



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:40 PM UTC

PDB ID : 3UJG / pdb_00003ujg
Title : Crystal structure of SnRK2.6 in complex with HAB1
Authors : Zhou, X.E.; Soon, F.-F.; Ng, L.-M.; Kovach, A.; Tan, M.H.E.; Suino-Powell, K.M.; He, Y.; Xu, Y.; Brunzelle, J.S.; Li, J.; Melcher, K.; Xu, H.E.
Deposited on : 2011-11-07
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

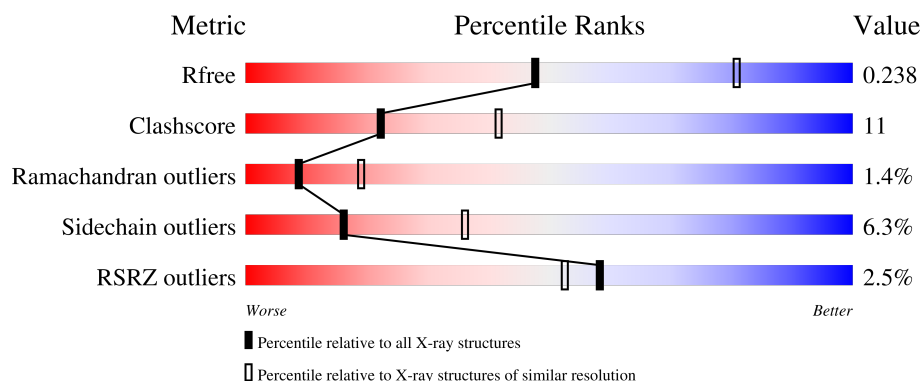
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	361	 2% 56% 21% • 20%
2	B	350	 2% 72% 16% • 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4941 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 Serine/threonine-protein kinase SRK2E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2326	1481	406	426	13			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	expression tag	UNP Q940H6
A	3	ALA	-	expression tag	UNP Q940H6
A	4	HIS	-	expression tag	UNP Q940H6
A	5	HIS	-	expression tag	UNP Q940H6
A	6	HIS	-	expression tag	UNP Q940H6
A	7	HIS	-	expression tag	UNP Q940H6
A	8	HIS	-	expression tag	UNP Q940H6
A	9	HIS	-	expression tag	UNP Q940H6
A	10	ALA	-	expression tag	UNP Q940H6
A	296	ALA	ASP	engineered mutation	UNP Q940H6
A	297	ALA	GLU	engineered mutation	UNP Q940H6

- Molecule 2 is a protein called Protein phosphatase 2C 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	315	Total	C	N	O	S	0	0	0
			2452	1545	433	456	18			

There are 10 discrepancies between the modelled and reference sequences:

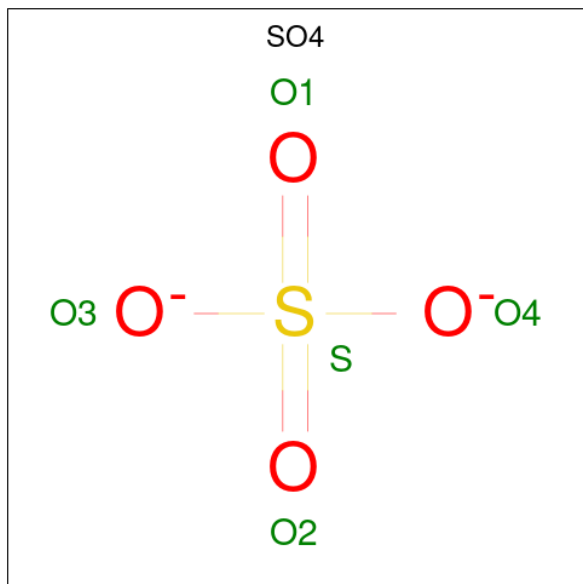
Chain	Residue	Modelled	Actual	Comment	Reference
B	162	GLY	-	expression tag	UNP Q9CAJ0
B	163	SER	-	expression tag	UNP Q9CAJ0
B	164	GLY	-	expression tag	UNP Q9CAJ0
B	165	SER	-	expression tag	UNP Q9CAJ0
B	166	ALA	-	expression tag	UNP Q9CAJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	167	GLY	-	expression tag	UNP Q9CAJ0
B	168	SER	-	expression tag	UNP Q9CAJ0
B	169	ALA	-	expression tag	UNP Q9CAJ0
B	170	ALA	-	expression tag	UNP Q9CAJ0
B	171	GLY	-	expression tag	UNP Q9CAJ0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	71	Total 71	O 71	0	0
5	B	75	Total 75	O 75	0	0

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.

- [illegible]

- [illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	154.84Å 154.84Å 70.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.78 – 2.60 29.78 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.78-2.60) 99.9 (29.78-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.34 (at 2.57Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.207 , 0.238 0.205 , 0.238	Depositor DCC
R_{free} test set	1878 reflections (7.11%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4941	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: SO4, MG

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	0.70	0/2373	0.86	2/3204 (0.1%)
2	B	0.75	0/2497	0.85	4/3366 (0.1%)
All	All	0.73	0/4870	0.85	6/6570 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	290	PHE	N-CA-C	5.59	117.46	111.36
2	B	271	ASP	N-CA-C	-5.54	105.12	112.94
2	B	231	LEU	N-CA-C	-5.50	99.09	110.80
1	A	317	VAL	N-CA-C	5.30	112.38	107.56
2	B	316	VAL	N-CA-C	5.15	115.66	110.05
1	A	57	LYS	N-CA-C	-5.14	106.85	113.02

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	2326	0	2323	61	0
2	B	2452	0	2446	42	0
3	A	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
4	B	2	0	0	0	0
5	A	71	0	0	4	0
5	B	75	0	0	1	0
All	All	4941	0	4769	101	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 11.

All (101) 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:38:MET:HE2	1:A:49:VAL:HG21	1.33	1.08
2:B:470:ILE:HD12	2:B:475:GLN:HE21	1.31	0.93
2:B:211:HIS:H	2:B:237:HIS:HD2	1.31	0.76
2:B:418:MET:HE3	2:B:419:PRO:HD2	1.68	0.76
1:A:205:VAL:O	1:A:209:VAL:HG23	1.88	0.72
1:A:146:THR:CG2	1:A:156:LEU:HD13	2.25	0.67
2:B:250:VAL:HG13	2:B:301:ILE:HD13	1.77	0.66
1:A:240:ILE:HD13	1:A:246:ILE:HD11	1.77	0.65
1:A:53:GLU:HA	1:A:89:HIS:ND1	2.12	0.65
1:A:146:THR:HG23	1:A:156:LEU:HD13	1.81	0.63
2:B:272:GLU:C	2:B:274:CYS:H	2.05	0.63
2:B:183:GLU:HA	2:B:231:LEU:HD12	1.81	0.62
2:B:208:VAL:HG23	2:B:208:VAL:O	1.99	0.62
1:A:85:LEU:HB2	1:A:311:ILE:HG23	1.82	0.61
2:B:470:ILE:HD12	2:B:475:GLN:NE2	2.10	0.61
1:A:178:GLY:N	5:A:378:HOH:O	2.33	0.60
1:A:160:ASP:HB3	1:A:163:TYR:CE1	2.37	0.60
1:A:83:VAL:HG22	1:A:90:LEU:HD11	1.85	0.59
1:A:287:ASN:HD21	1:A:292:THR:CG2	2.16	0.58
2:B:231:LEU:HD22	2:B:233:HIS:O	2.03	0.58
1:A:74:HIS:HB3	1:A:77:ILE:HD13	1.87	0.57
2:B:302:GLU:HB2	2:B:403:ARG:HD3	1.87	0.57
2:B:446:ILE:HD13	2:B:484:LEU:CD2	2.35	0.56
2:B:410:ILE:HD12	2:B:412:GLU:HB2	1.87	0.56
2:B:182:TYR:CD1	2:B:221:MET:HE3	2.40	0.56
1:A:287:ASN:ND2	1:A:292:THR:CG2	2.70	0.55
2:B:182:TYR:CG	2:B:221:MET:HE3	2.42	0.55
1:A:273:ASN:ND2	5:A:373:HOH:O	2.39	0.54
1:A:58:ILE:HB	1:A:316:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:HIS:CD2	1:A:76:ASN:H	2.26	0.54
1:A:256:ARG:NH2	1:A:264:LYS:O	2.39	0.54
1:A:139:ARG:HH21	1:A:142:LYS:HZ3	1.56	0.53
1:A:83:VAL:HG23	1:A:92:ILE:HD13	1.90	0.53
2:B:381:LYS:HD3	2:B:383:ILE:HD11	1.89	0.53
1:A:230:ILE:HG21	2:B:391:PHE:HE2	1.74	0.53
2:B:425:GLU:OE2	2:B:505:ARG:NH2	2.41	0.53
2:B:243:ASP:C	2:B:243:ASP:OD1	2.52	0.52
2:B:250:VAL:HG23	2:B:325:VAL:HG22	1.92	0.52
1:A:153:ALA:HB3	1:A:154:PRO:C	2.35	0.51
1:A:62:VAL:HG23	1:A:168:VAL:HG11	1.91	0.51
1:A:133:ALA:HB1	1:A:290:THR:HG21	1.93	0.51
2:B:398:ARG:HG2	2:B:410:ILE:HG13	1.92	0.51
1:A:105:ARG:HH21	1:A:105:ARG:HG2	1.76	0.51
2:B:259:HIS:CD2	2:B:259:HIS:H	2.30	0.50
1:A:83:VAL:H	1:A:303:GLN:HE22	1.59	0.50
1:A:289:ASN:ND2	1:A:292:THR:HG22	2.27	0.50
1:A:74:HIS:HD2	1:A:76:ASN:H	1.60	0.49
1:A:236:VAL:HG11	1:A:258:PHE:O	2.12	0.48
2:B:307:ARG:NH1	2:B:318:GLU:O	2.45	0.48
2:B:229:PRO:HG2	5:B:152:HOH:O	2.11	0.48
1:A:70:ARG:NH2	1:A:303:GLN:O	2.46	0.48
2:B:285:GLN:O	2:B:289:VAL:HG12	2.14	0.48
1:A:289:ASN:ND2	1:A:292:THR:N	2.62	0.47
2:B:231:LEU:CD2	2:B:233:HIS:O	2.61	0.47
2:B:353:ARG:HB3	2:B:358:MET:HE3	1.97	0.47
1:A:178:GLY:O	1:A:224:LYS:NZ	2.47	0.47
2:B:272:GLU:C	2:B:274:CYS:N	2.72	0.47
1:A:287:ASN:ND2	1:A:292:THR:HG21	2.30	0.47
1:A:78:VAL:HG13	1:A:160:ASP:HA	1.97	0.47
2:B:418:MET:HE3	2:B:419:PRO:CD	2.43	0.47
1:A:83:VAL:HG13	1:A:83:VAL:O	2.15	0.46
1:A:303:GLN:NE2	1:A:308:ILE:HG12	2.31	0.46
1:A:25:LYS:HE2	1:A:27:ILE:HG23	1.97	0.46
2:B:455:HIS:CD2	2:B:460:ALA:HB2	2.50	0.46
1:A:142:LYS:NZ	3:A:363:SO4:O3	2.40	0.46
1:A:118:ARG:HD3	1:A:279:LYS:O	2.15	0.46
1:A:268:ILE:N	1:A:269:PRO:HD2	2.31	0.45
2:B:213:LEU:HD13	2:B:215:LEU:HD21	1.97	0.45
1:A:172:GLN:HE22	2:B:491:LYS:H	1.62	0.45
1:A:83:VAL:HG12	1:A:303:GLN:HE22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:PRO:HG2	1:A:260:ALA:HA	1.99	0.45
1:A:76:ASN:C	1:A:77:ILE:HD12	2.41	0.45
1:A:303:GLN:HE21	1:A:308:ILE:HG12	1.82	0.45
1:A:54:ARG:HB2	1:A:89:HIS:HA	1.98	0.44
2:B:286:TRP:HA	2:B:289:VAL:HG12	2.00	0.44
1:A:120:PHE:HB3	1:A:156:LEU:HD23	1.99	0.44
1:A:179:THR:N	5:A:378:HOH:O	2.29	0.43
1:A:58:ILE:HA	1:A:62:VAL:HG11	1.99	0.43
2:B:190:TRP:CZ3	2:B:208:VAL:HG21	2.54	0.43
1:A:112:PHE:HB3	1:A:116:GLU:HB2	2.01	0.43
1:A:200:VAL:HG12	1:A:257:ILE:HG23	2.01	0.43
2:B:287:ASP:HA	2:B:415:VAL:HG21	2.00	0.43
2:B:208:VAL:O	2:B:208:VAL:CG2	2.67	0.42
1:A:236:VAL:HG12	1:A:236:VAL:O	2.19	0.42
2:B:286:TRP:HA	2:B:289:VAL:CG1	2.50	0.42
1:A:240:ILE:HG22	1:A:244:VAL:HG13	2.02	0.41
2:B:500:ASP:OD1	2:B:505:ARG:NH1	2.53	0.41
1:A:83:VAL:CG2	1:A:90:LEU:HD11	2.49	0.41
2:B:486:LEU:HD23	2:B:486:LEU:HA	1.94	0.41
1:A:289:ASN:ND2	1:A:292:THR:H	2.18	0.41
1:A:162:GLY:HA3	1:A:169:LEU:HD23	2.03	0.41
1:A:282:PRO:HG2	1:A:285:LEU:HD12	2.02	0.41
2:B:353:ARG:HH22	2:B:418:MET:HE2	1.85	0.41
1:A:177:VAL:HG22	5:A:378:HOH:O	2.21	0.41
2:B:211:HIS:H	2:B:237:HIS:CD2	2.22	0.41
2:B:217:ILE:HD12	2:B:221:MET:HB2	2.02	0.41
2:B:422:ARG:O	2:B:502:LYS:NZ	2.53	0.41
1:A:83:VAL:O	1:A:83:VAL:CG1	2.69	0.40
1:A:97:ALA:HB1	1:A:148:LEU:O	2.21	0.40
1:A:247:SER:HB2	1:A:248:PRO:HD2	2.02	0.40
1:A:289:ASN:CG	1:A:292:THR:HG22	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	280/361 (78%)	254 (91%)	21 (8%)	5 (2%)	6	14
2	B	307/350 (88%)	293 (95%)	11 (4%)	3 (1%)	12	28
All	All	587/711 (83%)	547 (93%)	32 (6%)	8 (1%)	9	19

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	PRO
1	A	59	ASP
1	A	109	ALA
2	B	273	LEU
1	A	53	GLU
1	A	224	LYS
2	B	231	LEU
2	B	459	GLY

5.3.2 Protein sidechains ⓘ

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	256/319 (80%)	237 (93%)	19 (7%)	13	29
2	B	264/288 (92%)	250 (95%)	14 (5%)	20	43
All	All	520/607 (86%)	487 (94%)	33 (6%)	16	36

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASP
1	A	27	ILE
1	A	56	GLU
1	A	78	VAL
1	A	85	LEU

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Mol	Chain	Res	Type
1	A	105	ARG
1	A	135	GLN
1	A	144	GLU
1	A	156	LEU
1	A	158	ILE
1	A	179	THR
1	A	189	LEU
1	A	191	LYS
1	A	209	VAL
1	A	244	VAL
1	A	256	ARG
1	A	270	GLU
1	A	294	GLN
1	A	310	GLN
2	B	213	LEU
2	B	217	ILE
2	B	218	LYS
2	B	235	THR
2	B	259	HIS
2	B	272	GLU
2	B	273	LEU
2	B	289	VAL
2	B	292	SER
2	B	325	VAL
2	B	331	VAL
2	B	333	LEU
2	B	355	LYS
2	B	434	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	74	HIS
1	A	76	ASN
1	A	122	GLN
1	A	132	HIS
1	A	135	GLN
1	A	145	ASN
1	A	170	HIS
1	A	172	GLN
1	A	235	ASN

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Mol	Chain	Res	Type
1	A	274	HIS
1	A	287	ASN
1	A	289	ASN
1	A	303	GLN
2	B	233	HIS
2	B	237	HIS
2	B	259	HIS
2	B	283	GLN
2	B	285	GLN
2	B	455	HIS
2	B	475	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	B	513	-	4,4,4	0.30	0	6,6,6	0.32	0
3	SO4	A	363	-	4,4,4	0.31	0	6,6,6	0.40	0
3	SO4	A	364	-	4,4,4	0.26	0	6,6,6	0.52	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	363	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	290/361 (80%)	0.24	9 (3%) 51 45	34, 60, 101, 105	0
2	B	315/350 (90%)	-0.13	6 (1%) 66 61	30, 45, 82, 107	0
All	All	605/711 (85%)	0.05	15 (2%) 58 52	30, 50, 96, 107	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	VAL	4.4
1	A	318	PRO	4.1
2	B	273	LEU	3.7
1	A	62	VAL	3.0
2	B	310	VAL	2.8
1	A	297	ALA	2.7
1	A	161	PHE	2.6
2	B	274	CYS	2.6
1	A	153	ALA	2.6
1	A	27	ILE	2.5
2	B	465	GLU	2.5
1	A	34	VAL	2.4
2	B	229	PRO	2.3
2	B	464	ALA	2.1
1	A	303	GLN	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 oligosaccharides 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	MG	B	100	1/1	0.75	0.27	69,69,69,69	0
4	MG	B	512	1/1	0.78	0.22	45,45,45,45	0
3	SO4	A	364	5/5	0.98	0.07	37,39,41,42	0
3	SO4	B	513	5/5	0.98	0.07	56,57,57,58	0
3	SO4	A	363	5/5	0.99	0.05	41,41,43,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.