Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:40 AM GMT

PDB ID	:	3BRF
Title	:	CSL (Lag-1) bound to DNA with Lin-12 RAM peptide, C2221
Authors	:	Wilson, J.J.; Kovall, R.A.
Deposited on	:	2007-12-21
Resolution	:	2.47 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:

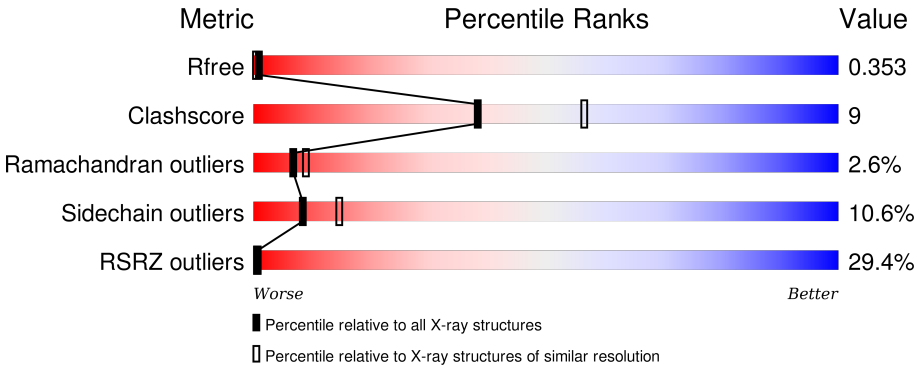
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.47 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	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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	B	15	7% 40% 40% 20%
2	C	15	7% 47% 47% 7%
3	A	478	28% 63% 21% • 12%
4	D	14	14% 64% 29% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4179 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 DNA chain called DNA (5'-D(*DTP*DTP*DAP*DCP*DTP*DGP*DTP*DGP*DGP*DGP*DAP*DAP*DAP*DGP*DA)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	15	311	149	61	87	14	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(*DAP*DAP*DTP*DCP*DTP*DTP*DTP*DCP*DCP*DCP*DAP*DCP*DAP*DGP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	15	298	145	50	89	14	0	0	0

- Molecule 3 is a protein called Lin-12 and glp-1 phenotype protein 1, isoform a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	423	3383	2149	583	633	18	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	SER	-	EXPRESSION TAG	UNP Q9TYY1
A	187	GLY	-	EXPRESSION TAG	UNP Q9TYY1
A	188	PRO	-	EXPRESSION TAG	UNP Q9TYY1
A	189	LEU	-	EXPRESSION TAG	UNP Q9TYY1
A	190	GLY	-	EXPRESSION TAG	UNP Q9TYY1
A	191	SER	-	EXPRESSION TAG	UNP Q9TYY1

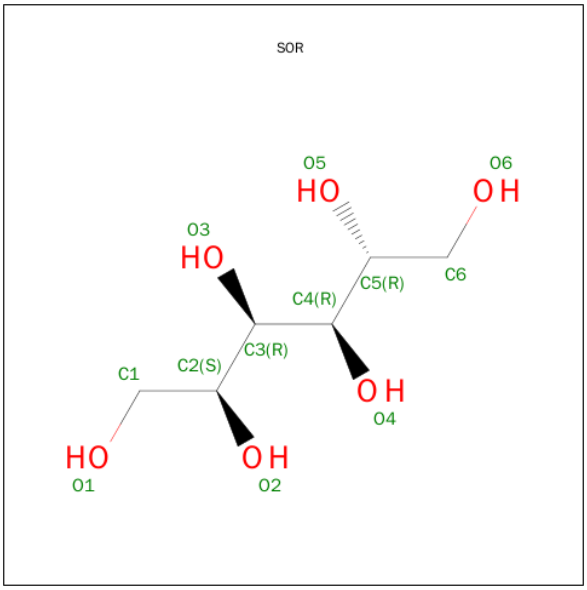
- Molecule 4 is a protein called Protein lin-12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	13	106	68	18	17	3	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	937	SER	-	EXPRESSION TAG	UNP P14585

- Molecule 5 is SUGAR (D-SORBITOL) (three-letter code: SOR) (formula: $C_6H_{14}O_6$).



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

- Molecule 6 is water.

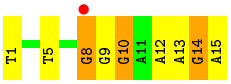
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	39	Total O 39 39	0	0
6	B	7	Total O 7 7	0	0
6	C	11	Total O 11 11	0	0

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.

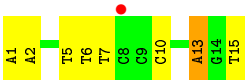
• Molecule 1: DNA (5'-D(*DTP*DTP*DAP*DCP*DTP*DGP*DTP*DGP*DGP*DGP*DAP*DAP*DAP*DGP*DA)-3')

Chain B:



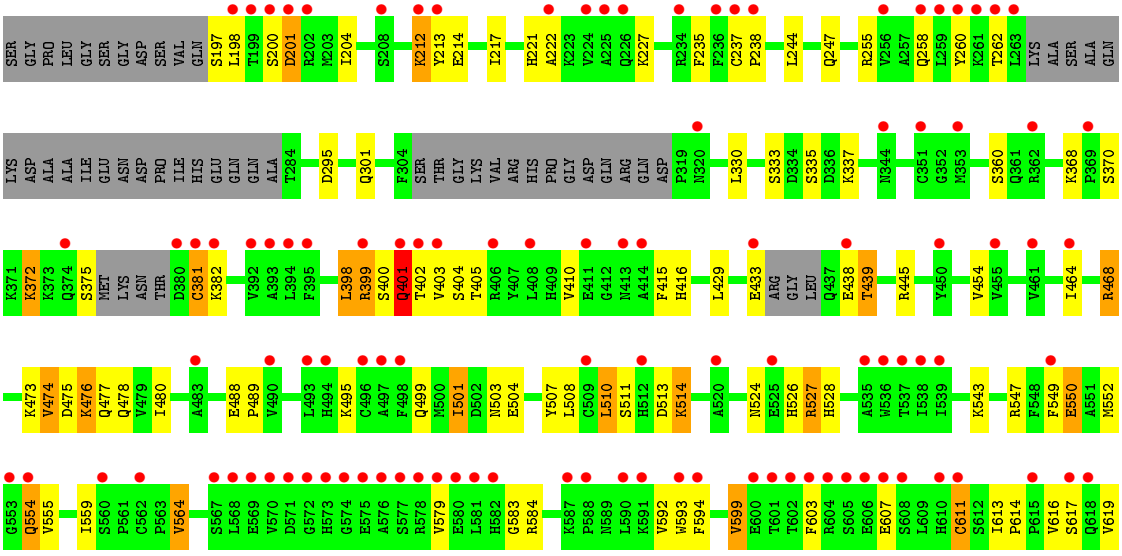
• Molecule 2: DNA (5'-D(*DAP*DAP*DTP*DCP*DTP*DTP*DTP*DCP*DCP*DCP*DAP*DCP*DAP*DGP*DT)-3')

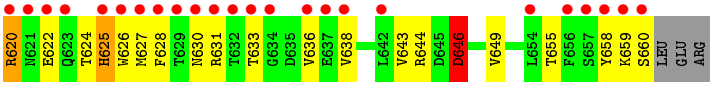
Chain C:



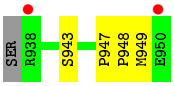
• Molecule 3: Lin-12 and glp-1 phenotype protein 1, isoform a

Chain A:





- Molecule 4: Protein lin-12



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	62.94Å 95.97Å 223.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.28 – 2.47 26.59 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.2 (28.28-2.47) 99.3 (26.59-2.47)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.47Å)	Xtriage
Refinement program	REFMAC 5.3.0020	Depositor
R, R_{free}	0.230 , 0.277 0.310 , 0.353	Depositor DCC
R_{free} test set	1246 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	54.8	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	6 of 24719 reflections (0.024%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4179	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: SOR

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	B	1.17	0/350	1.86	9/540 (1.7%)
2	C	1.21	0/332	1.78	9/509 (1.8%)
3	A	0.57	3/3463 (0.1%)	0.64	2/4675 (0.0%)
4	D	0.41	0/109	0.64	0/147
All	All	0.71	3/4254 (0.1%)	0.96	20/5871 (0.3%)

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
3	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	550	GLU	CD-OE2	7.00	1.33	1.25
3	A	644	ARG	CZ-NH1	6.82	1.42	1.33
3	A	197	SER	CB-OG	5.54	1.49	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	5	DT	O4'-C1'-N1	-10.16	100.89	108.00
1	B	1	DT	O4'-C1'-N1	9.30	114.51	108.00
2	C	6	DT	O4'-C1'-N1	-8.27	102.21	108.00
1	B	1	DT	C1'-O4'-C4'	-7.78	102.32	110.10
2	C	10	DC	O4'-C1'-C2'	-7.26	100.09	105.90
1	B	12	DA	N1-C6-N6	-7.02	114.39	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	10	DG	C2-N3-C4	6.54	115.17	111.90
2	C	7	DT	N3-C2-O2	-6.36	118.49	122.30
2	C	7	DT	N1-C2-N3	6.32	118.39	114.60
2	C	5	DT	C4-C5-C7	6.11	122.67	119.00
1	B	14	DG	P-O3'-C3'	6.02	126.92	119.70
1	B	10	DG	C5-C6-N1	5.87	114.44	111.50
2	C	15	DT	O4'-C1'-N1	5.51	111.86	108.00
1	B	9	DG	C5-C6-N1	5.46	114.23	111.50
1	B	8	DG	P-O3'-C3'	5.42	126.20	119.70
3	A	510	LEU	CA-CB-CG	5.42	127.75	115.30
2	C	5	DT	C6-C5-C7	-5.23	119.77	122.90
2	C	13	DA	O4'-C1'-N9	5.20	111.64	108.00
3	A	405	THR	N-CA-C	-5.14	97.13	111.00
2	C	13	DA	P-O3'-C3'	5.12	125.84	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	401	GLN	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	B	311	0	171	4	0
2	C	298	0	172	3	0
3	A	3383	0	3329	66	0
4	D	106	0	105	1	0
5	A	24	0	28	5	0
6	A	39	0	0	2	0
6	B	7	0	0	0	0
6	C	11	0	0	0	0
All	All	4179	0	3805	72	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 9.

All (72) 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)
3:A:438:GLU:HB2	3:A:439:THR:HG23	1.23	1.14
3:A:335:SER:HB3	5:A:1:SOR:O6	1.64	0.96
3:A:227:LYS:HZ2	5:A:2:SOR:H11	1.36	0.90
5:A:1:SOR:H2	6:A:671:HOH:O	1.72	0.89
3:A:454:VAL:HG13	3:A:501:ILE:HD11	1.57	0.84
3:A:227:LYS:NZ	5:A:2:SOR:H11	1.93	0.83
3:A:476:LYS:O	3:A:478:GLN:N	2.24	0.71
3:A:468:ARG:HG3	3:A:501:ILE:HD13	1.77	0.67
3:A:555:VAL:HG11	3:A:646:ASP:HB3	1.76	0.66
3:A:337:LYS:O	6:A:692:HOH:O	2.15	0.64
3:A:511:SER:O	3:A:514:LYS:HG2	1.97	0.62
2:C:1:DA:H2"	2:C:2:DA:C8	2.34	0.62
3:A:594:PHE:O	3:A:638:VAL:HB	2.01	0.61
3:A:247:GLN:HA	3:A:247:GLN:OE1	2.03	0.59
3:A:594:PHE:HD1	3:A:599:VAL:HG21	1.69	0.58
3:A:221:HIS:CE1	3:A:360:SER:HB2	2.39	0.58
3:A:438:GLU:CB	3:A:439:THR:HG23	2.16	0.56
3:A:398:LEU:HD13	3:A:402:THR:HG23	1.86	0.56
3:A:454:VAL:CG1	3:A:501:ILE:HD11	2.35	0.55
3:A:214:GLU:OE1	3:A:547:ARG:HD2	2.06	0.55
3:A:594:PHE:CD1	3:A:599:VAL:HG21	2.42	0.54
3:A:592:VAL:HG11	3:A:611:CYS:SG	2.48	0.54
3:A:550:GLU:OE2	3:A:554:GLN:HA	2.09	0.53
3:A:255:ARG:HD3	3:A:554:GLN:HB3	1.90	0.53
3:A:499:GLN:HB3	3:A:507:TYR:CE2	2.44	0.52
3:A:335:SER:HB3	5:A:1:SOR:HO6	1.69	0.50
3:A:630:ASN:ND2	3:A:633:THR:H	2.10	0.50
3:A:636:VAL:O	3:A:658:TYR:HB2	2.12	0.50
3:A:212:LYS:H	3:A:212:LYS:HD2	1.77	0.50
3:A:212:LYS:N	3:A:212:LYS:HD2	2.27	0.49
3:A:524:ASN:HB2	3:A:527:ARG:CB	2.42	0.49
3:A:474:VAL:HG22	3:A:495:LYS:HB3	1.94	0.49
3:A:415:PHE:HE1	3:A:464:ILE:HG22	1.79	0.48
3:A:475:ASP:O	3:A:476:LYS:O	2.32	0.48
1:B:14:DG:H1'	1:B:15:DA:H5'	1.94	0.48
3:A:524:ASN:HB3	3:A:526:HIS:H	1.79	0.48
3:A:507:TYR:OH	3:A:528:HIS:HD2	1.97	0.48
3:A:235:PHE:HA	3:A:330:LEU:O	2.14	0.48
3:A:416:HIS:HB2	3:A:513:ASP:O	2.13	0.47
3:A:217:ILE:HD12	3:A:244:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:221:HIS:HD2	3:A:222:ALA:O	1.97	0.47
1:B:10:DG:O6	3:A:368:LYS:NZ	2.48	0.47
2:C:13:DA:N3	3:A:401:GLN:HG2	2.29	0.47
3:A:213:TYR:HB3	3:A:549:PHE:CE1	2.51	0.46
3:A:473:LYS:HB3	3:A:480:ILE:HG12	1.98	0.46
3:A:616:VAL:O	3:A:619:VAL:HG22	2.17	0.45
3:A:564:VAL:O	3:A:583:GLY:HA3	2.16	0.45
3:A:488:GLU:HA	3:A:489:PRO:HD3	1.86	0.45
3:A:198:LEU:HD22	3:A:643:VAL:HG21	1.98	0.45
3:A:627:MET:HG3	3:A:628:PHE:CD1	2.52	0.45
1:B:8:DG:H5'	3:A:400:SER:HB3	1.98	0.44
3:A:370:SER:OG	3:A:372:LYS:HD3	2.18	0.44
3:A:476:LYS:C	3:A:478:GLN:H	2.21	0.44
2:C:1:DA:C2'	2:C:2:DA:C8	3.01	0.43
3:A:617:SER:HA	3:A:620:ARG:HH12	1.84	0.43
3:A:201:ASP:HA	3:A:204:ILE:HD12	2.01	0.43
3:A:593:TRP:CD1	3:A:643:VAL:HG12	2.53	0.43
3:A:613:ILE:HG13	3:A:614:PRO:HD2	2.01	0.42
3:A:624:THR:O	3:A:625:HIS:HB2	2.18	0.42
1:B:13:DA:H1'	1:B:14:DG:H5'	2.01	0.42
3:A:217:ILE:HD12	3:A:244:LEU:HD21	2.01	0.42
3:A:564:VAL:CG2	3:A:584:ARG:HE	2.33	0.42
4:D:947:PRO:HA	4:D:948:PRO:HD3	1.87	0.42
3:A:255:ARG:NH1	3:A:550:GLU:HB2	2.35	0.42
3:A:504:GLU:OE1	3:A:504:GLU:HA	2.19	0.41
3:A:524:ASN:HB2	3:A:527:ARG:HB3	2.02	0.41
3:A:237:CYS:HA	3:A:238:PRO:C	2.41	0.41
3:A:564:VAL:HG21	3:A:584:ARG:HE	1.85	0.41
3:A:659:LYS:O	3:A:660:SER:C	2.58	0.41
3:A:398:LEU:HD11	3:A:404:SER:O	2.20	0.41
3:A:579:VAL:HG11	3:A:594:PHE:HZ	1.86	0.41
3:A:381:CYS:O	3:A:382:LYS:HB2	2.21	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
3	A	415/478 (87%)	376 (91%)	28 (7%)	11 (3%)	6 8
4	D	11/14 (79%)	9 (82%)	2 (18%)	0	100 100
All	All	426/492 (87%)	385 (90%)	30 (7%)	11 (3%)	7 9

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	399	ARG
3	A	403	VAL
3	A	476	LYS
3	A	401	GLN
3	A	477	GLN
3	A	625	HIS
3	A	200	SER
3	A	552	MET
3	A	603	PHE
3	A	381	CYS
3	A	646	ASP

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
3	A	375/417 (90%)	336 (90%)	39 (10%)	9 15
4	D	12/13 (92%)	10 (83%)	2 (17%)	3 4
All	All	387/430 (90%)	346 (89%)	41 (11%)	8 15

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	201	ASP

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Mol	Chain	Res	Type
3	A	212	LYS
3	A	258	GLN
3	A	260	TYR
3	A	262	THR
3	A	295	ASP
3	A	301	GLN
3	A	333	SER
3	A	372	LYS
3	A	375	SER
3	A	398	LEU
3	A	399	ARG
3	A	410	VAL
3	A	429	LEU
3	A	433	GLU
3	A	439	THR
3	A	445	ARG
3	A	468	ARG
3	A	474	VAL
3	A	501	ILE
3	A	503	ASN
3	A	508	LEU
3	A	510	LEU
3	A	514	LYS
3	A	527	ARG
3	A	543	LYS
3	A	554	GLN
3	A	559	ILE
3	A	564	VAL
3	A	599	VAL
3	A	607	GLU
3	A	611	CYS
3	A	620	ARG
3	A	622	GLU
3	A	626	TRP
3	A	631	ARG
3	A	646	ASP
3	A	649	VAL
3	A	655	THR
4	D	943	SER
4	D	949	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	221	HIS
3	A	396	ASN
3	A	416	HIS
3	A	441	ASN
3	A	503	ASN
3	A	524	ASN
3	A	528	HIS
3	A	557	ASN
3	A	623	GLN
3	A	630	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 carbohydrates in this entry.

5.6 Ligand geometry

2 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	$\#\|Z\| > 2$
5	SOR	A	1	-	11,11,11	0.33	0	14,14,14	1.50	2 (14%)
5	SOR	A	2	-	11,11,11	0.42	0	14,14,14	1.31	3 (21%)

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
5	SOR	A	1	-	-	0/16/16/16	0/0/0/0
5	SOR	A	2	-	-	0/16/16/16	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1	SOR	O6-C6-C5	-3.56	103.36	111.10
5	A	2	SOR	C2-C3-C4	-2.36	108.63	112.47
5	A	2	SOR	C5-C4-C3	-2.09	109.08	112.47
5	A	2	SOR	O4-C4-C5	2.31	114.57	108.75
5	A	1	SOR	O5-C5-C4	3.22	117.12	109.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	SOR	3	0
5	A	2	SOR	2	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	B	15/15 (100%)	0.94	1 (6%) 21 23	36, 40, 46, 48	0
2	C	15/15 (100%)	1.03	1 (6%) 21 23	36, 40, 46, 47	0
3	A	423/478 (88%)	1.62	133 (31%) 1 0	29, 40, 50, 58	0
4	D	13/14 (92%)	1.05	2 (15%) 3 3	41, 44, 46, 48	0
All	All	466/522 (89%)	1.56	137 (29%) 1 0	29, 40, 49, 58	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	626	TRP	8.7
3	A	260	TYR	8.4
3	A	399	ARG	7.9
3	A	262	THR	7.6
3	A	571	ASP	6.1
3	A	403	VAL	6.0
3	A	572	GLY	6.0
3	A	605	SER	5.9
3	A	263	LEU	5.8
3	A	351	CYS	5.8
3	A	634	GLY	5.6
3	A	604	ARG	5.5
3	A	402	THR	5.5
3	A	537	THR	5.3
3	A	258	GLN	5.1
3	A	575	GLU	5.0
3	A	538	ILE	4.9
3	A	637	GLU	4.8
3	A	570	VAL	4.5
3	A	629	THR	4.5
3	A	461	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
3	A	656	PHE	4.3
3	A	553	GLY	4.3
3	A	539	ILE	4.2
3	A	536	TRP	4.2
3	A	631	ARG	4.2
3	A	610	HIS	4.2
3	A	633	THR	4.1
3	A	622	GLU	4.0
3	A	636	VAL	4.0
3	A	498	PHE	4.0
3	A	588	PRO	3.9
3	A	237	CYS	3.9
3	A	395	PHE	3.9
3	A	393	ALA	3.8
3	A	580	GLU	3.8
3	A	208	SER	3.8
3	A	493	LEU	3.8
3	A	615	PRO	3.7
3	A	621	ASN	3.7
3	A	568	LEU	3.7
3	A	625	HIS	3.7
3	A	438	GLU	3.7
3	A	620	ARG	3.7
3	A	394	LEU	3.7
3	A	602	THR	3.7
3	A	261	LYS	3.6
3	A	496	CYS	3.6
3	A	611	CYS	3.6
3	A	433	GLU	3.6
3	A	632	THR	3.5
3	A	578	ARG	3.5
3	A	381	CYS	3.5
3	A	238	PRO	3.4
3	A	617	SER	3.4
3	A	380	ASP	3.3
3	A	353	MET	3.3
4	D	950	GLU	3.3
3	A	259	LEU	3.2
3	A	374	GLN	3.2
3	A	213	TYR	3.2
3	A	606	GLU	3.2
3	A	414	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
3	A	535	ALA	3.2
3	A	579	VAL	3.2
3	A	660	SER	3.1
3	A	392	VAL	3.1
3	A	659	LYS	3.1
3	A	483	ALA	3.1
3	A	554	GLN	3.1
3	A	497	ALA	3.0
3	A	576	ALA	3.0
3	A	201	ASP	3.0
3	A	654	LEU	3.0
3	A	657	SER	2.9
3	A	600	GLU	2.9
3	A	320	ASN	2.9
3	A	630	ASN	2.9
3	A	658	TYR	2.9
3	A	587	LYS	2.8
3	A	212	LYS	2.8
3	A	525	GLU	2.8
3	A	577	SER	2.8
3	A	608	SER	2.8
3	A	590	LEU	2.7
3	A	199	THR	2.7
3	A	573	HIS	2.7
3	A	638	VAL	2.7
3	A	603	PHE	2.7
1	B	8	DG	2.6
3	A	574	GLY	2.6
3	A	569	GLU	2.6
3	A	198	LEU	2.6
3	A	509	CYS	2.6
3	A	401	GLN	2.6
3	A	222	ALA	2.5
3	A	618	GLN	2.5
3	A	627	MET	2.5
3	A	382	LYS	2.5
3	A	464	ILE	2.5
3	A	567	SER	2.5
3	A	623	GLN	2.5
3	A	520	ALA	2.5
3	A	594	PHE	2.4
3	A	369	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	202	ARG	2.4
3	A	236	PHE	2.4
3	A	225	ALA	2.4
3	A	455	VAL	2.3
3	A	607	GLU	2.3
3	A	200	SER	2.3
3	A	562	CYS	2.3
3	A	628	PHE	2.3
3	A	642	LEU	2.3
3	A	256	VAL	2.3
3	A	234	ARG	2.3
3	A	582	HIS	2.2
3	A	411	GLU	2.2
3	A	344	ASN	2.2
3	A	224	VAL	2.2
3	A	406	ARG	2.2
3	A	593	TRP	2.2
2	C	8	DC	2.2
3	A	549	PHE	2.2
3	A	581	LEU	2.1
4	D	938	ARG	2.1
3	A	601	THR	2.1
3	A	226	GLN	2.1
3	A	512	HIS	2.1
3	A	362[A]	ARG	2.1
3	A	450	TYR	2.1
3	A	490	VAL	2.1
3	A	413	ASN	2.1
3	A	591	LYS	2.1
3	A	408	LEU	2.1
3	A	560	SER	2.0
3	A	494	HIS	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

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
5	SOR	A	1	12/12	0.89	0.28	1.73	19,23,26,27	12
5	SOR	A	2	12/12	0.66	0.28	1.19	57,64,71,71	0

6.5 Other polymers

There are no such residues in this entry.