLU	2.8
1	A	339	VAL	2.8
1	D	259	LYS	2.8
1	B	360	PHE	2.8
1	D	378	ALA	2.8
1	B	352	GLN	2.8
1	A	340	LEU	2.8
1	A	411	LEU	2.7
1	A	36	ILE	2.7
1	B	384	ILE	2.7
1	D	166	PHE	2.7
1	D	72	LEU	2.7
1	D	165	CYS	2.7
1	A	167	GLY	2.7
1	D	296	VAL	2.7
1	C	205	ARG	2.7
1	C	199	SER	2.7
1	B	257	ASP	2.7
1	A	161	VAL	2.7
1	C	314	SER	2.7
1	B	379	ILE	2.7
1	C	382	TRP	2.7
1	D	238	THR	2.7
1	A	19	LEU	2.7
1	A	419	LEU	2.7
1	B	226	PHE	2.7
1	A	73	PRO	2.7
1	A	368	ILE	2.6
1	B	28	LEU	2.6
1	B	169	PRO	2.6
1	A	412	SER	2.6
1	A	361	ALA	2.6
1	C	97	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	75	PHE	2.6
1	B	188	ALA	2.6
1	A	218	ILE	2.6
1	B	120	PHE	2.5
1	C	408	LEU	2.5
1	C	120	PHE	2.5
1	A	120	PHE	2.5
1	B	170	VAL	2.5
1	D	17	ASP	2.5
1	D	246	LEU	2.5
1	B	175	MET	2.5
1	A	344	VAL	2.5
1	D	73	PRO	2.5
1	D	388	PRO	2.5
1	B	378	ALA	2.4
1	B	340	LEU	2.4
1	C	340	LEU	2.4
1	D	291	PRO	2.4
1	D	294	GLY	2.4
1	A	423	ALA	2.4
1	B	385	GLY	2.4
1	D	126	THR	2.4
1	A	448	GLU	2.4
1	A	170	VAL	2.4
1	A	23	ILE	2.4
1	C	208	TYR	2.4
1	A	58	MET	2.4
1	A	116	PHE	2.4
1	A	260	ALA	2.4
1	B	272	MET	2.4
1	A	290	LEU	2.4
1	A	160	ILE	2.4
1	C	163	GLY	2.3
1	C	261	GLY	2.3
1	B	191	VAL	2.3
1	B	416	ARG	2.3
1	C	162	ILE	2.3
1	C	348	TYR	2.3
1	C	211	THR	2.3
1	B	161	VAL	2.3
1	C	165	CYS	2.3
1	B	160	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	133	ASN	2.3
1	D	157	LEU	2.3
1	A	393	ILE	2.3
1	B	92	TYR	2.3
1	A	363	VAL	2.3
1	B	187	GLY	2.3
1	D	380	GLY	2.3
1	C	438	ALA	2.3
1	D	339	VAL	2.3
1	D	58	MET	2.3
1	B	425	ILE	2.3
1	D	55	PHE	2.3
1	D	243	GLU	2.3
1	B	222	PHE	2.2
1	D	144	TYR	2.2
1	B	448	GLU	2.2
1	C	405	SER	2.2
1	D	135	LYS	2.2
1	B	337	LEU	2.2
1	C	336	LEU	2.2
1	B	122	ALA	2.2
1	C	359	THR	2.2
1	A	28	LEU	2.2
1	A	159	GLY	2.2
1	C	239	TRP	2.2
1	B	162	ILE	2.2
1	B	193	LEU	2.2
1	A	54	GLY	2.2
1	D	403	GLY	2.2
1	C	316	LEU	2.2
1	D	235	LYS	2.1
1	A	110	VAL	2.1
1	C	118	ASN	2.1
1	D	145	ILE	2.1
1	B	158	PHE	2.1
1	A	262	GLN	2.1
1	D	36	ILE	2.1
1	B	126	THR	2.1
1	A	314	SER	2.1
1	D	257	ASP	2.1
1	C	344	VAL	2.1
1	B	147	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	140	SER	2.1
1	B	414	CYS	2.1
1	C	332	PHE	2.1
1	B	192	PRO	2.1
1	B	413	ALA	2.1
1	A	98	ILE	2.1
1	D	340	LEU	2.1
1	A	107	ILE	2.0
1	A	119	LEU	2.0
1	C	111	MET	2.0
1	B	317	CYS	2.0
1	C	403	GLY	2.0
1	C	437	ILE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	BOG	A	1456	20/20	0.63	0.78	4.24	71,113,125,131	0
7	PTY	A	1455	50/50	0.61	0.81	4.01	66,90,101,110	50
5	UND	D	1450	11/11	0.78	0.42	3.26	55,61,81,83	0
3	FLC	B	1449	13/13	0.53	0.35	2.80	76,87,98,105	0
5	UND	A	1451	11/11	0.89	0.31	1.84	55,62,68,75	0
3	FLC	A	1453	13/13	0.55	0.26	1.42	79,108,121,121	0
2	NA	C	501	1/1	0.92	0.27	1.27	54,54,54,54	0
8	MES	D	1453	12/12	0.69	0.23	1.24	75,103,106,113	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	FLC	D	1449	13/13	0.87	0.31	1.13	68,82,91,93	0
4	BOG	A	1450	20/20	0.91	0.25	0.49	44,57,70,77	0
3	FLC	C	1446	13/13	0.95	0.28	0.30	44,57,65,66	0
2	NA	D	501	1/1	0.97	0.19	-0.06	54,54,54,54	0
4	BOG	C	1447	20/20	0.94	0.22	-0.13	57,63,76,76	0
2	NA	D	502	1/1	0.92	0.20	-0.20	50,50,50,50	0
3	FLC	B	1450	13/13	0.77	0.17	-0.53	98,108,114,116	0
2	NA	C	502	1/1	0.94	0.12	-0.72	56,56,56,56	0
2	NA	B	502	1/1	0.93	0.15	-0.76	72,72,72,72	0
2	NA	A	501	1/1	0.95	0.13	-1.16	39,39,39,39	0
3	FLC	A	1449	13/13	0.98	0.12	-1.45	38,43,52,54	0
6	CL	D	1452	1/1	0.98	0.09	-3.39	56,56,56,56	0
2	NA	A	502	1/1	0.97	0.05	-3.77	42,42,42,42	0
4	BOG	C	1448	20/20	0.70	0.43	-	80,99,115,118	0
4	BOG	D	1454	20/20	0.69	0.42	-	84,105,112,113	0
6	CL	A	1452	1/1	0.89	0.11	-	108,108,108,108	0
3	FLC	A	1454	13/13	0.62	0.36	-	98,120,125,128	0
6	CL	D	1451	1/1	0.95	0.14	-	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.