Full wwPDB X-ray Structure Validation Report (i)

Jan 17, 2024 – 04:04 PM EST

PDB ID	:	8SXQ
Title	:	Crystal structure of Sel-1 repeat protein LceB from Legionella pneumophila
Authors	:	Penner, T.V.; Prehna, G.
Deposited on	:	2023-05-23
Resolution	:	2.70 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

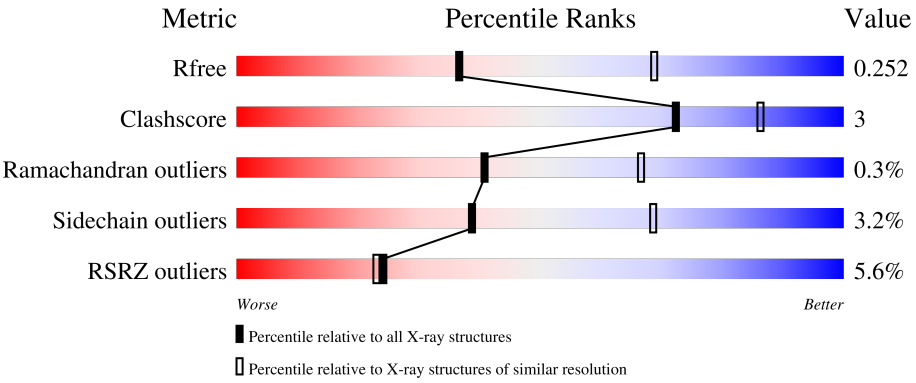
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	379	89% · 8%
1	B	379	85% 7% 8%
1	C	379	13% 77% 15% · 7%

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	MPD	A	401	-	-	-	X
2	MPD	B	402	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16148 atoms, of which 7866 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 SEL-1 repeat protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	349	Total	C	H	N	O	S	0	0	0
			5336	1747	2603	448	527	11			
1	B	348	Total	C	H	N	O	S	0	0	0
			5329	1745	2600	447	526	11			
1	C	351	Total	C	H	N	O	S	0	0	0
			5369	1758	2621	450	529	11			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q5ZVT4
A	2	GLY	-	expression tag	UNP Q5ZVT4
A	3	SER	-	expression tag	UNP Q5ZVT4
A	4	SER	-	expression tag	UNP Q5ZVT4
A	5	HIS	-	expression tag	UNP Q5ZVT4
A	6	HIS	-	expression tag	UNP Q5ZVT4
A	7	HIS	-	expression tag	UNP Q5ZVT4
A	8	HIS	-	expression tag	UNP Q5ZVT4
A	9	HIS	-	expression tag	UNP Q5ZVT4
A	10	HIS	-	expression tag	UNP Q5ZVT4
A	11	SER	-	expression tag	UNP Q5ZVT4
A	12	SER	-	expression tag	UNP Q5ZVT4
A	13	GLY	-	expression tag	UNP Q5ZVT4
A	14	LEU	-	expression tag	UNP Q5ZVT4
A	15	VAL	-	expression tag	UNP Q5ZVT4
A	16	PRO	-	expression tag	UNP Q5ZVT4
A	17	ARG	-	expression tag	UNP Q5ZVT4
A	18	GLY	-	expression tag	UNP Q5ZVT4
A	19	SER	-	expression tag	UNP Q5ZVT4
A	20	HIS	-	expression tag	UNP Q5ZVT4
A	21	MET	ALA	engineered mutation	UNP Q5ZVT4
B	1	MET	-	initiating methionine	UNP Q5ZVT4
B	2	GLY	-	expression tag	UNP Q5ZVT4

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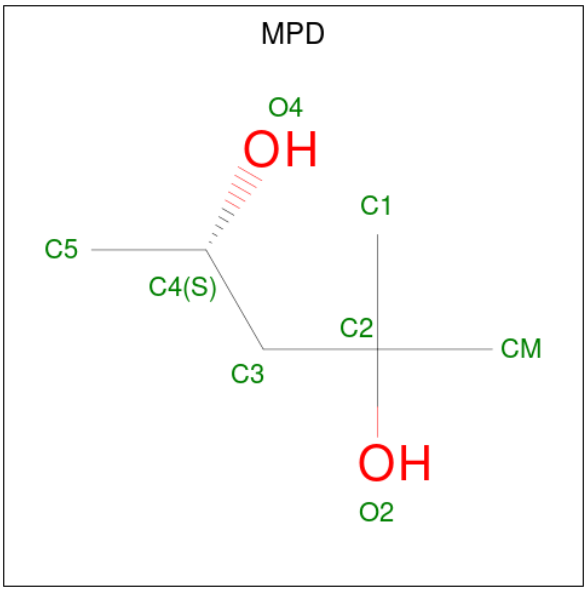
Chain	Residue	Modelled	Actual	Comment	Reference
B	3	SER	-	expression tag	UNP Q5ZVT4
B	4	SER	-	expression tag	UNP Q5ZVT4
B	5	HIS	-	expression tag	UNP Q5ZVT4
B	6	HIS	-	expression tag	UNP Q5ZVT4
B	7	HIS	-	expression tag	UNP Q5ZVT4
B	8	HIS	-	expression tag	UNP Q5ZVT4
B	9	HIS	-	expression tag	UNP Q5ZVT4
B	10	HIS	-	expression tag	UNP Q5ZVT4
B	11	SER	-	expression tag	UNP Q5ZVT4
B	12	SER	-	expression tag	UNP Q5ZVT4
B	13	GLY	-	expression tag	UNP Q5ZVT4
B	14	LEU	-	expression tag	UNP Q5ZVT4
B	15	VAL	-	expression tag	UNP Q5ZVT4
B	16	PRO	-	expression tag	UNP Q5ZVT4
B	17	ARG	-	expression tag	UNP Q5ZVT4
B	18	GLY	-	expression tag	UNP Q5ZVT4
B	19	SER	-	expression tag	UNP Q5ZVT4
B	20	HIS	-	expression tag	UNP Q5ZVT4
B	21	MET	ALA	engineered mutation	UNP Q5ZVT4
C	1	MET	-	initiating methionine	UNP Q5ZVT4
C	2	GLY	-	expression tag	UNP Q5ZVT4
C	3	SER	-	expression tag	UNP Q5ZVT4
C	4	SER	-	expression tag	UNP Q5ZVT4
C	5	HIS	-	expression tag	UNP Q5ZVT4
C	6	HIS	-	expression tag	UNP Q5ZVT4
C	7	HIS	-	expression tag	UNP Q5ZVT4
C	8	HIS	-	expression tag	UNP Q5ZVT4
C	9	HIS	-	expression tag	UNP Q5ZVT4
C	10	HIS	-	expression tag	UNP Q5ZVT4
C	11	SER	-	expression tag	UNP Q5ZVT4
C	12	SER	-	expression tag	UNP Q5ZVT4
C	13	GLY	-	expression tag	UNP Q5ZVT4
C	14	LEU	-	expression tag	UNP Q5ZVT4
C	15	VAL	-	expression tag	UNP Q5ZVT4
C	16	PRO	-	expression tag	UNP Q5ZVT4
C	17	ARG	-	expression tag	UNP Q5ZVT4
C	18	GLY	-	expression tag	UNP Q5ZVT4
C	19	SER	-	expression tag	UNP Q5ZVT4
C	20	HIS	-	expression tag	UNP Q5ZVT4
C	21	MET	ALA	engineered mutation	UNP Q5ZVT4

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 22 6 14 2	0	0
2	B	1	Total C H O 22 6 14 2	0	0
2	B	1	Total C H O 22 6 14 2	0	0

- Molecule 3 is water.

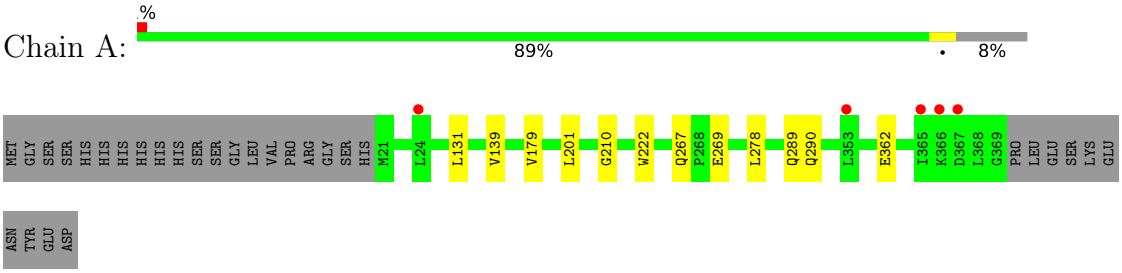
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	20	Total O 20 20	0	0
3	B	23	Total O 23 23	0	0
3	C	5	Total O 5 5	0	0

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.

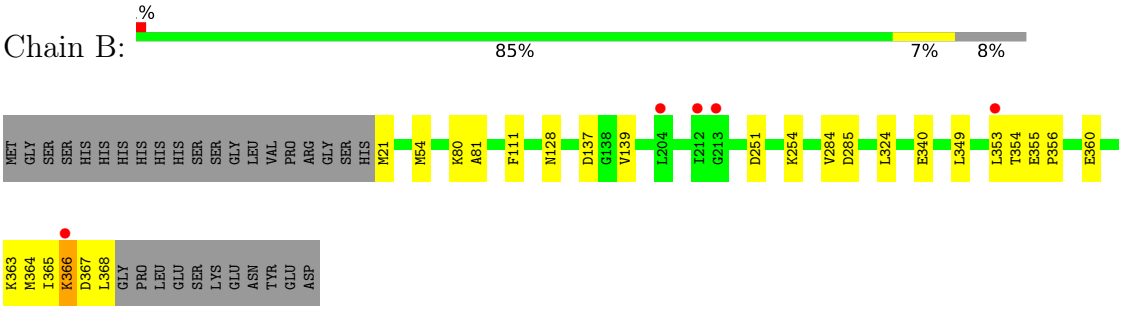
• Molecule 1: SEL-1 repeat protein

Chain A:



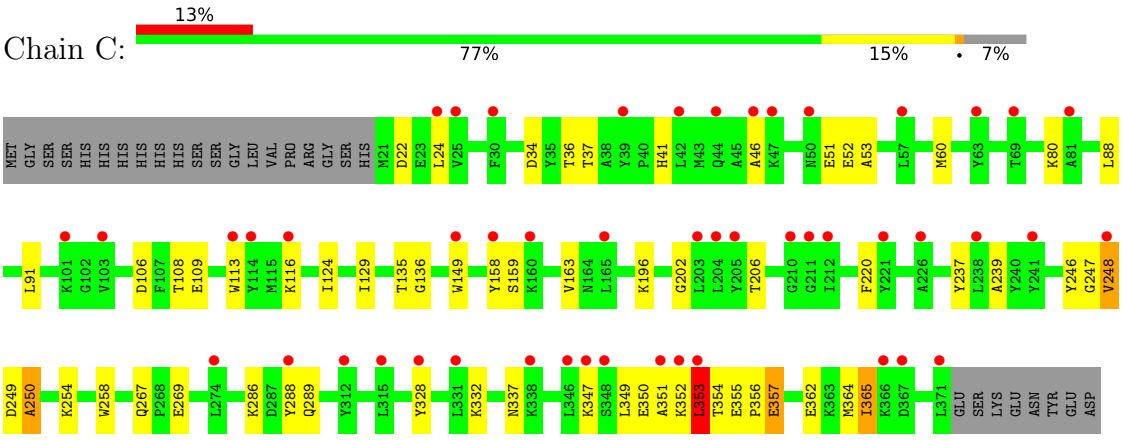
• Molecule 1: SEL-1 repeat protein

Chain B:



• Molecule 1: SEL-1 repeat protein

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	116.79Å 116.79Å 88.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.72 – 2.70 48.72 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.72-2.70) 94.5 (48.72-2.70)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.82 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.217 , 0.251 0.217 , 0.252	Depositor DCC
R_{free} test set	1849 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	86.1	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 70.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l 0.034 for h,-h-k,-l 0.035 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16148	wwPDB-VP
Average B, all atoms (Å^2)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.25	0/2800	0.38	0/3777
1	B	0.25	0/2796	0.39	0/3772
1	C	0.25	0/2816	0.40	1/3800 (0.0%)
All	All	0.25	0/8412	0.39	1/11349 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	353	LEU	CA-CB-CG	5.30	127.50	115.30

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	2733	2603	2603	5	0
1	B	2729	2600	2600	14	0
1	C	2748	2621	2621	35	1
2	A	8	14	14	1	0
2	B	16	28	28	3	0
3	A	20	0	0	0	0
3	B	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	0	0	0
All	All	8282	7866	7866	55	1

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.

All (55) 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:362:GLU:O	1:C:365:ILE:HG23	1.85	0.75
1:C:51:GLU:OE1	1:C:51:GLU:N	2.21	0.73
1:C:129:ILE:HD11	1:C:149:TRP:CG	2.24	0.72
1:C:354:THR:O	1:C:357:GLU:N	2.28	0.67
1:C:34:ASP:OD2	1:C:37:THR:OG1	2.05	0.66
1:C:24:LEU:HD23	1:C:24:LEU:O	1.97	0.63
1:A:179:VAL:HG21	1:A:210:GLY:O	1.97	0.63
1:C:91:LEU:HD21	1:C:124:ILE:HG21	1.82	0.62
1:C:106:ASP:O	1:C:108:THR:N	2.33	0.61
1:C:108:THR:HG23	1:C:109:GLU:OE1	2.01	0.60
1:C:353:LEU:O	1:C:353:LEU:HD13	2.03	0.58
1:C:247:GLY:O	1:C:248:VAL:HG13	2.04	0.56
1:A:201:LEU:HD23	1:A:222:TRP:CE2	2.43	0.54
1:C:364:MET:SD	1:C:365:ILE:N	2.81	0.54
1:C:106:ASP:O	1:C:108:THR:HG22	2.09	0.53
1:C:267:GLN:OE1	1:C:269:GLU:N	2.42	0.53
1:B:367:ASP:OD1	1:B:368:LEU:N	2.42	0.52
1:C:46:ALA:HB2	1:C:53:ALA:HB3	1.91	0.52
1:B:80:LYS:O	1:B:81:ALA:HB3	2.11	0.50
1:C:289:GLN:N	1:C:289:GLN:OE1	2.44	0.50
1:B:251:ASP:OD2	1:B:254:LYS:NZ	2.35	0.50
1:B:128:ASN:HB3	2:B:401:MPD:H51	1.95	0.49
1:C:22:ASP:OD1	1:C:41:HIS:ND1	2.46	0.49
1:C:353:LEU:O	1:C:353:LEU:HD22	2.14	0.47
1:B:365:ILE:HG22	1:B:367:ASP:H	1.79	0.47
1:C:249:ASP:O	1:C:250:ALA:HB2	2.14	0.47
1:B:111:PHE:CZ	1:B:139:VAL:HG11	2.51	0.46
1:B:137:ASP:CB	2:B:401:MPD:H13	2.46	0.46
1:C:202:GLY:O	1:C:206:THR:HG23	2.16	0.46
1:C:353:LEU:HD23	1:C:357:GLU:OE1	2.16	0.46
1:B:324:LEU:HB3	1:B:353:LEU:HD11	1.99	0.45
1:C:220:PHE:CE1	1:C:248:VAL:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:TYR:O	1:C:332:LYS:N	2.45	0.45
1:B:349:LEU:HG	1:B:353:LEU:HD13	1.99	0.45
1:C:239:ALA:HB2	1:C:258:TRP:HB2	2.00	0.44
1:B:364:MET:HG3	1:B:366:LYS:HG2	2.00	0.43
1:C:349:LEU:HD12	1:C:350:GLU:N	2.33	0.43
1:A:131:LEU:HD12	2:A:401:MPD:H52	2.00	0.43
1:B:54:MET:HB2	1:B:81:ALA:HB2	2.00	0.43
1:C:349:LEU:HD12	1:C:349:LEU:C	2.39	0.43
1:C:353:LEU:HB2	1:C:357:GLU:OE2	2.18	0.43
1:C:159:SER:O	1:C:163:VAL:HG23	2.19	0.43
1:B:284:VAL:HG22	1:B:285:ASP:N	2.34	0.42
1:B:365:ILE:HG22	1:B:367:ASP:HB2	2.01	0.42
1:C:350:GLU:O	1:C:351:ALA:HB3	2.19	0.42
1:A:278:LEU:HD13	1:A:290:GLN:HB3	2.02	0.42
1:C:129:ILE:HD12	1:C:129:ILE:C	2.40	0.41
1:A:267:GLN:OE1	1:A:269:GLU:N	2.50	0.41
1:C:364:MET:O	1:C:365:ILE:C	2.58	0.41
1:C:355:GLU:N	1:C:356:PRO:HD2	2.35	0.41
1:B:355:GLU:N	1:B:356:PRO:HD2	2.35	0.41
2:B:401:MPD:H11	2:B:401:MPD:H4	1.92	0.41
1:C:135:THR:HG22	1:C:136:GLY:N	2.36	0.41
1:C:124:ILE:HD13	1:C:158:TYR:CZ	2.57	0.40
1:C:88:LEU:HD22	1:C:88:LEU:N	2.37	0.40

All (1) 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)
1:C:36:THR:OG1	1:C:286:LYS:NZ[2_654]	2.16	0.04

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	347/379 (92%)	335 (96%)	12 (4%)	0	100 100
1	B	346/379 (91%)	328 (95%)	18 (5%)	0	100 100
1	C	349/379 (92%)	315 (90%)	31 (9%)	3 (1%)	17 40
All	All	1042/1137 (92%)	978 (94%)	61 (6%)	3 (0%)	41 66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	250	ALA
1	C	353	LEU
1	C	365	ILE

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	259/286 (91%)	256 (99%)	3 (1%)	71 88
1	B	259/286 (91%)	253 (98%)	6 (2%)	50 78
1	C	261/286 (91%)	245 (94%)	16 (6%)	18 41
All	All	779/858 (91%)	754 (97%)	25 (3%)	39 68

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	VAL
1	A	289	GLN
1	A	362	GLU
1	B	21	MET
1	B	340	GLU
1	B	354	THR
1	B	360	GLU
1	B	363	LYS
1	B	366	LYS
1	C	52	GLU

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Mol	Chain	Res	Type
1	C	60	MET
1	C	80	LYS
1	C	113	TRP
1	C	116	LYS
1	C	196	LYS
1	C	237	TYR
1	C	246	TYR
1	C	248	VAL
1	C	254	LYS
1	C	288	TYR
1	C	337	ASN
1	C	347	LYS
1	C	352	LYS
1	C	353	LEU
1	C	357	GLU

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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MPD	B	401	-	7,7,7	0.26	0	9,10,10	0.47	0
2	MPD	A	401	-	7,7,7	0.28	0	9,10,10	0.19	0
2	MPD	B	402	-	7,7,7	0.27	0	9,10,10	0.23	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
2	MPD	B	401	-	-	2/5/5/5	-
2	MPD	A	401	-	-	0/5/5/5	-
2	MPD	B	402	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	MPD	C2-C3-C4-O4
2	B	401	MPD	C2-C3-C4-C5
2	B	402	MPD	C2-C3-C4-C5
2	B	402	MPD	C2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	MPD	3	0
2	A	401	MPD	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	349/379 (92%)	0.25	5 (1%) 75 77	69, 89, 118, 181	0
1	B	348/379 (91%)	0.30	5 (1%) 75 77	71, 94, 127, 186	0
1	C	351/379 (92%)	0.82	49 (13%) 2 1	100, 144, 199, 234	0
All	All	1048/1137 (92%)	0.45	59 (5%) 24 23	69, 103, 175, 234	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	ILE	7.7
1	C	42	LEU	5.4
1	C	24	LEU	5.3
1	C	210	GLY	5.2
1	C	113	TRP	4.9
1	B	366	LYS	4.5
1	A	366	LYS	4.3
1	C	366	LYS	4.0
1	C	328	TYR	3.9
1	C	211	GLY	3.9
1	C	312	TYR	3.7
1	B	213	GLY	3.7
1	C	39	TYR	3.6
1	C	149	TRP	3.4
1	C	346	LEU	3.4
1	A	367	ASP	3.3
1	C	103	VAL	3.2
1	C	50	ASN	3.2
1	C	241	TYR	3.2
1	C	351	ALA	3.1
1	C	57	LEU	3.1
1	C	248	VAL	3.0
1	C	315	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	367	ASP	3.0
1	C	212	ILE	2.9
1	A	24	LEU	2.9
1	C	25	VAL	2.9
1	C	348	SER	2.8
1	C	205	TYR	2.7
1	C	81	ALA	2.7
1	C	338	LYS	2.7
1	B	353	LEU	2.7
1	C	160	LYS	2.7
1	C	371	LEU	2.6
1	A	365	ILE	2.6
1	C	331	LEU	2.6
1	C	116	LYS	2.5
1	C	69	THR	2.5
1	C	30	PHE	2.5
1	A	353	LEU	2.4
1	B	204	LEU	2.4
1	C	353	LEU	2.3
1	C	158	TYR	2.3
1	C	63	TYR	2.3
1	C	203	LEU	2.3
1	C	114	TYR	2.3
1	C	44	GLN	2.2
1	C	352	LYS	2.2
1	C	226	ALA	2.2
1	C	165	LEU	2.1
1	C	47	LYS	2.1
1	C	101	LYS	2.1
1	C	204	LEU	2.1
1	C	221	TYR	2.1
1	C	288	TYR	2.1
1	C	46	ALA	2.1
1	C	347	LYS	2.0
1	C	274	LEU	2.0
1	C	238	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MPD	B	402	8/8	0.75	0.66	99,127,139,163	0
2	MPD	A	401	8/8	0.78	0.50	88,108,117,126	0
2	MPD	B	401	8/8	0.86	0.36	84,107,127,127	0

6.5 Other polymers (i)

There are no such residues in this entry.