Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 03:57 PM EDT

PDB ID	:	5V4B
Title	:	Crystal structure of the Skp1-FBXW7-DISC1 complex
Authors	:	Li, Y.; Baillie, G.S.; Hao, B.
Deposited on	:	2017-03-08
Resolution	:	2.60 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 (i)) were used in the production of this report:

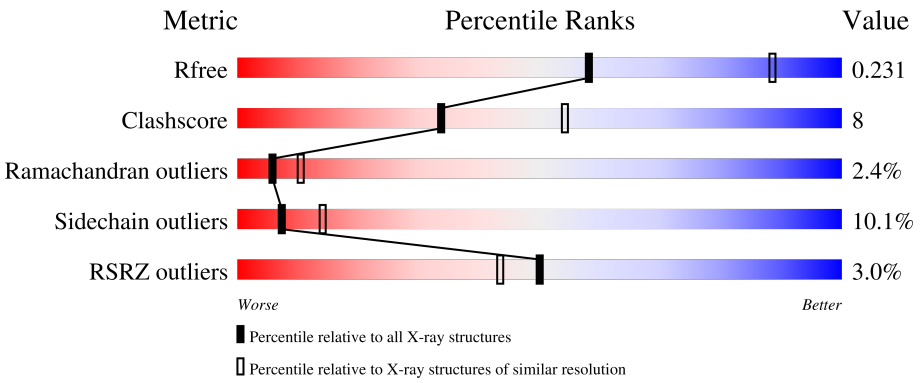
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	149	8%, 80%, 14%, • •
2	B	444	%, 73%, 21%, 5% •
3	C	15	13%, 47%, 20%, 33%

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
3	SEP	C	202	-	-	-	X
5	IMD	B	2810	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4910 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 S-phase kinase-associated protein 1,S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	146	1092	697	175	215	5	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1002	ALA	PRO	engineered mutation	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	GLU	deletion	UNP P63208
A	?	-	GLY	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	1070	GLY	-	linker	UNP P63208
A	1071	GLY	-	linker	UNP P63208
A	1072	SER	-	linker	UNP P63208
A	1073	GLY	-	linker	UNP P63208
A	1129	ALA	GLY	conflict	UNP P63208

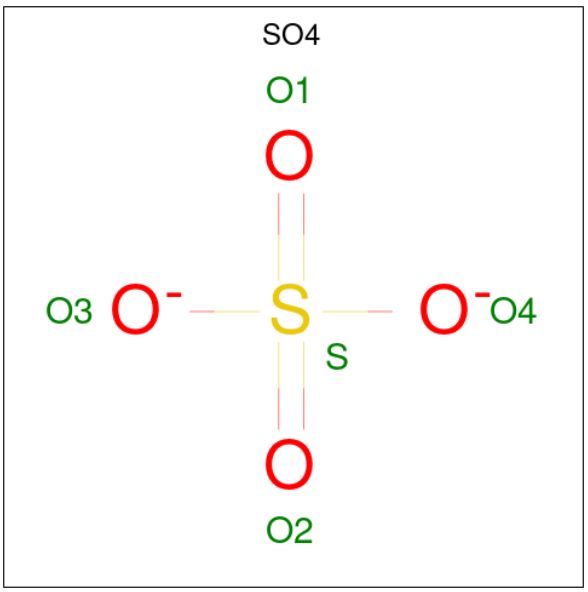
- Molecule 2 is a protein called F-box/WD repeat-containing protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	444	3525	2210	639	654	22	0	5	0

- Molecule 3 is a protein called DISC1 peptide.

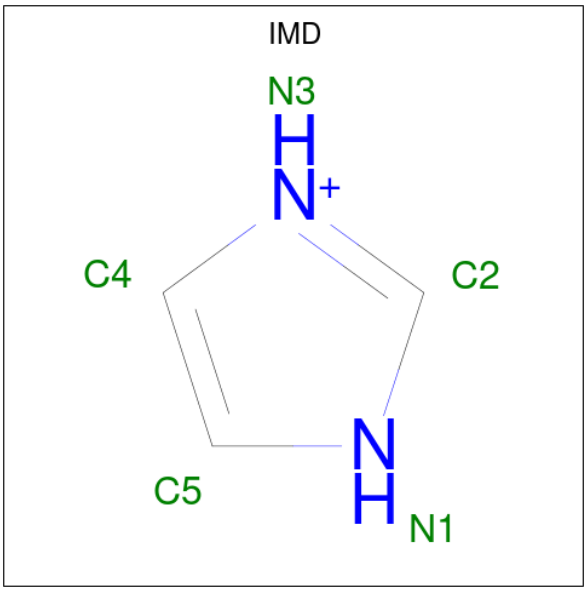
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	10	76	44	10	20	2	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
5	B	1	5	3	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	8	8	8	0	0
			Total	O		
6	B	154	154	154	0	0
			Total	O		
6	C	5	5	5	0	0

3 Residue-property plots (i)

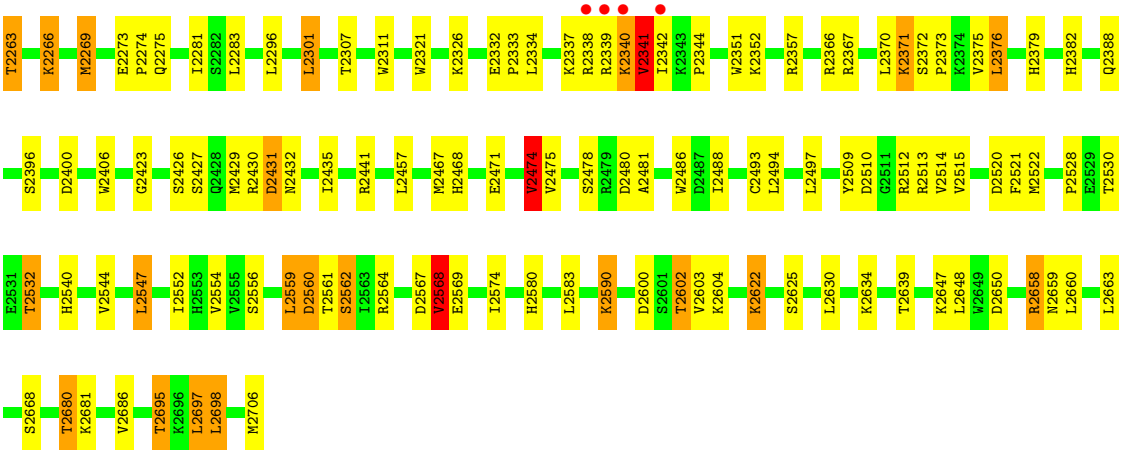
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: S-phase kinase-associated protein 1,S-phase kinase-associated protein 1

Chain A:

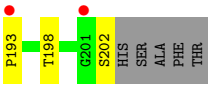
• Molecule 2: F-box/WD repeat-containing protein 7

Chain B:



• Molecule 3: DISC1 peptide

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	233.51Å 233.51Å 108.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.93 – 2.60 42.89 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.93-2.60) 99.8 (42.89-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.184 , 0.219 0.194 , 0.231	Depositor DCC
R_{free} test set	2328 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.1	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	0.94	EDS
Total number of atoms	4910	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: SEP, IMD, SO4, TPO

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	0.52	0/1111	0.69	0/1517
2	B	0.81	0/3596	0.96	6/4875 (0.1%)
3	C	0.81	0/58	1.21	1/79 (1.3%)
All	All	0.75	0/4765	0.91	7/6471 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	193	PRO	CA-N-CD	-9.02	98.88	111.50
2	B	2658	ARG	NE-CZ-NH2	-8.63	115.98	120.30
2	B	2658	ARG	NE-CZ-NH1	7.68	124.14	120.30
2	B	2474	VAL	CB-CA-C	-7.36	97.42	111.40
2	B	2568	VAL	CB-CA-C	-5.63	100.71	111.40
2	B	2697	LEU	CA-CB-CG	5.57	128.11	115.30
2	B	2510	ASP	CB-CG-OD1	5.02	122.82	118.30

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	1092	0	1033	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3525	0	3482	68	0
3	C	76	0	61	0	0
4	B	45	0	0	1	0
5	B	5	0	5	0	0
6	A	8	0	0	1	0
6	B	154	0	0	0	0
6	C	5	0	0	0	0
All	All	4910	0	4581	79	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 8.

All (79) 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)
2:B:2430:ARG:NH2	2:B:2471:GLU:O	2.00	0.95
2:B:2468:HIS:HD2	2:B:2509:TYR:H	1.33	0.77
2:B:2340:LYS:HA	2:B:2341:VAL:HG22	1.70	0.72
2:B:2513[B]:ARG:HH22	2:B:2569:GLU:CD	1.95	0.71
2:B:2680:THR:HG22	2:B:2681:LYS:HG3	1.74	0.68
2:B:2379:HIS:HE1	2:B:2396:SER:OG	1.75	0.68
2:B:2382:HIS:O	2:B:2695:THR:HG21	1.94	0.67
2:B:2474:VAL:HG22	2:B:2488:ILE:HD11	1.78	0.66
2:B:2530:THR:OG1	2:B:2532:THR:HG23	1.97	0.64
2:B:2486:TRP:CZ3	2:B:2493:CYS:HB2	2.33	0.64
2:B:2600:ASP:OD1	2:B:2602:THR:HG22	2.01	0.61
2:B:2379:HIS:HD2	2:B:2400:ASP:OD2	1.84	0.60
2:B:2480:ASP:O	2:B:2481:ALA:HB3	2.00	0.60
2:B:2334:LEU:HD22	2:B:2357:ARG:HD3	1.85	0.58
2:B:2366[A]:ARG:O	2:B:2658:ARG:HD2	2.06	0.56
1:A:1095:VAL:HG13	1:A:1099:THR:HB	1.87	0.56
2:B:2376:LEU:N	2:B:2376:LEU:HD23	2.21	0.56
1:A:1090:GLN:CB	6:A:1206:HOH:O	2.54	0.55
2:B:2530:THR:OG1	2:B:2532:THR:CG2	2.55	0.55
1:A:1141:ILE:HD13	2:B:2307:THR:CG2	2.39	0.53
2:B:2560:ASP:CB	2:B:2562:SER:OG	2.57	0.52
2:B:2567:ASP:HB2	2:B:2574:ILE:HD11	1.92	0.52
2:B:2622:LYS:HB2	2:B:2622:LYS:NZ	2.26	0.51
1:A:1095:VAL:CG1	1:A:1099:THR:HB	2.41	0.50
1:A:1130:LYS:HB3	1:A:1134:GLU:HB2	1.92	0.50
2:B:2540:HIS:HE1	2:B:2556:SER:OG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1107:ALA:HB2	1:A:1115:LEU:HD13	1.94	0.50
1:A:1141:ILE:HD13	2:B:2307:THR:HG21	1.93	0.50
2:B:2281:ILE:HG12	2:B:2311:TRP:CZ2	2.47	0.49
1:A:1085:ILE:HD11	1:A:1118:VAL:HG13	1.95	0.49
2:B:2514:VAL:HG23	2:B:2528:PRO:HG3	1.95	0.49
2:B:2281:ILE:HG12	2:B:2311:TRP:CE2	2.49	0.48
2:B:2423:GLY:N	4:B:2806:SO4:O1	2.39	0.48
2:B:2515:VAL:HG12	2:B:2547:LEU:HD11	1.94	0.48
2:B:2530:THR:O	2:B:2532:THR:HG22	2.14	0.48
2:B:2559:LEU:C	2:B:2561:THR:H	2.17	0.48
2:B:2371:LYS:HE3	2:B:2373:PRO:HA	1.96	0.47
2:B:2426:SER:HB2	2:B:2467:MET:HG2	1.96	0.47
2:B:2468:HIS:CD2	2:B:2509:TYR:H	2.22	0.47
2:B:2630:LEU:HD12	2:B:2630:LEU:C	2.34	0.47
2:B:2388:GLN:HB3	2:B:2429:MET:HE1	1.97	0.47
2:B:2457:LEU:HB3	2:B:2486:TRP:CZ3	2.49	0.47
2:B:2468:HIS:HD2	2:B:2509:TYR:N	2.06	0.47
2:B:2474:VAL:CG2	2:B:2488:ILE:HD11	2.45	0.47
2:B:2333:PRO:HD3	2:B:2351:TRP:CH2	2.50	0.47
2:B:2340:LYS:CA	2:B:2341:VAL:HG22	2.42	0.46
2:B:2321:TRP:CE2	2:B:2352:LYS:HG3	2.50	0.46
2:B:2480:ASP:O	2:B:2481:ALA:CB	2.63	0.46
2:B:2269:MET:HA	2:B:2269:MET:HE3	1.98	0.45
2:B:2540:HIS:CE1	2:B:2564:ARG:HD2	2.51	0.45
1:A:1085:ILE:HD13	1:A:1086:PRO:HD2	1.97	0.45
2:B:2263:THR:HA	2:B:2266:LYS:HB2	1.97	0.45
2:B:2647:LYS:NZ	2:B:2659:ASN:HD21	2.14	0.45
2:B:2590:LYS:HE2	2:B:2590:LYS:HB2	1.72	0.45
2:B:2296:LEU:HB2	2:B:2301:LEU:HD13	1.99	0.44
1:A:1141:ILE:HG21	2:B:2307:THR:HG22	2.00	0.44
2:B:2366[B]:ARG:NH2	2:B:2650:ASP:OD2	2.33	0.44
2:B:2339:ARG:HA	2:B:2340:LYS:CB	2.48	0.44
2:B:2376:LEU:HB3	2:B:2406:TRP:CZ3	2.53	0.43
2:B:2488:ILE:HD13	2:B:2488:ILE:HA	1.72	0.43
2:B:2520:ASP:OD1	2:B:2522:MET:HB2	2.18	0.42
1:A:1125:ASN:HA	1:A:1128:LYS:HG2	2.01	0.42
2:B:2520:ASP:O	2:B:2521:PHE:HB2	2.18	0.42
1:A:1083:ASP:O	1:A:1084:ASP:CB	2.68	0.42
2:B:2512:ARG:HG2	2:B:2513[B]:ARG:HD2	2.02	0.42
2:B:2521:PHE:N	2:B:2521:PHE:CD2	2.88	0.42
2:B:2333:PRO:HD3	2:B:2351:TRP:CZ2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:PRO:HD2	1:A:1109:TYR:OH	2.20	0.41
1:A:1157:ASN:OD1	2:B:2352:LYS:NZ	2.49	0.41
2:B:2512:ARG:CZ	2:B:2513[B]:ARG:NH1	2.83	0.41
2:B:2273:GLU:N	2:B:2274:PRO:HD3	2.36	0.41
2:B:2375:VAL:C	2:B:2376:LEU:HD23	2.40	0.41
2:B:2603:VAL:HG21	2:B:2639:THR:HG21	2.02	0.41
1:A:1103:LEU:HD23	1:A:1103:LEU:HA	1.95	0.41
2:B:2686:VAL:HG21	2:B:2698:LEU:HD22	2.03	0.40
2:B:2475:VAL:HG23	2:B:2509:TYR:CD2	2.56	0.40
2:B:2427:SER:HA	2:B:2435:ILE:O	2.21	0.40
2:B:2552:ILE:O	2:B:2568:VAL:HG22	2.21	0.40
2:B:2580:HIS:CE1	2:B:2604:LYS:HG3	2.56	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	144/149 (97%)	127 (88%)	10 (7%)	7 (5%)	2 2
2	B	447/444 (101%)	416 (93%)	24 (5%)	7 (2%)	9 19
3	C	7/15 (47%)	7 (100%)	0	0	100 100
All	All	598/608 (98%)	550 (92%)	34 (6%)	14 (2%)	6 11

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1083	ASP
1	A	1095	VAL
1	A	1082	THR
2	B	2338	ARG
2	B	2431	ASP

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Mol	Chain	Res	Type
1	A	1072	SER
2	B	2344	PRO
2	B	2560	ASP
1	A	1141	ILE
1	A	1068	ASP
1	A	1084	ASP
2	B	2340	LYS
2	B	2342	ILE
2	B	2341	VAL

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	112/133 (84%)	105 (94%)	7 (6%)	18 36
2	B	390/394 (99%)	345 (88%)	45 (12%)	5 10
3	C	7/11 (64%)	7 (100%)	0	100 100
All	All	509/538 (95%)	457 (90%)	52 (10%)	7 14

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1003	SER
1	A	1015	GLU
1	A	1031	LEU
1	A	1054	ILE
1	A	1085	ILE
1	A	1089	ASP
1	A	1115	LEU
2	B	2263	THR
2	B	2266	LYS
2	B	2269	MET
2	B	2275	GLN
2	B	2283	LEU
2	B	2301	LEU

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Mol	Chain	Res	Type
2	B	2326	LYS
2	B	2332	GLU
2	B	2337	LYS
2	B	2341	VAL
2	B	2367	ARG
2	B	2370	LEU
2	B	2371	LYS
2	B	2372[A]	SER
2	B	2372[B]	SER
2	B	2376	LEU
2	B	2431	ASP
2	B	2432	ASN
2	B	2441	ARG
2	B	2474	VAL
2	B	2478	SER
2	B	2494	LEU
2	B	2497	LEU
2	B	2532	THR
2	B	2544	VAL
2	B	2547	LEU
2	B	2554	VAL
2	B	2559	LEU
2	B	2562	SER
2	B	2568	VAL
2	B	2583	LEU
2	B	2590	LYS
2	B	2602	THR
2	B	2622	LYS
2	B	2625	SER
2	B	2634	LYS
2	B	2648	LEU
2	B	2660	LEU
2	B	2663	LEU
2	B	2668	SER
2	B	2680	THR
2	B	2695	THR
2	B	2697	LEU
2	B	2698	LEU
2	B	2706	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1060	GLN
2	B	2275	GLN
2	B	2318	ASN
2	B	2379	HIS
2	B	2382	HIS
2	B	2388	GLN
2	B	2392	ASN
2	B	2432	ASN
2	B	2468	HIS
2	B	2492	GLN
2	B	2540	HIS
2	B	2572	ASN
2	B	2615	GLN
2	B	2659	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)

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	$\#\|Z\| > 2$
3	TPO	C	198	3	8,10,11	1.17	0	10,14,16	1.50	2 (20%)
3	SEP	C	202	3	8,9,10	0.98	0	8,12,14	2.55	2 (25%)

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	TPO	C	198	3	-	3/9/11/13	-
3	SEP	C	202	3	-	4/5/8/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	202	SEP	OG-CB-CA	4.59	112.61	108.14
3	C	202	SEP	P-OG-CB	4.22	129.93	118.30
3	C	198	TPO	O3P-P-O2P	2.83	118.44	107.64
3	C	198	TPO	OG1-P-O1P	-2.62	99.26	109.39

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	198	TPO	N-CA-CB-OG1
3	C	198	TPO	O-C-CA-CB
3	C	202	SEP	N-CA-CB-OG
3	C	202	SEP	CB-OG-P-O2P
3	C	202	SEP	CB-OG-P-O3P
3	C	202	SEP	CB-OG-P-O1P
3	C	198	TPO	CB-OG1-P-O2P

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)

10 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	IMD	B	2810	-	3,5,5	0.63	0	4,5,5	0.67	0
4	SO4	B	2805	-	4,4,4	0.39	0	6,6,6	0.34	0
4	SO4	B	2804	-	4,4,4	0.56	0	6,6,6	0.58	0
4	SO4	B	2803	-	4,4,4	0.45	0	6,6,6	0.42	0
4	SO4	B	2807	-	4,4,4	0.42	0	6,6,6	1.17	0
4	SO4	B	2806	-	4,4,4	0.46	0	6,6,6	0.82	0
4	SO4	B	2801	-	4,4,4	0.39	0	6,6,6	0.22	0
4	SO4	B	2808	-	4,4,4	0.45	0	6,6,6	0.42	0
4	SO4	B	2802	-	4,4,4	0.65	0	6,6,6	0.78	0
4	SO4	B	2809	-	4,4,4	0.61	0	6,6,6	0.83	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	IMD	B	2810	-	-	-	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2806	SO4	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	146/149 (97%)	-0.03	12 (8%) 11 8	30, 71, 121, 168	0
2	B	444/444 (100%)	-0.46	4 (0%) 84 82	19, 45, 99, 180	0
3	C	8/15 (53%)	0.59	2 (25%) 0 0	57, 70, 101, 106	0
All	All	598/608 (98%)	-0.34	18 (3%) 50 43	19, 53, 107, 180	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1071	GLY	5.0
1	A	1070	GLY	4.5
1	A	1072	SER	4.3
2	B	2338	ARG	4.1
2	B	2342	ILE	4.0
2	B	2340	LYS	4.0
1	A	1160	CYS	3.6
1	A	1073	GLY	3.2
2	B	2339	ARG	3.2
1	A	1161	GLU	2.9
1	A	1082	THR	2.9
3	C	193	PRO	2.8
1	A	1069	PRO	2.7
1	A	1067	ASP	2.5
1	A	1151	ALA	2.3
1	A	1002	ALA	2.3
3	C	201	GLY	2.2
1	A	1159	TRP	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
3	SEP	C	202	10/11	0.73	0.47	24,36,62,64	0
3	TPO	C	198	11/12	0.97	0.15	56,57,60,67	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
5	IMD	B	2810	5/5	0.50	0.55	69,77,86,88	0
4	SO4	B	2809	5/5	0.88	0.21	54,82,88,118	0
4	SO4	B	2802	5/5	0.88	0.19	41,84,93,98	0
4	SO4	B	2801	5/5	0.90	0.22	101,104,114,134	0
4	SO4	B	2803	5/5	0.91	0.19	68,78,91,112	0
4	SO4	B	2808	5/5	0.91	0.26	76,77,129,130	0
4	SO4	B	2806	5/5	0.92	0.23	40,51,113,150	0
4	SO4	B	2804	5/5	0.95	0.13	41,47,98,108	0
4	SO4	B	2805	5/5	0.95	0.17	59,75,108,177	0
4	SO4	B	2807	5/5	0.96	0.10	31,43,92,92	0

6.5 Other polymers (i)

There are no such residues in this entry.