wwPDB X-ray Structure Validation Summary Report (i)

Jun 22, 2024 – 12:07 PM EDT

PDB ID	:	5LUG
Title	:	Crystal structure of human Spindlin-2B protein in complex with ART(M3L)QTA(2MR)KS peptide
Authors	:	Srikannathasan, V.; Gileadi, C.; Talon, R.; Shrestha, L.; Kopec, J.; Szykowska, A.; Burgess-Brown, N.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; von Delft, F.; Oppermann, U.; Huber, K.
Deposited on	:	2016-09-08
Resolution	:	1.70 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

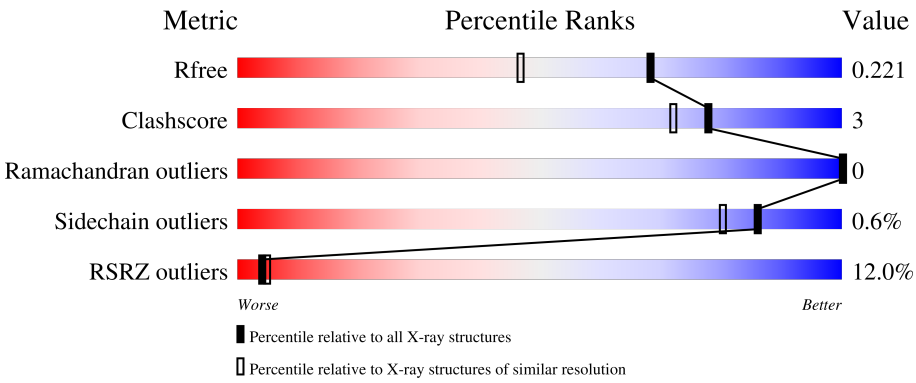
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	222	12% 83% 10% 7%
1	B	222	9% 87% 6% 7%
1	C	222	11% 90% • 8%
1	D	222	12% 86% 6% 8%

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Mol	Chain	Length	Quality of chain
2	E	10	20% 70% 30%
2	F	10	20% 60% 20% 20%
2	G	10	30% 30% 20% 20%
2	H	10	40% 30% 10% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2MR	F	8[A]	-	-	-	X
2	2MR	F	8[B]	-	-	-	X
4	2MR	B	301	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7746 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 Spindlin-like protein 2, isoform CRA_a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	207	1673	1079	278	307	9	0	2	0
1	B	207	1674	1079	279	307	9	0	2	0
1	C	205	1635	1054	271	302	8	0	0	0
1	D	204	1639	1059	273	299	8	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	-	initiating methionine	UNP A0A024R9Y9
A	259	ALA	-	expression tag	UNP A0A024R9Y9
A	260	GLU	-	expression tag	UNP A0A024R9Y9
A	261	ASN	-	expression tag	UNP A0A024R9Y9
A	262	LEU	-	expression tag	UNP A0A024R9Y9
A	263	TYR	-	expression tag	UNP A0A024R9Y9
A	264	PHE	-	expression tag	UNP A0A024R9Y9
A	265	GLN	-	expression tag	UNP A0A024R9Y9
B	44	MET	-	initiating methionine	UNP A0A024R9Y9
B	259	ALA	-	expression tag	UNP A0A024R9Y9
B	260	GLU	-	expression tag	UNP A0A024R9Y9
B	261	ASN	-	expression tag	UNP A0A024R9Y9
B	262	LEU	-	expression tag	UNP A0A024R9Y9
B	263	TYR	-	expression tag	UNP A0A024R9Y9
B	264	PHE	-	expression tag	UNP A0A024R9Y9
B	265	GLN	-	expression tag	UNP A0A024R9Y9
C	44	MET	-	initiating methionine	UNP A0A024R9Y9
C	259	ALA	-	expression tag	UNP A0A024R9Y9
C	260	GLU	-	expression tag	UNP A0A024R9Y9
C	261	ASN	-	expression tag	UNP A0A024R9Y9
C	262	LEU	-	expression tag	UNP A0A024R9Y9

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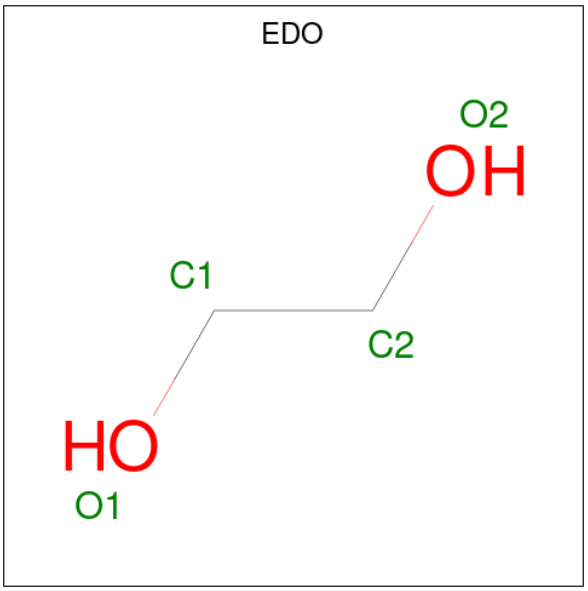
Chain	Residue	Modelled	Actual	Comment	Reference
C	263	TYR	-	expression tag	UNP A0A024R9Y9
C	264	PHE	-	expression tag	UNP A0A024R9Y9
C	265	GLN	-	expression tag	UNP A0A024R9Y9
D	44	MET	-	initiating methionine	UNP A0A024R9Y9
D	259	ALA	-	expression tag	UNP A0A024R9Y9
D	260	GLU	-	expression tag	UNP A0A024R9Y9
D	261	ASN	-	expression tag	UNP A0A024R9Y9
D	262	LEU	-	expression tag	UNP A0A024R9Y9
D	263	TYR	-	expression tag	UNP A0A024R9Y9
D	264	PHE	-	expression tag	UNP A0A024R9Y9
D	265	GLN	-	expression tag	UNP A0A024R9Y9

- Molecule 2 is a protein called ALA-ARG-THR-M3L-GLN-THR-ALA-2MR-LYS-SER.

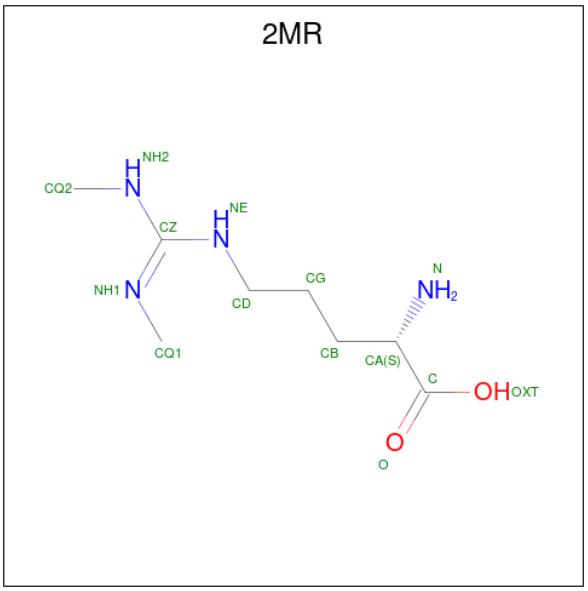
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	F	8	82	50	20	12	0	1	0
2	G	8	82	50	20	12	0	1	0
2	H	8	82	50	20	12	0	1	0
2	E	7	56	34	12	10	0	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is N3, N4-DIMETHYLARGININE (three-letter code: 2MR) (formula: $C_8H_{18}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			13	8	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	189	Total	O	0	0
			189	189		
5	B	194	Total	O	0	0
			194	194		
5	C	168	Total	O	0	0
			168	168		

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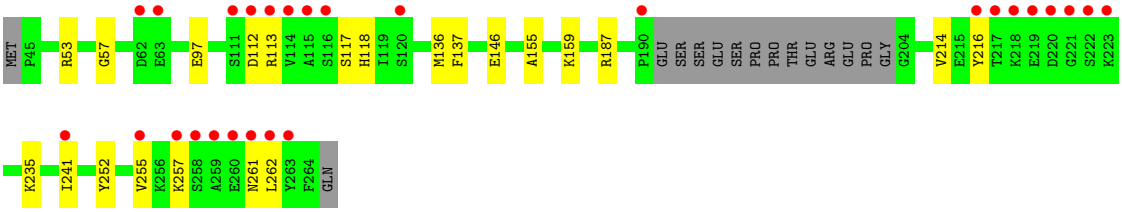
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	D	187	187	187	0	0
			Total	O		
5	F	12	12	12	0	0
			Total	O		
5	G	14	14	14	0	0
			Total	O		
5	H	11	11	11	0	0
			Total	O		
5	E	11	11	11	0	0

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.

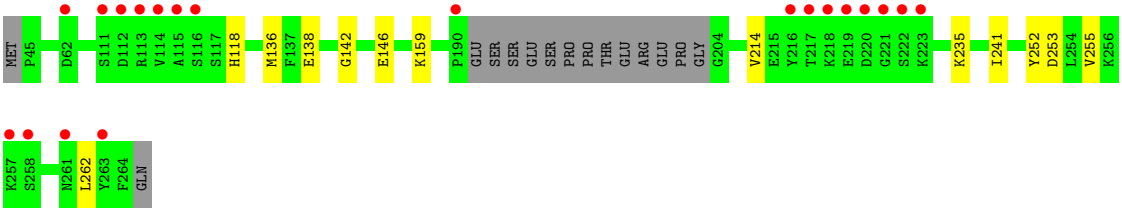
• Molecule 1: Spindlin-like protein 2, isoform CRA_a

Chain A:



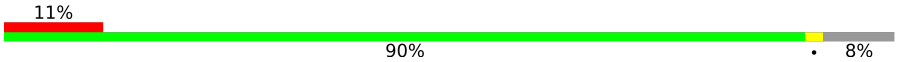
• Molecule 1: Spindlin-like protein 2, isoform CRA_a

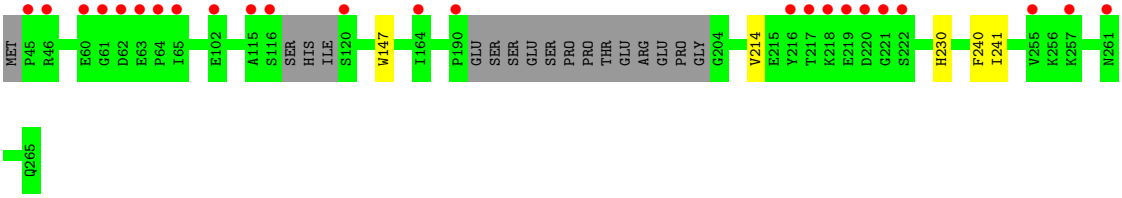
Chain B:



• Molecule 1: Spindlin-like protein 2, isoform CRA_a

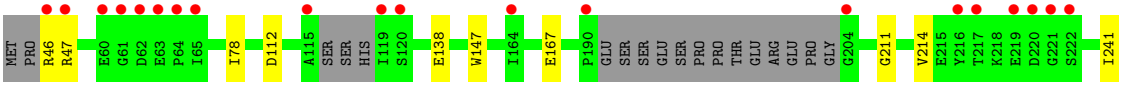
Chain C:

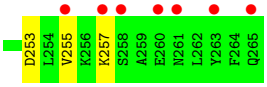




• Molecule 1: Spindlin-like protein 2, isoform CRA_a

Chain D:



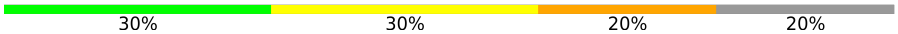


- Molecule 2: ALA-ARG-THR-M3L-GLN-THR-ALA-2MR-LYS-SER

Chain F:

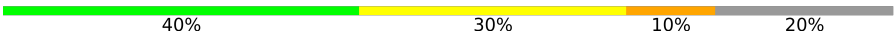
- Molecule 2: ALA-ARG-THR-M3L-GLN-THR-ALA-2MR-LYS-SER

Chain G:



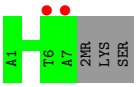
- Molecule 2: ALA-ARG-THR-M3L-GLN-THR-ALA-2MR-LYS-SER

Chain H:



- Molecule 2: ALA-ARG-THR-M3L-GLN-THR-ALA-2MR-LYS-SER

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.53Å 81.22Å 93.97Å 90.00° 99.86° 90.00°	Depositor
Resolution (Å)	19.90 – 1.70 19.90 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.90-1.70) 91.7 (19.90-1.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.9_1682	Depositor
R, R_{free}	0.194 , 0.221 0.195 , 0.221	Depositor DCC
R_{free} test set	5309 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7746	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7138e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 2MR, EDO, M3L

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	0.37	0/1720	0.59	0/2326
1	B	0.36	0/1718	0.56	0/2323
1	C	0.34	0/1673	0.52	0/2262
1	D	0.35	0/1677	0.56	0/2267
2	E	0.35	0/43	0.59	0/57
2	F	0.33	0/43	0.52	0/57
2	G	0.36	0/43	0.82	0/57
2	H	0.49	0/43	0.65	0/57
All	All	0.36	0/6960	0.56	0/9406

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	1673	0	1642	15	1
1	B	1674	0	1636	9	0
1	C	1635	0	1588	3	0
1	D	1639	0	1598	9	0
2	E	56	0	66	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	82	0	98	1	0
2	G	82	0	99	4	0
2	H	82	0	99	2	0
3	A	8	0	12	0	0
3	B	12	0	18	2	0
3	D	4	0	6	0	0
4	B	13	0	17	1	0
5	A	189	0	0	2	3
5	B	194	0	0	2	1
5	C	168	0	0	0	0
5	D	187	0	0	2	0
5	E	11	0	0	0	0
5	F	12	0	0	0	0
5	G	14	0	0	1	0
5	H	11	0	0	0	1
All	All	7746	0	6879	40	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 40 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:D:47:ARG:NH2	1:D:112:ASP:OD1	2.19	0.75
1:A:112:ASP:OD2	1:A:113:ARG:NH1	2.21	0.73
1:A:53:ARG:NH2	1:A:113:ARG:NH1	2.42	0.67
2:G:8[B]:2MR:N	5:G:101:HOH:O	2.28	0.66
1:B:142:GLY:HA2	3:B:303:EDO:H21	1.78	0.65

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:401:HOH:O	5:A:414:HOH:O[2_545]	1.98	0.22
1:A:187:ARG:NH2	5:A:401:HOH:O[2_555]	2.01	0.19
5:B:564:HOH:O	5:B:577:HOH:O[2_544]	2.13	0.07
5:A:404:HOH:O	5:H:104:HOH:O[2_645]	2.15	0.05

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	205/222 (92%)	200 (98%)	5 (2%)	0	100	100
1	B	205/222 (92%)	200 (98%)	5 (2%)	0	100	100
1	C	199/222 (90%)	196 (98%)	3 (2%)	0	100	100
1	D	198/222 (89%)	195 (98%)	3 (2%)	0	100	100
2	E	4/10 (40%)	4 (100%)	0	0	100	100
2	F	5/10 (50%)	5 (100%)	0	0	100	100
2	G	5/10 (50%)	4 (80%)	1 (20%)	0	100	100
2	H	5/10 (50%)	5 (100%)	0	0	100	100
All	All	826/928 (89%)	809 (98%)	17 (2%)	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	180/196 (92%)	178 (99%)	2 (1%)	73	63
1	B	179/196 (91%)	179 (100%)	0	100	100
1	C	173/196 (88%)	173 (100%)	0	100	100
1	D	172/196 (88%)	172 (100%)	0	100	100
2	E	4/6 (67%)	4 (100%)	0	100	100
2	F	4/6 (67%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	4/6 (67%)	3 (75%)	1 (25%)	0	0
2	H	4/6 (67%)	3 (75%)	1 (25%)	0	0
All	All	720/808 (89%)	716 (99%)	4 (1%)	86	80

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	VAL
1	A	257	LYS
2	G	6	THR
2	H	6	THR

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)

10 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	$\#\|Z\| > 2$
2	M3L	F	4	2	10,11,12	0.44	0	9,14,16	0.95	0
2	2MR	F	8[B]	-	10,12,13	1.81	1 (10%)	5,13,15	3.12	1 (20%)
2	2MR	G	8[A]	2	10,12,13	2.46	2 (20%)	5,13,15	5.76	2 (40%)
2	2MR	G	8[B]	-	10,12,13	2.55	3 (30%)	5,13,15	1.10	1 (20%)
2	2MR	H	8[A]	2	10,12,13	2.68	2 (20%)	5,13,15	4.24	3 (60%)
2	M3L	G	4	2	10,11,12	0.65	0	9,14,16	0.46	0
2	2MR	H	8[B]	-	10,12,13	2.69	2 (20%)	5,13,15	3.95	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	M3L	E	4	2	10,11,12	0.48	0	9,14,16	0.62	0
2	M3L	H	4	2	10,11,12	0.73	0	9,14,16	0.32	0
2	2MR	F	8[A]	2	10,12,13	1.83	1 (10%)	5,13,15	2.42	2 (40%)

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	M3L	F	4	2	-	4/9/10/12	-
2	2MR	F	8[B]	-	-	2/10/13/15	-
2	2MR	G	8[A]	2	-	2/10/13/15	-
2	2MR	G	8[B]	-	-	3/10/13/15	-
2	2MR	H	8[A]	2	-	2/10/13/15	-
2	M3L	G	4	2	-	0/9/10/12	-
2	2MR	H	8[B]	-	-	2/10/13/15	-
2	M3L	E	4	2	-	5/9/10/12	-
2	M3L	H	4	2	-	0/9/10/12	-
2	2MR	F	8[A]	2	-	3/10/13/15	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	8[B]	2MR	CZ-NE	5.91	1.47	1.34
2	H	8[A]	2MR	CZ-NE	5.79	1.46	1.34
2	H	8[A]	2MR	CZ-NH2	5.65	1.46	1.33
2	H	8[B]	2MR	CZ-NH2	5.56	1.45	1.33
2	F	8[A]	2MR	CZ-NE	5.32	1.45	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	8[A]	2MR	NE-CZ-NH2	-11.90	108.57	119.48
2	F	8[B]	2MR	NE-CZ-NH2	6.71	125.63	119.48
2	H	8[A]	2MR	NE-CZ-NH2	6.41	125.36	119.48
2	H	8[B]	2MR	NE-CZ-NH2	6.34	125.29	119.48
2	H	8[A]	2MR	CD-NE-CZ	5.94	134.54	123.41

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	4	M3L	C-CA-CB-CG
2	F	8[B]	2MR	N-CA-CB-CG
2	F	8[B]	2MR	C-CA-CB-CG
2	G	8[B]	2MR	O-C-CA-CB
2	H	8[A]	2MR	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	4	M3L	1	0
2	G	8[B]	2MR	1	0
2	G	4	M3L	1	0
2	H	4	M3L	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
3	EDO	A	301	-	3,3,3	0.48	0	2,2,2	0.23	0
3	EDO	A	302	-	3,3,3	0.42	0	2,2,2	0.41	0
4	2MR	B	301	-	10,12,13	2.48	2 (20%)	5,13,15	3.88	2 (40%)
3	EDO	B	303	-	3,3,3	0.43	0	2,2,2	0.28	0
3	EDO	B	304	-	3,3,3	0.44	0	2,2,2	0.39	0
3	EDO	B	302	-	3,3,3	0.43	0	2,2,2	0.25	0
3	EDO	D	301	-	3,3,3	0.45	0	2,2,2	0.29	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
3	EDO	A	301	-	-	0/1/1/1	-
3	EDO	A	302	-	-	0/1/1/1	-
4	2MR	B	301	-	-	3/10/13/15	-
3	EDO	B	303	-	-	0/1/1/1	-
3	EDO	B	304	-	-	0/1/1/1	-
3	EDO	B	302	-	-	0/1/1/1	-
3	EDO	D	301	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	2MR	CZ-NH2	5.48	1.45	1.33
4	B	301	2MR	CZ-NE	4.98	1.44	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	301	2MR	NE-CZ-NH2	-7.85	112.28	119.48
4	B	301	2MR	CQ2-NH2-CZ	3.47	131.53	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	2MR	N-CA-CB-CG
4	B	301	2MR	C-CA-CB-CG
4	B	301	2MR	NE-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	2MR	1	0
3	B	303	EDO	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	1
2	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	7:ALA	C	8[B]:2MR	N	2.97
1	G	7:ALA	C	8[B]:2MR	N	2.94

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	207/222 (93%)	0.80	27 (13%)	3	4	12, 17, 46, 100	0
1	B	207/222 (93%)	0.66	20 (9%)	7	8	11, 17, 46, 80	0
1	C	205/222 (92%)	0.75	24 (11%)	4	5	12, 20, 49, 75	0
1	D	204/222 (91%)	0.78	27 (13%)	3	3	12, 20, 52, 73	0
2	E	6/10 (60%)	2.33	2 (33%)	0	0	15, 20, 60, 65	0
2	F	6/10 (60%)	2.04	2 (33%)	0	0	15, 19, 62, 63	0
2	G	6/10 (60%)	0.57	0	100	100	17, 19, 31, 35	1 (16%)
2	H	6/10 (60%)	0.62	0	100	100	17, 19, 30, 35	1 (16%)
All	All	847/928 (91%)	0.76	102 (12%)	4	5	11, 18, 51, 100	2 (0%)

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	GLY	13.2
1	C	116	SER	9.4
1	A	222	SER	8.4
1	A	218	LYS	8.3
1	B	220	ASP	7.7

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
2	2MR	H	8[A]	13/14	0.52	0.34	30,32,35,35	13

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	2MR	H	8[B]	13/14	0.52	0.34	23,32,34,35	13
2	2MR	F	8[A]	13/14	0.53	0.45	27,38,49,53	13
2	2MR	F	8[B]	13/14	0.53	0.45	22,38,48,49	13
2	2MR	G	8[A]	13/14	0.63	0.32	19,34,38,38	13
2	2MR	G	8[B]	13/14	0.63	0.32	26,34,37,38	13
2	M3L	F	4	12/13	0.91	0.11	12,18,22,23	0
2	M3L	H	4	12/13	0.91	0.12	13,14,17,19	0
2	M3L	E	4	12/13	0.91	0.13	11,20,24,24	0
2	M3L	G	4	12/13	0.92	0.13	13,15,16,16	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	2MR	B	301	13/14	0.51	0.44	61,66,72,74	0
3	EDO	D	301	4/4	0.83	0.21	38,40,40,41	0
3	EDO	B	304	4/4	0.86	0.13	33,38,42,48	0
3	EDO	A	302	4/4	0.87	0.14	38,41,41,45	0
3	EDO	B	303	4/4	0.89	0.27	34,38,40,43	0
3	EDO	A	301	4/4	0.97	0.07	18,21,23,25	0
3	EDO	B	302	4/4	0.97	0.08	19,19,26,27	0

6.5 Other polymers (i)

There are no such residues in this entry.