Full wwPDB X-ray Structure Validation Report (i)

Oct 6, 2021 – 04:09 am BST

PDB ID	:	6HR1
Title	:	Crystal structure of the YFPnano fusion protein
Authors	:	Benoit, R.M.
Deposited on	:	2018-09-26
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

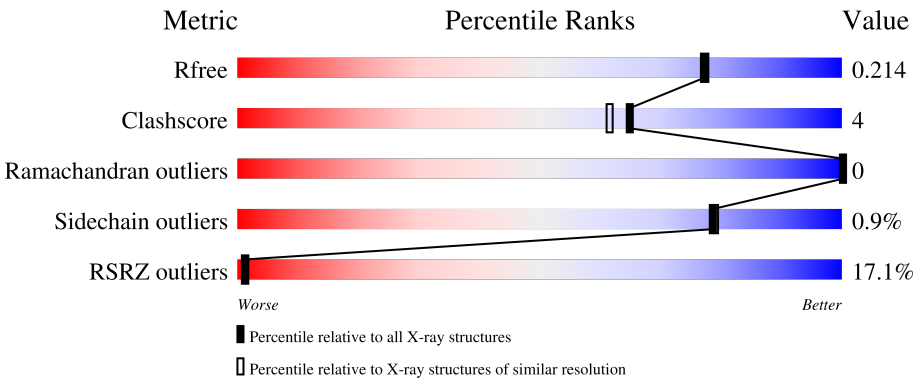
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	434	13% 83% 11% 6%
1	B	434	19% 84% 8% 7%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6986 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 Myosin light chain kinase 2, skeletal/cardiac muscle,Unconventional myosin-X,Green fluorescent protein,Calmodulin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	407	3284	2063	552	652	17	78	4	0
1	B	402	3250	2045	541	649	15	136	5	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	GLY	-	expression tag	UNP P07313
A	-34	PRO	-	expression tag	UNP P07313
A	-33	HIS	-	expression tag	UNP P07313
A	-32	MET	-	expression tag	UNP P07313
A	-31	ALA	-	expression tag	UNP P07313
A	-26	ALA	ASN	engineered mutation	UNP P07313
A	1	VAL	MET	conflict	UNP P42212
A	66	CR2	SER	chromophore	UNP P42212
A	66	CR2	TYR	chromophore	UNP P42212
A	66	CR2	GLY	chromophore	UNP P42212
A	68	LEU	VAL	conflict	UNP P42212
A	72	ALA	SER	conflict	UNP P42212
A	203	TYR	THR	conflict	UNP P42212
A	231	LEU	HIS	conflict	UNP P42212
A	239	GLY	-	linker	UNP P42212
A	240	GLU	-	linker	UNP P42212
A	241	ASN	-	linker	UNP P42212
A	242	LEU	-	linker	UNP P42212
A	243	TYR	-	linker	UNP P42212
A	244	PHE	-	linker	UNP P42212
A	245	GLN	-	linker	UNP P42212
A	246	SER	-	linker	UNP P42212
A	247	GLY	-	linker	UNP P42212
A	248	GLY	-	linker	UNP P42212

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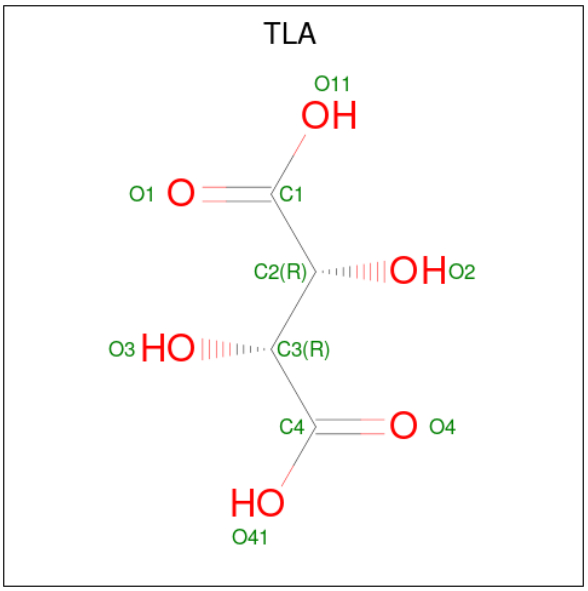
Chain	Residue	Modelled	Actual	Comment	Reference
A	249	SER	-	linker	UNP P42212
A	250	ALA	-	linker	UNP P42212
A	251	ALA	-	linker	UNP P42212
A	252	ALA	-	linker	UNP P42212
B	-35	GLY	-	expression tag	UNP P07313
B	-34	PRO	-	expression tag	UNP P07313
B	-33	HIS	-	expression tag	UNP P07313
B	-32	MET	-	expression tag	UNP P07313
B	-31	ALA	-	expression tag	UNP P07313
B	-26	ALA	ASN	engineered mutation	UNP P07313
B	1	VAL	MET	conflict	UNP P42212
B	66	CR2	SER	chromophore	UNP P42212
B	66	CR2	TYR	chromophore	UNP P42212
B	66	CR2	GLY	chromophore	UNP P42212
B	68	LEU	VAL	conflict	UNP P42212
B	72	ALA	SER	conflict	UNP P42212
B	203	TYR	THR	conflict	UNP P42212
B	231	LEU	HIS	conflict	UNP P42212
B	239	GLY	-	linker	UNP P42212
B	240	GLU	-	linker	UNP P42212
B	241	ASN	-	linker	UNP P42212
B	242	LEU	-	linker	UNP P42212
B	243	TYR	-	linker	UNP P42212
B	244	PHE	-	linker	UNP P42212
B	245	GLN	-	linker	UNP P42212
B	246	SER	-	linker	UNP P42212
B	247	GLY	-	linker	UNP P42212
B	248	GLY	-	linker	UNP P42212
B	249	SER	-	linker	UNP P42212
B	250	ALA	-	linker	UNP P42212
B	251	ALA	-	linker	UNP P42212
B	252	ALA	-	linker	UNP P42212

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).

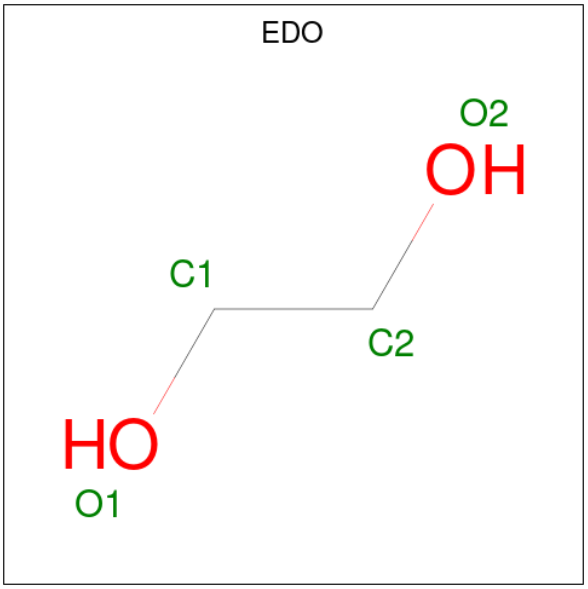


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	10	4	6	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

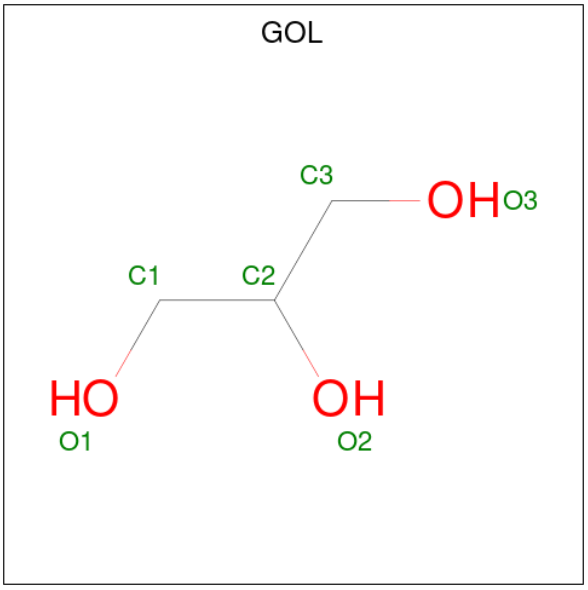
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	4	4	4	0	0
3	B	4	Total	Ca	0	0
			4	4		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	B	1	4	2	2	0	0
			Total	C	O		
4	B	1	4	2	2	0	0
			Total	C	O		
4	B	1	4	2	2	0	0
			Total	C	O		
4	B	1	4	2	2	0	0
			Total	C	O		
4	B	1	4	2	2	0	0
			Total	C	O		
4	B	1	4	2	2	0	0
			Total	C	O		
4	B	1	4	2	2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	B	2	2	2	0	0

- Molecule 7 is water.

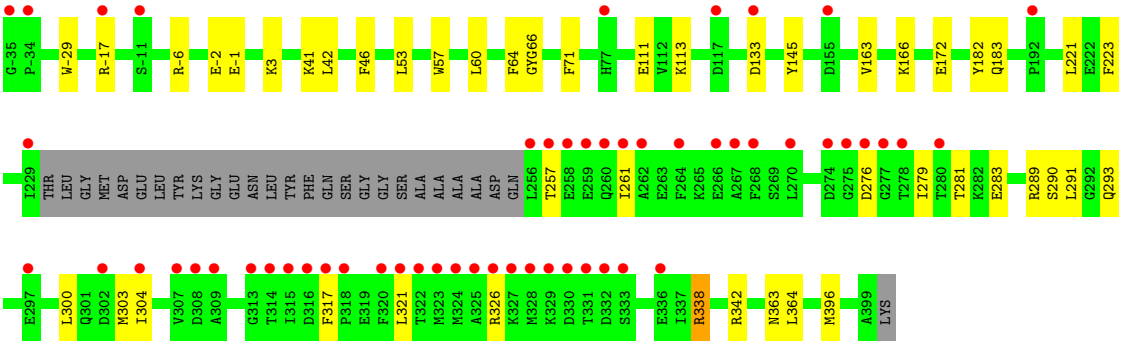
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	185	185	185	0	0
			Total	O		
7	B	181	181	181	0	0

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.

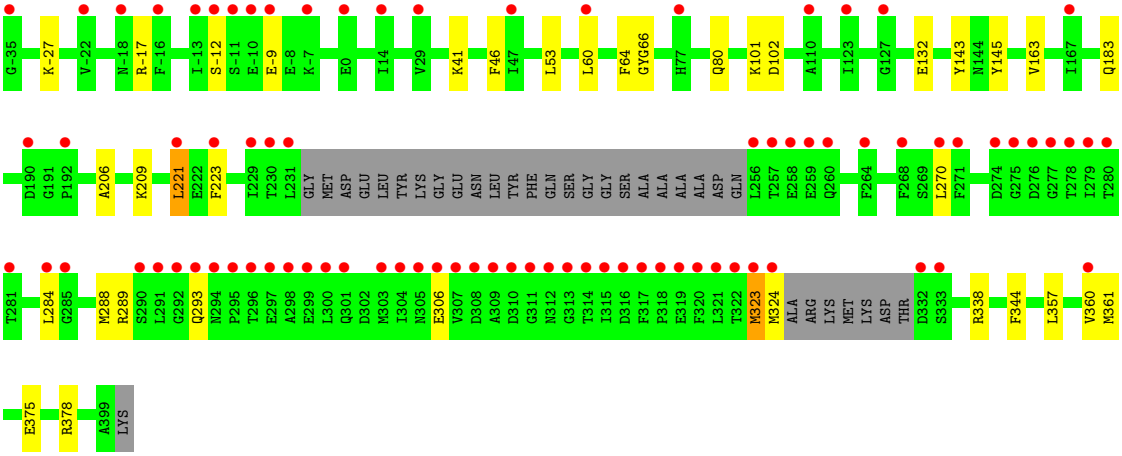
• Molecule 1: Myosin light chain kinase 2, skeletal/cardiac muscle,Unconventional myosin-X,Green fluorescent protein,Calmodulin-1

Chain A:



• Molecule 1: Myosin light chain kinase 2, skeletal/cardiac muscle,Unconventional myosin-X,Green fluorescent protein,Calmodulin-1

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	53.70Å 117.80Å 84.50Å 90.00° 99.90° 90.00°	Depositor
Resolution (Å)	48.59 – 1.90 48.59 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.59-1.90) 99.9 (48.59-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.181 , 0.214 0.180 , 0.214	Depositor DCC
R_{free} test set	4058 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6986	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.76% 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: TLA, CR2, NA, EDO, GOL, CA

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	0.46	0/3328	0.60	0/4477
1	B	0.47	0/3290	0.60	0/4429
All	All	0.46	0/6618	0.60	0/8906

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 (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	3284	0	3164	31	0
1	B	3250	0	3119	22	0
2	A	10	0	4	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	8	0	12	0	0
4	B	28	0	42	2	0
5	A	18	0	24	2	0
5	B	12	0	16	2	0
6	B	2	0	0	0	0
7	A	185	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	181	0	0	1	0
All	All	6986	0	6381	51	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 4.

All (51) 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:A:166:LYS:HG3	5:A:910:GOL:H32	1.50	0.93
1:B:375:GLU:OE2	1:B:378:ARG:NH2	2.09	0.84
1:A:-6:ARG:NH1	1:A:-2:GLU:OE2	2.29	0.66
1:A:182:TYR:OH	5:A:910:GOL:H12	1.98	0.64
1:A:172:GLU:OE1	7:A:1001:HOH:O	2.16	0.60
1:B:221[A]:LEU:HD21	1:B:223:PHE:CE2	2.37	0.59
1:A:281:THR:HG22	1:A:304:ILE:HG13	1.85	0.59
1:B:344:PHE:HA	1:B:360:VAL:HG21	1.85	0.57
1:B:46:PHE:CZ	1:B:64:PHE:HB3	2.41	0.56
1:A:223:PHE:HD2	1:B:206:ALA:HB1	1.73	0.54
1:A:46:PHE:CZ	1:A:64:PHE:HB3	2.43	0.53
1:A:289:ARG:HA	1:A:293:GLN:O	2.08	0.53
1:B:-17:ARG:NH1	1:B:324:MET:HA	2.24	0.53
1:A:-17:ARG:NH1	1:A:326:ARG:O	2.41	0.52
1:A:41:LYS:NZ	7:A:1006:HOH:O	2.42	0.52
1:B:-9:GLU:HG2	1:B:306:GLU:OE2	2.09	0.52
1:A:-1:GLU:HG3	1:A:3:LYS:NZ	2.25	0.51
1:A:317:PHE:CE2	1:A:321:LEU:HD22	2.46	0.50
1:A:221:LEU:HD21	1:A:223:PHE:CE2	2.48	0.49
1:A:-29:TRP:CD1	1:A:396:MET:SD	3.07	0.48
1:B:101:LYS:HB3	5:B:515:GOL:H31	1.97	0.47
1:A:163:VAL:HB	1:A:183:GLN:HB3	1.96	0.47
1:A:53:LEU:HD22	1:A:57:TRP:CE2	2.50	0.47
1:A:261:ILE:HD12	1:A:321:LEU:HD21	1.97	0.46
1:A:111:GLU:OE1	1:A:113:LYS:NZ	2.48	0.46
1:A:300:LEU:HA	1:A:303:MET:HE3	1.97	0.46
1:B:-27:LYS:HE3	1:B:270:LEU:HD11	1.97	0.46
1:B:102:ASP:HB2	5:B:515:GOL:H11	1.98	0.46
1:B:143:TYR:CZ	1:B:209:LYS:HE2	2.50	0.46
1:B:338:ARG:NH2	4:B:513:EDO:O2	2.48	0.46
1:A:53:LEU:HD21	1:A:60:LEU:HD12	1.97	0.45
1:B:41:LYS:HE3	1:B:221[A]:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD21	1:A:71:PHE:CD2	2.52	0.44
1:A:290:SER:HB2	1:A:363:ASN:HB3	2.00	0.44
1:B:357:LEU:O	1:B:361:MET:HG2	2.17	0.44
1:A:53:LEU:HD22	1:A:57:TRP:CD2	2.52	0.43
1:A:338:ARG:HG2	1:A:342:ARG:CZ	2.49	0.43
1:A:257:THR:O	1:A:261:ILE:HG12	2.17	0.43
1:B:163:VAL:HB	1:B:183:GLN:HB3	2.01	0.43
1:B:53:LEU:HD21	1:B:60:LEU:HD12	2.01	0.43
1:A:221:LEU:CD2	1:B:221[A]:LEU:HD22	2.48	0.42
1:B:323:MET:O	1:B:323:MET:HG2	2.19	0.42
1:A:279:ILE:HA	1:A:283:GLU:OE2	2.19	0.42
1:B:284:LEU:O	1:B:288:MET:HG2	2.19	0.42
1:A:317:PHE:CZ	1:A:321:LEU:HD13	2.55	0.42
1:A:291:LEU:HD21	1:A:364:LEU:HD21	2.02	0.41
1:B:132:GLU:OE1	7:B:601:HOH:O	2.22	0.41
1:B:289:ARG:HA	1:B:293:GLN:O	2.20	0.41
1:B:80:GLN:HB3	4:B:510:EDO:H12	2.03	0.41
1:A:133:ASP:OD1	1:A:133:ASP:N	2.49	0.41
1:A:276:ASP:C	1:A:276:ASP:OD1	2.59	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	404/434 (93%)	402 (100%)	2 (0%)	0	100	100
1	B	398/434 (92%)	392 (98%)	6 (2%)	0	100	100
All	All	802/868 (92%)	794 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	354/369 (96%)	352 (99%)	2 (1%)	86	87
1	B	351/369 (95%)	346 (99%)	5 (1%)	67	65
All	All	705/738 (96%)	698 (99%)	7 (1%)	78	76

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

Mol	Chain	Res	Type
1	A	145	TYR
1	A	338	ARG
1	B	-12	SER
1	B	145	TYR
1	B	221[A]	LEU
1	B	221[B]	LEU
1	B	323	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CR2	B	66	1	20,20,21	2.58	9 (45%)	25,27,29	2.48	8 (32%)
1	CR2	A	66	1	20,20,21	2.54	10 (50%)	25,27,29	3.41	9 (36%)

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
1	CR2	B	66	1	-	0/6/25/26	0/2/2/2
1	CR2	A	66	1	-	0/6/25/26	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CR2	C1-N2	5.17	1.41	1.32
1	B	66	CR2	CB2-CA2	-5.10	1.30	1.35
1	A	66	CR2	C1-N3	4.98	1.45	1.37
1	B	66	CR2	C1-N2	4.66	1.40	1.32
1	A	66	CR2	CA1-C1	4.39	1.54	1.49
1	A	66	CR2	CG2-CB2	4.22	1.55	1.46
1	B	66	CR2	CA1-C1	4.15	1.54	1.49
1	B	66	CR2	CG2-CB2	4.08	1.54	1.46
1	B	66	CR2	C1-N3	3.88	1.43	1.37
1	B	66	CR2	CA2-C2	3.23	1.51	1.48
1	A	66	CR2	CB2-CA2	-3.01	1.32	1.35
1	A	66	CR2	CA2-C2	2.88	1.51	1.48
1	A	66	CR2	C2-N3	2.66	1.46	1.39
1	B	66	CR2	CA2-N2	2.49	1.43	1.38
1	B	66	CR2	C2-N3	2.26	1.45	1.39
1	B	66	CR2	OH-CZ	2.24	1.42	1.37
1	A	66	CR2	CA2-N2	2.11	1.43	1.38
1	A	66	CR2	OH-CZ	2.08	1.41	1.37
1	A	66	CR2	O3-C3	2.01	1.31	1.19

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	CR2	O2-C2-CA2	-9.65	125.54	130.96
1	A	66	CR2	CA2-C2-N3	8.63	107.45	103.37
1	B	66	CR2	C1-CA1-N1	-7.58	96.08	112.85
1	A	66	CR2	C2-N3-C1	-6.33	104.90	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	CR2	CA2-C2-N3	4.73	105.61	103.37
1	A	66	CR2	C1-CA1-N1	-4.42	103.08	112.85
1	B	66	CR2	O2-C2-CA2	-4.40	128.49	130.96
1	A	66	CR2	O3-C3-CA3	-3.99	114.36	126.39
1	B	66	CR2	CD2-CG2-CD1	3.31	122.53	117.64
1	B	66	CR2	C2-N3-C1	-3.13	106.46	107.99
1	A	66	CR2	CD2-CG2-CD1	2.89	121.92	117.64
1	A	66	CR2	CG2-CB2-CA2	-2.85	126.45	129.94
1	A	66	CR2	CE1-CD1-CG2	-2.57	117.90	121.25
1	B	66	CR2	CG2-CB2-CA2	-2.54	126.83	129.94
1	B	66	CR2	O3-C3-CA3	-2.47	118.93	126.39
1	B	66	CR2	CE2-CD2-CG2	-2.34	118.19	121.25
1	A	66	CR2	CB2-CA2-N2	2.08	131.71	128.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
5	GOL	A	908	-	5,5,5	0.41	0	5,5,5	0.21	0
4	EDO	B	511	-	3,3,3	0.41	0	2,2,2	0.49	0
5	GOL	B	514	-	5,5,5	0.38	0	5,5,5	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TLA	A	901	-	3,9,9	0.82	0	6,12,12	1.49	1 (16%)
4	EDO	B	509	-	3,3,3	0.43	0	2,2,2	0.49	0
5	GOL	A	909	-	5,5,5	0.25	0	5,5,5	0.48	0
4	EDO	B	507	-	3,3,3	0.40	0	2,2,2	0.45	0
4	EDO	B	512	-	3,3,3	0.42	0	2,2,2	0.63	0
4	EDO	A	906	-	3,3,3	0.47	0	2,2,2	0.41	0
4	EDO	B	508	-	3,3,3	0.40	0	2,2,2	0.46	0
4	EDO	A	907	-	3,3,3	0.42	0	2,2,2	0.48	0
5	GOL	B	515	-	5,5,5	0.24	0	5,5,5	0.64	0
4	EDO	B	513	-	3,3,3	0.46	0	2,2,2	0.37	0
5	GOL	A	910	-	5,5,5	0.49	0	5,5,5	1.30	1 (20%)
4	EDO	B	510	-	3,3,3	0.44	0	2,2,2	0.64	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
5	GOL	A	908	-	-	2/4/4/4	-
4	EDO	B	511	-	-	1/1/1/1	-
5	GOL	B	514	-	-	2/4/4/4	-
2	TLA	A	901	-	-	0/4/12/12	-
4	EDO	B	509	-	-	0/1/1/1	-
5	GOL	A	909	-	-	2/4/4/4	-
4	EDO	B	507	-	-	0/1/1/1	-
4	EDO	B	512	-	-	1/1/1/1	-
4	EDO	A	906	-	-	0/1/1/1	-
4	EDO	B	508	-	-	0/1/1/1	-
4	EDO	A	907	-	-	1/1/1/1	-
5	GOL	B	515	-	-	0/4/4/4	-
4	EDO	B	513	-	-	0/1/1/1	-
5	GOL	A	910	-	-	3/4/4/4	-
4	EDO	B	510	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	TLA	C4-C3-C2	-3.28	106.04	113.11
5	A	910	GOL	C3-C2-C1	-2.89	100.46	111.70

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	908	GOL	C1-C2-C3-O3
5	A	909	GOL	O1-C1-C2-C3
5	A	910	GOL	C1-C2-C3-O3
5	B	514	GOL	O1-C1-C2-C3
5	A	910	GOL	O1-C1-C2-C3
5	A	908	GOL	O2-C2-C3-O3
5	A	909	GOL	O1-C1-C2-O2
5	A	910	GOL	O2-C2-C3-O3
4	B	510	EDO	O1-C1-C2-O2
4	B	511	EDO	O1-C1-C2-O2
5	B	514	GOL	O1-C1-C2-O2
4	A	907	EDO	O1-C1-C2-O2
4	B	512	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	515	GOL	2	0
4	B	513	EDO	1	0
5	A	910	GOL	2	0
4	B	510	EDO	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	406/434 (93%)	1.22	55 (13%)	3	3	19, 33, 63, 88	21 (5%)
1	B	401/434 (92%)	1.52	83 (20%)	1	1	17, 32, 71, 84	35 (8%)
All	All	807/868 (92%)	1.37	138 (17%)	1	1	17, 32, 70, 88	56 (6%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	321	LEU	11.0
1	A	-34	PRO	9.4
1	A	317	PHE	9.3
1	B	320	PHE	9.3
1	A	261	ILE	8.9
1	B	315	ILE	8.4
1	B	295	PRO	7.9
1	A	328	MET	7.8
1	B	231	LEU	7.7
1	A	256	LEU	7.7
1	B	-13	ILE	7.6
1	B	317	PHE	7.5
1	B	-16	PHE	7.3
1	B	312	ASN	7.1
1	B	305	ASN	7.0
1	A	325	ALA	7.0
1	B	307	VAL	6.6
1	B	-9	GLU	6.4
1	B	318	PRO	6.3
1	B	257	THR	6.1
1	A	257	THR	6.0
1	B	268	PHE	5.9
1	B	300	LEU	5.9
1	B	322	THR	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	310	ASP	5.8
1	B	316	ASP	5.8
1	B	333	SER	5.8
1	B	324	MET	5.7
1	B	311	GLY	5.6
1	B	301	GLN	5.4
1	B	230	THR	5.3
1	A	229	ILE	5.3
1	B	292	GLY	5.3
1	A	327	LYS	5.3
1	B	298	ALA	5.2
1	B	314	THR	5.2
1	B	306	GLU	5.1
1	B	309	ALA	5.1
1	B	281	THR	5.0
1	A	309	ALA	4.9
1	A	318	PRO	4.9
1	B	308	ASP	4.9
1	A	307	VAL	4.8
1	A	333	SER	4.8
1	B	278	THR	4.7
1	A	264	PHE	4.7
1	A	326	ARG	4.6
1	B	304	ILE	4.5
1	B	313	GLY	4.5
1	A	313	GLY	4.4
1	A	322	THR	4.4
1	B	319	GLU	4.4
1	B	190	ASP	4.3
1	B	256	LEU	4.1
1	B	284	LEU	4.0
1	A	-35	GLY	4.0
1	B	321	LEU	3.9
1	B	-11	SER	3.8
1	B	290	SER	3.8
1	A	258	GLU	3.5
1	B	297	GLU	3.5
1	B	285	GLY	3.5
1	A	278	THR	3.4
1	A	308	ASP	3.4
1	B	229	ILE	3.4
1	A	260	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	299	GLU	3.4
1	B	279	ILE	3.4
1	B	-10	GLU	3.3
1	B	277	GLY	3.3
1	B	77	HIS	3.2
1	B	270	LEU	3.2
1	A	280	THR	3.1
1	A	316	ASP	3.1
1	A	329	LYS	3.1
1	B	303	MET	3.1
1	B	-22	VAL	3.1
1	A	331	THR	3.1
1	A	315	ILE	3.0
1	B	-18	ASN	3.0
1	B	276	ASP	3.0
1	A	259	GLU	3.0
1	A	274	ASP	3.0
1	B	192	PRO	3.0
1	A	266	GLU	2.9
1	A	277	GLY	2.9
1	B	294	ASN	2.9
1	A	192	PRO	2.9
1	B	323	MET	2.9
1	A	77	HIS	2.9
1	B	259	GLU	2.9
1	A	304	ILE	2.9
1	A	324	MET	2.8
1	B	123	ILE	2.8
1	B	296	THR	2.8
1	A	268	PHE	2.8
1	A	262	ALA	2.7
1	B	221[A]	LEU	2.7
1	B	-35	GLY	2.7
1	A	330	ASP	2.7
1	A	302	ASP	2.7
1	B	293	GLN	2.6
1	B	264	PHE	2.6
1	B	258	GLU	2.5
1	A	276	ASP	2.5
1	B	-7	LYS	2.5
1	B	47[A]	ILE	2.4
1	A	155	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	0	GLU	2.4
1	A	320	PHE	2.4
1	B	271	PHE	2.4
1	A	-11	SER	2.4
1	B	127	GLY	2.4
1	A	133	ASP	2.4
1	B	260	GLN	2.4
1	A	270	LEU	2.4
1	B	332	ASP	2.4
1	B	275	GLY	2.3
1	B	167	ILE	2.3
1	B	280	THR	2.3
1	B	110	ALA	2.3
1	A	314	THR	2.3
1	A	117	ASP	2.3
1	A	267	ALA	2.2
1	B	-12	SER	2.2
1	B	14	ILE	2.2
1	B	274	ASP	2.2
1	A	-17	ARG	2.2
1	B	29	VAL	2.1
1	B	360	VAL	2.1
1	A	323	MET	2.1
1	A	297	GLU	2.1
1	A	332	ASP	2.0
1	A	336	GLU	2.0
1	B	223	PHE	2.0
1	A	275	GLY	2.0
1	B	60	LEU	2.0
1	B	291	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CR2	A	66	19/20	0.91	0.15	19,23,30,37	0
1	CR2	B	66	19/20	0.92	0.16	16,21,28,29	0

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
4	EDO	B	512	4/4	0.73	0.14	50,55,57,58	0
3	CA	B	503	1/1	0.74	0.33	79,79,79,79	0
4	EDO	B	510	4/4	0.75	0.12	53,54,59,59	0
4	EDO	B	513	4/4	0.76	0.13	50,52,56,65	0
5	GOL	A	908	6/6	0.77	0.20	47,50,55,57	0
4	EDO	A	907	4/4	0.79	0.12	40,47,47,59	0
4	EDO	B	509	4/4	0.79	0.20	37,49,50,65	0
2	TLA	A	901	10/10	0.82	0.18	33,41,43,44	0
5	GOL	A	910	6/6	0.82	0.20	27,41,44,46	0
5	GOL	B	515	6/6	0.82	0.19	33,45,47,60	0
4	EDO	A	906	4/4	0.84	0.16	38,41,46,55	0
4	EDO	B	507	4/4	0.85	0.16	34,45,47,51	0
5	GOL	A	909	6/6	0.86	0.17	33,44,48,63	0
5	GOL	B	514	6/6	0.88	0.17	38,45,52,64	0
4	EDO	B	511	4/4	0.88	0.14	35,44,49,52	0
6	NA	B	506	1/1	0.90	0.10	51,51,51,51	0
6	NA	B	505	1/1	0.92	0.18	53,53,53,53	0
3	CA	B	501	1/1	0.92	0.10	50,50,50,50	0
3	CA	A	903	1/1	0.94	0.13	54,54,54,54	0
4	EDO	B	508	4/4	0.95	0.14	38,40,43,59	0
3	CA	B	502	1/1	0.97	0.09	23,23,23,23	0
3	CA	A	902	1/1	0.97	0.10	43,43,43,43	0
3	CA	A	905	1/1	0.99	0.15	23,23,23,23	0
3	CA	A	904	1/1	0.99	0.14	23,23,23,23	0
3	CA	B	504	1/1	1.00	0.14	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.