Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 01:07 AM EDT

PDB ID	:	5WFL
Title	:	Kelch domain of human Keap1 in open unliganded conformation
Authors	:	Carolan, J.P.; Lynch, A.J.; Allen, K.N.
Deposited on	:	2017-07-12
Resolution	:	1.93 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:

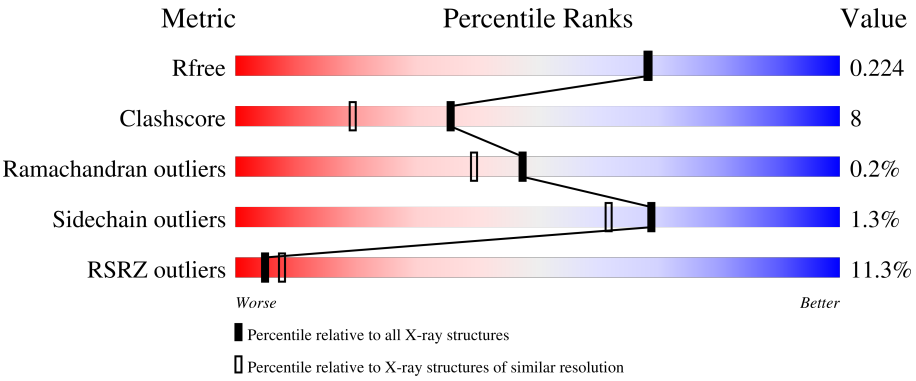
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	336	17% 67% 16% · 16%
1	B	336	?% 80% 6% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4577 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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2170	1351	392	412	15			
1	B	290	Total	C	N	O	S	0	1	0
			2229	1385	405	423	16			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	MET	-	initiating methionine	UNP Q14145
A	290	GLY	-	expression tag	UNP Q14145
A	291	SER	-	expression tag	UNP Q14145
A	292	SER	-	expression tag	UNP Q14145
A	293	HIS	-	expression tag	UNP Q14145
A	294	HIS	-	expression tag	UNP Q14145
A	295	HIS	-	expression tag	UNP Q14145
A	296	HIS	-	expression tag	UNP Q14145
A	297	HIS	-	expression tag	UNP Q14145
A	298	HIS	-	expression tag	UNP Q14145
A	299	SER	-	expression tag	UNP Q14145
A	300	SER	-	expression tag	UNP Q14145
A	301	GLY	-	expression tag	UNP Q14145
A	302	GLY	-	expression tag	UNP Q14145
A	303	GLU	-	expression tag	UNP Q14145
A	304	ASN	-	expression tag	UNP Q14145
A	305	LEU	-	expression tag	UNP Q14145
A	306	TYR	-	expression tag	UNP Q14145
A	307	PHE	-	expression tag	UNP Q14145
A	308	GLN	-	expression tag	UNP Q14145
A	309	GLY	-	expression tag	UNP Q14145
A	310	HIS	-	expression tag	UNP Q14145
A	311	MET	-	expression tag	UNP Q14145
A	319	SER	CYS	engineered mutation	UNP Q14145
A	540	ALA	GLU	engineered mutation	UNP Q14145

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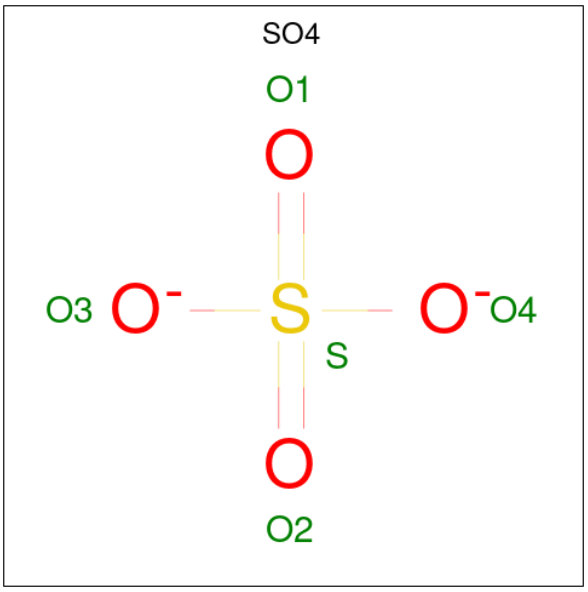
Chain	Residue	Modelled	Actual	Comment	Reference
A	542	ALA	GLU	engineered mutation	UNP Q14145
A	613	SER	CYS	engineered mutation	UNP Q14145
A	622	SER	CYS	engineered mutation	UNP Q14145
A	624	SER	CYS	engineered mutation	UNP Q14145
B	289	MET	-	initiating methionine	UNP Q14145
B	290	GLY	-	expression tag	UNP Q14145
B	291	SER	-	expression tag	UNP Q14145
B	292	SER	-	expression tag	UNP Q14145
B	293	HIS	-	expression tag	UNP Q14145
B	294	HIS	-	expression tag	UNP Q14145
B	295	HIS	-	expression tag	UNP Q14145
B	296	HIS	-	expression tag	UNP Q14145
B	297	HIS	-	expression tag	UNP Q14145
B	298	HIS	-	expression tag	UNP Q14145
B	299	SER	-	expression tag	UNP Q14145
B	300	SER	-	expression tag	UNP Q14145
B	301	GLY	-	expression tag	UNP Q14145
B	302	GLY	-	expression tag	UNP Q14145
B	303	GLU	-	expression tag	UNP Q14145
B	304	ASN	-	expression tag	UNP Q14145
B	305	LEU	-	expression tag	UNP Q14145
B	306	TYR	-	expression tag	UNP Q14145
B	307	PHE	-	expression tag	UNP Q14145
B	308	GLN	-	expression tag	UNP Q14145
B	309	GLY	-	expression tag	UNP Q14145
B	310	HIS	-	expression tag	UNP Q14145
B	311	MET	-	expression tag	UNP Q14145
B	319	SER	CYS	engineered mutation	UNP Q14145
B	540	ALA	GLU	engineered mutation	UNP Q14145
B	542	ALA	GLU	engineered mutation	UNP Q14145
B	613	SER	CYS	engineered mutation	UNP Q14145
B	622	SER	CYS	engineered mutation	UNP Q14145
B	624	SER	CYS	engineered mutation	UNP Q14145

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

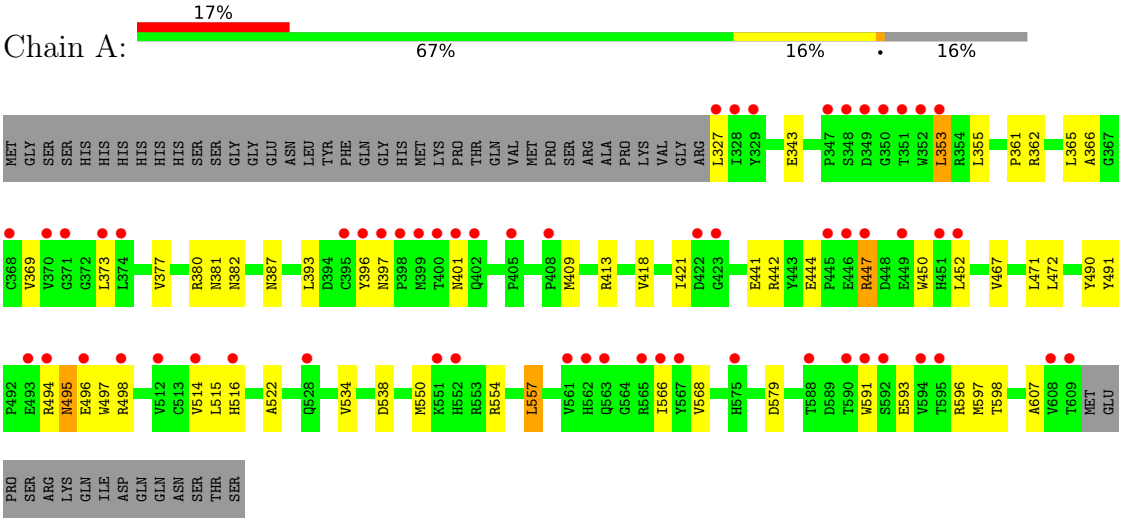
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	30	Total O 30 30	0	0
3	B	123	Total O 123 123	0	0

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.

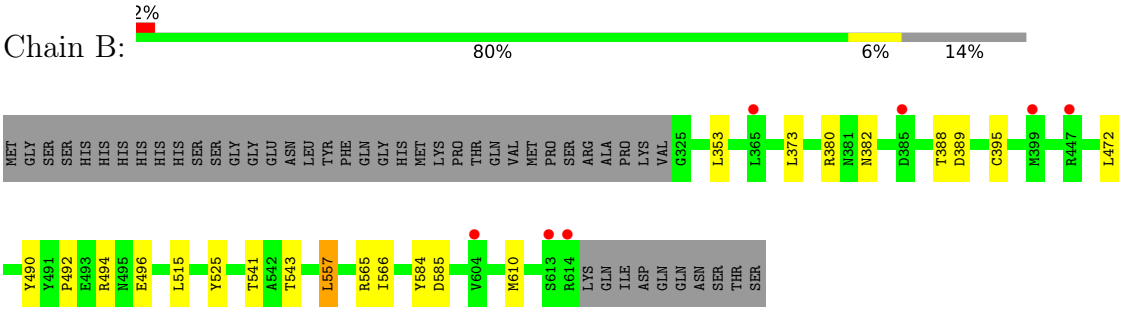
• Molecule 1: Kelch-like ECH-associated protein 1

Chain A:



• Molecule 1: Kelch-like ECH-associated protein 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.31Å 68.73Å 77.17Å 90.00° 117.73° 90.00°	Depositor
Resolution (Å)	35.92 – 1.93 35.92 – 1.79	Depositor EDS
% Data completeness (in resolution range)	97.3 (35.92-1.93) 90.5 (35.92-1.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.13 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.197 , 0.222 0.198 , 0.224	Depositor DCC
R_{free} test set	2017 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4577	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% 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: SO4

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	0.61	0/2223	0.81	1/3029 (0.0%)
1	B	0.70	0/2286	0.82	1/3112 (0.0%)
All	All	0.66	0/4509	0.81	2/6141 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	538	ASP	CB-CG-OD1	5.56	123.30	118.30
1	B	353	LEU	CA-CB-CG	5.54	128.03	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	2170	0	2063	54	1
1	B	2229	0	2127	18	1
2	A	15	0	0	0	0
2	B	10	0	0	0	0
3	A	30	0	0	0	0
3	B	123	0	0	0	0
All	All	4577	0	4190	70	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 8.

All (70) 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:494:ARG:HG2	1:A:496:GLU:HG2	1.16	1.10
1:A:498:ARG:HH11	1:A:498:ARG:HA	1.24	0.98
1:A:494:ARG:HG2	1:A:496:GLU:CG	1.91	0.98
1:A:494:ARG:CG	1:A:496:GLU:HG2	1.93	0.98
1:A:396:TYR:OH	1:A:401:ASN:OD1	1.90	0.89
1:A:497:TRP:O	1:A:498:ARG:NH1	2.14	0.80
1:A:522:ALA:HB1	1:A:550:MET:HE3	1.68	0.75
1:A:498:ARG:HA	1:A:498:ARG:NH1	2.00	0.74
1:A:471:LEU:HD22	1:A:491:TYR:CD1	2.24	0.73
1:A:557:LEU:HD23	1:A:557:LEU:H	1.62	0.63
1:B:557:LEU:H	1:B:557:LEU:HD23	1.64	0.63
1:A:441:GLU:HB3	1:A:452:LEU:HD23	1.79	0.62
1:A:550:MET:CE	1:A:568:VAL:HG11	2.31	0.60
1:B:541:THR:O	1:B:543:THR:HG23	2.02	0.60
1:B:565:ARG:HH11	1:B:585:ASP:HB2	1.68	0.59
1:A:494:ARG:O	1:A:495:ASN:C	2.41	0.59
1:B:565:ARG:NH1	1:B:585:ASP:CG	2.57	0.59
1:A:494:ARG:CG	1:A:496:GLU:CG	2.66	0.56
1:A:444:GLU:OE1	1:A:447:ARG:HD2	2.06	0.55
1:A:516:HIS:HD2	1:B:494:ARG:NH1	2.04	0.55
1:A:353:LEU:HD21	1:A:355:LEU:HD21	1.87	0.55
1:A:471:LEU:CD2	1:A:491:TYR:CD1	2.90	0.55
1:B:515:LEU:HD22	1:B:566:ILE:HG13	1.89	0.55
1:A:382:ASN:OD1	1:A:387:ASN:ND2	2.35	0.55
1:B:565:ARG:HH12	1:B:585:ASP:CG	2.09	0.55
1:A:579:ASP:O	1:A:597:MET:HG3	2.09	0.53
1:A:554:ARG:HG3	1:A:557:LEU:HD22	1.89	0.53
1:B:380:ARG:NE	1:B:382:ASN:OD1	2.41	0.53
1:B:565:ARG:NH1	1:B:585:ASP:HB2	2.24	0.53
1:A:353:LEU:CD2	1:A:355:LEU:HD21	2.39	0.53
1:A:444:GLU:HB3	1:A:447:ARG:CZ	2.40	0.52
1:A:380:ARG:NH2	1:A:387:ASN:HB3	2.25	0.52
1:A:494:ARG:HG2	1:A:494:ARG:O	2.10	0.51
1:B:566:ILE:HB	1:B:584:TYR:HB3	1.93	0.51
1:A:498:ARG:HH11	1:A:498:ARG:CA	2.10	0.51
1:A:471:LEU:HD22	1:A:491:TYR:CE1	2.46	0.51
1:A:409:MET:SD	1:A:413:ARG:HD2	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:HIS:CD2	1:B:494:ARG:NH1	2.80	0.49
1:A:366:ALA:HB3	1:A:418:VAL:HG13	1.95	0.49
1:A:369:VAL:HG23	1:A:607:ALA:HB1	1.95	0.49
1:A:498:ARG:NH1	1:A:498:ARG:CA	2.74	0.49
1:A:491:TYR:HB2	1:A:494:ARG:HB3	1.94	0.48
1:A:327:LEU:HD12	1:A:327:LEU:N	2.29	0.48
1:A:472:LEU:HB3	1:A:490:TYR:HB3	1.94	0.48
1:B:472:LEU:HB3	1:B:490:TYR:HB3	1.95	0.48
1:A:396:TYR:CE1	1:A:401:ASN:HA	2.49	0.48
1:A:377:VAL:HG12	1:A:409:MET:CE	2.44	0.47
1:A:343:GLU:OE2	1:A:598:THR:HG21	2.14	0.47
1:A:444:GLU:HB3	1:A:447:ARG:NE	2.30	0.47
1:A:361:PRO:O	1:A:362:ARG:HG3	2.15	0.47
1:A:365:LEU:HD23	1:A:365:LEU:H	1.79	0.46
1:A:467:VAL:O	1:A:514:VAL:HG21	2.15	0.46
1:B:565:ARG:NH1	1:B:585:ASP:CB	2.79	0.46
1:A:534:VAL:HG21	1:A:591:TRP:CZ2	2.52	0.45
1:B:494:ARG:HB3	1:B:496:GLU:HG2	1.97	0.45
1:A:421:ILE:HD11	1:A:472:LEU:HB2	1.99	0.45
1:A:534:VAL:HG21	1:A:591:TRP:HZ2	1.81	0.44
1:A:515:LEU:HD22	1:A:566:ILE:HG13	2.00	0.43
1:A:373:LEU:HD22	1:A:397:ASN:HA	2.01	0.43
1:A:393:LEU:HD22	1:A:450:TRP:CZ2	2.54	0.43
1:A:494:ARG:O	1:A:496:GLU:N	2.52	0.42
1:B:373:LEU:HB3	1:B:395:CYS:SG	2.60	0.42
1:A:442:ARG:HH11	1:A:444:GLU:HG2	1.84	0.42
1:A:550:MET:CE	1:A:568:VAL:HG21	2.50	0.41
1:A:377:VAL:HG12	1:A:409:MET:HE3	2.02	0.41
1:B:373:LEU:HD13	1:B:395:CYS:SG	2.61	0.41
1:A:491:TYR:O	1:A:495:ASN:N	2.53	0.41
1:B:490:TYR:CE2	1:B:492:PRO:HA	2.55	0.40
1:A:593:GLU:OE1	1:A:596:ARG:NH2	2.54	0.40
1:B:388:THR:HG22	1:B:389:ASP:O	2.21	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:A:387:ASN:OD1	1:B:525:TYR:OH[1_556]	2.13	0.07

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	281/336 (84%)	267 (95%)	13 (5%)	1 (0%)	34 24
1	B	289/336 (86%)	282 (98%)	7 (2%)	0	100 100
All	All	570/672 (85%)	549 (96%)	20 (4%)	1 (0%)	47 39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	495	ASN

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	228/275 (83%)	224 (98%)	4 (2%)	59 47
1	B	235/275 (86%)	233 (99%)	2 (1%)	78 75
All	All	463/550 (84%)	457 (99%)	6 (1%)	69 62

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	353	LEU
1	A	381	ASN
1	A	447	ARG
1	A	557	LEU
1	B	557	LEU

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Mol	Chain	Res	Type
1	B	610	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	ASN
1	A	516	HIS
1	A	517	ASN

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)

5 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	SO4	A	702	-	4,4,4	0.16	0	6,6,6	0.74	0
2	SO4	B	702	-	4,4,4	0.15	0	6,6,6	0.36	0
2	SO4	A	701	1	4,4,4	0.35	0	6,6,6	0.59	0
2	SO4	A	703	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	B	701	-	4,4,4	0.32	0	6,6,6	0.56	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	283/336 (84%)	1.09	58 (20%) 1 1	27, 64, 107, 140	0
1	B	290/336 (86%)	0.06	7 (2%) 59 66	28, 35, 61, 107	0
All	All	573/672 (85%)	0.57	65 (11%) 5 8	27, 45, 101, 140	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	494	ARG	9.3
1	A	353	LEU	7.4
1	A	401	ASN	7.2
1	A	351	THR	7.0
1	A	371	GLY	6.4
1	A	567	TYR	5.8
1	A	349	ASP	5.0
1	A	402	GLN	4.9
1	A	423	GLY	4.9
1	A	446	GLU	4.9
1	A	327	LEU	4.7
1	B	613	SER	4.7
1	A	447	ARG	4.6
1	A	563	GLN	4.5
1	A	588	THR	4.5
1	A	399	MET	4.4
1	A	348	SER	4.4
1	A	562	HIS	4.1
1	A	594	VAL	4.1
1	A	493	GLU	4.0
1	A	396	TYR	3.9
1	A	400	THR	3.7
1	B	614	ARG	3.7
1	A	565	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	398	PRO	3.6
1	A	347	PRO	3.5
1	A	328	ILE	3.5
1	A	452	LEU	3.4
1	A	352	TRP	3.3
1	A	373	LEU	3.2
1	A	551	LYS	3.2
1	A	329	TYR	3.2
1	A	608	VAL	3.0
1	A	552	HIS	3.0
1	A	590	THR	3.0
1	A	449	GLU	2.9
1	A	575	HIS	2.9
1	A	395	CYS	2.9
1	B	604	VAL	2.9
1	A	445	PRO	2.7
1	A	374	LEU	2.7
1	A	405	PRO	2.6
1	A	496	GLU	2.5
1	A	514	VAL	2.5
1	B	399	MET	2.5
1	A	498	ARG	2.5
1	A	591	TRP	2.5
1	A	566	ILE	2.4
1	A	595	THR	2.4
1	A	451	HIS	2.4
1	B	365	LEU	2.4
1	A	516	HIS	2.4
1	A	592	SER	2.3
1	A	512	VAL	2.2
1	A	609	THR	2.2
1	B	385	ASP	2.2
1	A	422	ASP	2.2
1	A	528	GLN	2.2
1	A	350	GLY	2.1
1	A	368	CYS	2.1
1	B	447	ARG	2.1
1	A	370	VAL	2.1
1	A	561	VAL	2.1
1	A	397	ASN	2.1
1	A	408	PRO	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	SO4	A	701	5/5	0.85	0.32	70,76,80,80	0
2	SO4	A	703	5/5	0.88	0.16	122,122,123,124	0
2	SO4	B	701	5/5	0.94	0.10	54,54,63,65	0
2	SO4	A	702	5/5	0.95	0.10	66,68,71,72	0
2	SO4	B	702	5/5	0.97	0.11	76,76,77,82	0

6.5 Other polymers (i)

There are no such residues in this entry.