



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2026 – 12:07 PM EDT

PDB ID : 12FH / pdb_000012fh
Title : Structure of eIF2B bound to a activator
Authors : Jain, R.; Jakob, C.G.; Qiu, W.
Deposited on : 2026-04-01
Resolution : 3.50 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

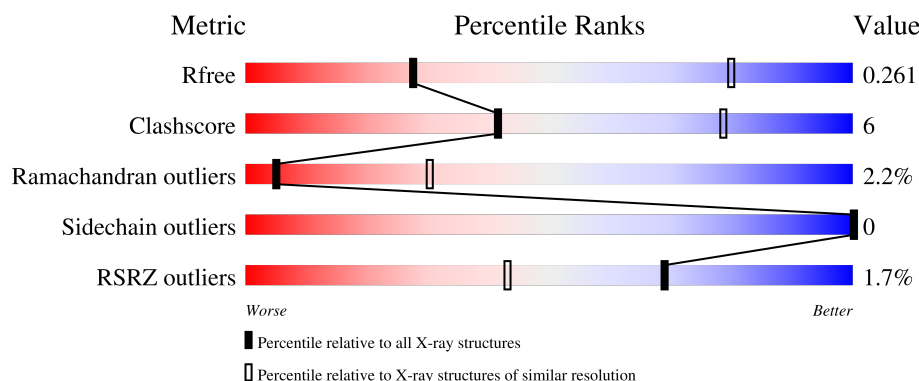
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	542	<div> <div>51%</div> <div>15%</div> <div>35%</div> </div>
1	B	542	<div> <div>52%</div> <div>12%</div> <div>35%</div> </div>
2	C	366	<div> <div>74%</div> <div>10%</div> <div>15%</div> </div>
2	D	366	<div> <div>70%</div> <div>14%</div> <div>15%</div> </div>
3	F	16	<div> <div>100%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10540 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 Isoform 2 of Translation initiation factor eIF2B subunit delta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	P	S	0	0	0
			2772	1751	494	512	1	14			
1	B	353	Total	C	N	O	P	S	0	0	0
			2756	1740	491	510	1	14			

- Molecule 2 is a protein called Translation initiation factor eIF2B subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	311	Total	C	N	O	P	S	0	0	0
			2445	1552	430	447	1	15			
2	D	311	Total	C	N	O	P	S	0	0	0
			2440	1546	430	448	1	15			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASP	-	expression tag	UNP P49770
C	-13	TYR	-	expression tag	UNP P49770
C	-12	LYS	-	expression tag	UNP P49770
C	-11	ASP	-	expression tag	UNP P49770
C	-10	ASP	-	expression tag	UNP P49770
C	-9	ASP	-	expression tag	UNP P49770
C	-8	ASP	-	expression tag	UNP P49770
C	-7	LYS	-	expression tag	UNP P49770
C	-6	GLU	-	expression tag	UNP P49770
C	-5	ASN	-	expression tag	UNP P49770
C	-4	LEU	-	expression tag	UNP P49770
C	-3	TYR	-	expression tag	UNP P49770
C	-2	PHE	-	expression tag	UNP P49770
C	-1	GLN	-	expression tag	UNP P49770
C	0	SER	-	expression tag	UNP P49770
D	-14	ASP	-	expression tag	UNP P49770

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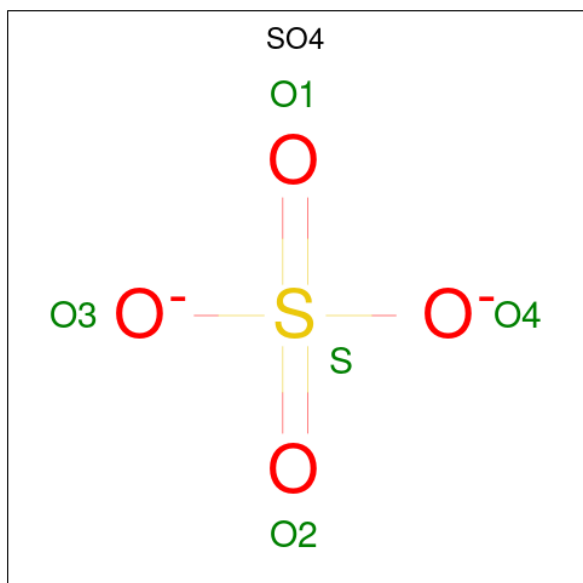
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-13	TYR	-	expression tag	UNP P49770
D	-12	LYS	-	expression tag	UNP P49770
D	-11	ASP	-	expression tag	UNP P49770
D	-10	ASP	-	expression tag	UNP P49770
D	-9	ASP	-	expression tag	UNP P49770
D	-8	ASP	-	expression tag	UNP P49770
D	-7	LYS	-	expression tag	UNP P49770
D	-6	GLU	-	expression tag	UNP P49770
D	-5	ASN	-	expression tag	UNP P49770
D	-4	LEU	-	expression tag	UNP P49770
D	-3	TYR	-	expression tag	UNP P49770
D	-2	PHE	-	expression tag	UNP P49770
D	-1	GLN	-	expression tag	UNP P49770
D	0	SER	-	expression tag	UNP P49770

- Molecule 3 is a protein called unidentified protein fragment.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	16	Total	C	N	O	0	0	0
			80	48	16	16			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



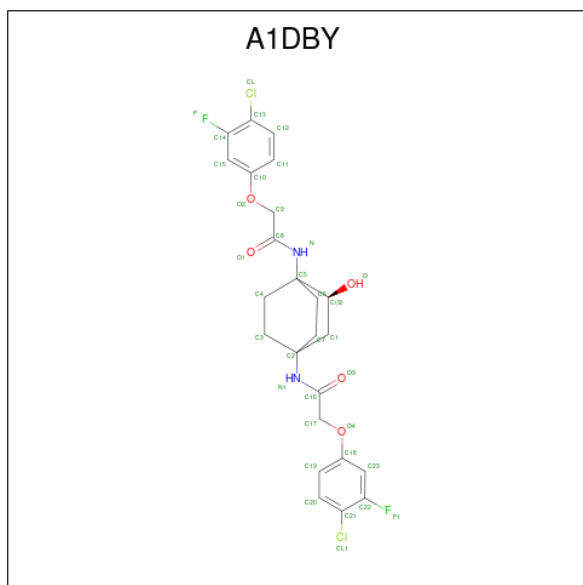
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 5 is N,N'-[(1S,2S,4R)-2-hydroxybicyclo[2.2.2]octane-1,4-diyl]bis[2-(4-chloro-3-fluorophenoxy)acetamide] (CCD ID: A1DBY) (formula: C₂₄H₂₄Cl₂F₂N₂O₅) (labeled as "Ligand of Interest" by depositor).

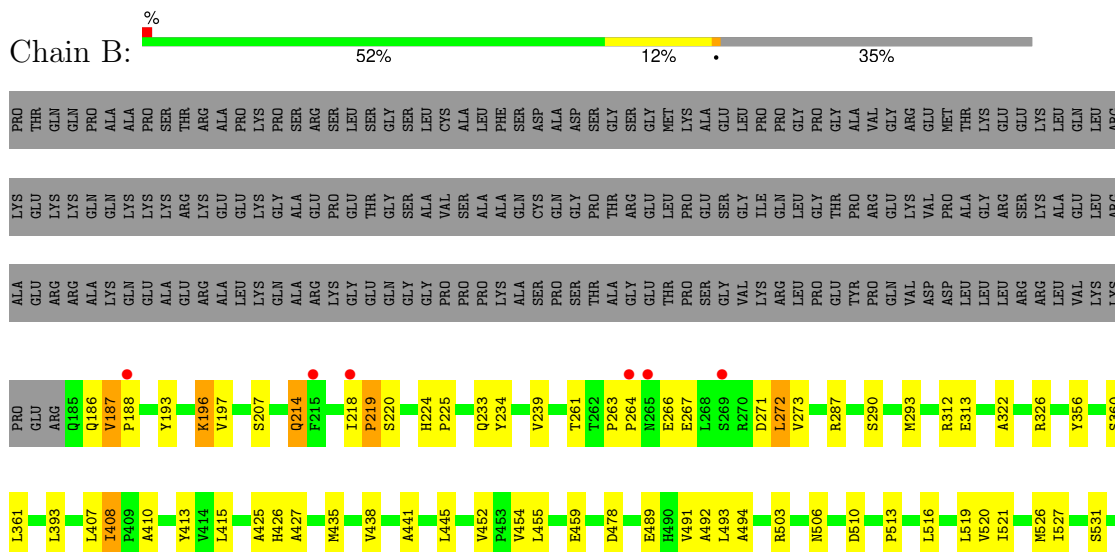


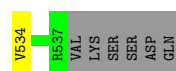
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	D	1	Total	C	Cl	F	N	O	0	0
			35	24	2	2	2	5		

- Molecule 6 is water.

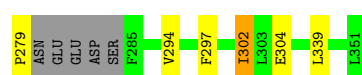
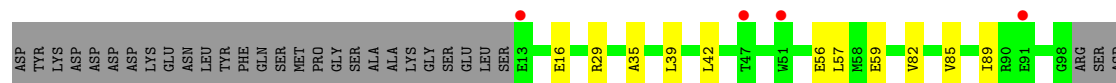
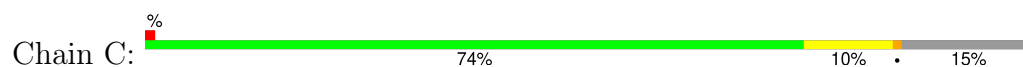
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	D	1	Total	O	0	0
			1	1		

- Molecule 1: Isoform 2 of Translation initiation factor eIF2B subunit delta





- Molecule 2: Translation initiation factor eIF2B subunit beta



- Molecule 2: Translation initiation factor eIF2B subunit beta



- Molecule 3: unidentified protein fragment



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	131.47Å 230.81Å 89.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.50 49.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.98-3.50) 96.1 (49.98-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.215 , 0.271 0.209 , 0.261	Depositor DCC
R_{free} test set	1817 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	76.6	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10540	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: TPO, A1DBY, SEP, 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	0.20	0/2813	0.53	0/3821
1	B	0.24	0/2797	0.56	0/3800
2	C	0.18	0/2481	0.48	0/3352
2	D	0.21	0/2475	0.48	0/3344
All	All	0.21	0/10566	0.52	0/14317

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	2772	0	2831	47	0
1	B	2756	0	2809	36	0
2	C	2445	0	2464	27	0
2	D	2440	0	2460	34	0
3	F	80	0	18	0	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
5	D	35	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1	0	0	0	0
All	All	10540	0	10582	136	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 6.

All (136) 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:408:ILE:HG13	1:A:409:PRO:HD3	1.54	0.89
1:A:394:ARG:HH12	2:C:302:ILE:HG23	1.47	0.79
1:A:230:LEU:HD11	1:A:248:ALA:HB1	1.66	0.77
2:C:228:ARG:HE	2:D:160:HIS:HE1	1.33	0.76
2:D:195:ALA:HB1	2:D:196:PRO:HD2	1.66	0.76
2:C:195:ALA:HB1	2:C:196:PRO:HD2	1.68	0.75
2:D:42:LEU:HD23	2:D:85:VAL:HG11	1.69	0.75
2:D:127:ALA:O	2:D:128:GLN:HG2	1.87	0.74
2:C:42:LEU:HD23	2:C:85:VAL:HG11	1.71	0.73
1:B:455:LEU:HD22	1:B:519:LEU:HB3	1.76	0.66
1:A:233:GLN:HB3	1:A:239:VAL:HG22	1.77	0.66
2:C:127:ALA:O	2:C:128:GLN:HG2	1.96	0.65
1:B:521:ILE:HG12	1:B:526:MET:HG2	1.79	0.65
2:D:39:LEU:HD21	2:D:140:LEU:HD23	1.81	0.62
1:B:263:PRO:HD3	1:B:272:LEU:HD22	1.82	0.62
2:D:85:VAL:HG23	2:D:137:ILE:HD11	1.80	0.62
1:B:478:ASP:HB3	1:B:506:ASN:ND2	2.15	0.61
1:A:423:LEU:HD13	1:A:440:THR:HG23	1.82	0.60
1:A:531:SER:O	1:A:534:VAL:HG22	2.01	0.60
1:B:531:SER:O	1:B:534:VAL:HG22	2.02	0.60
2:C:155:ALA:HA	2:C:177:PHE:CZ	2.38	0.58
1:A:438:VAL:HA	1:A:510:ASP:HB2	1.86	0.57
1:A:219:PRO:HA	1:A:223:ILE:HD13	1.86	0.56
1:B:415:LEU:HD22	1:B:452:VAL:HG11	1.86	0.56
1:A:322:ALA:O	1:A:326:ARG:HG3	2.06	0.56
1:A:294:HIS:O	1:A:298:LYS:HG2	2.06	0.56
1:A:234:TYR:HB3	1:A:287:ARG:HB3	1.86	0.56
1:B:407:LEU:O	1:B:408:ILE:HB	2.07	0.55
1:A:225:PRO:HA	1:A:228:VAL:HG22	1.89	0.54
1:B:290:SER:H	1:B:293:MET:HE3	1.72	0.54
1:A:407:LEU:HD13	2:C:294:VAL:HG13	1.90	0.53
2:D:173:TPO:HG21	2:D:270:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ALA:O	1:B:426:HIS:HB2	2.07	0.53
1:B:427:ALA:HB3	1:B:435:MET:HB3	1.89	0.53
1:A:352:VAL:HG13	1:A:418:VAL:HA	1.91	0.53
2:C:57:LEU:HD22	2:C:89:ILE:HD13	1.90	0.53
2:D:35:ALA:HB1	2:D:144:LEU:HD11	1.90	0.53
1:A:352:VAL:HG11	1:A:417:GLU:O	2.09	0.52
1:A:425:ALA:O	1:A:426:HIS:HB2	2.09	0.52
2:C:155:ALA:HB1	2:C:181:ALA:HB2	1.92	0.52
2:D:276:PRO:HG3	2:D:344:TYR:CD2	2.45	0.52
1:B:356:TYR:CE1	1:B:408:ILE:HD11	2.46	0.51
2:D:155:ALA:HA	2:D:177:PHE:CZ	2.45	0.51
1:A:352:VAL:HG13	1:A:352:VAL:O	2.10	0.51
2:C:85:VAL:HG23	2:C:137:ILE:HD11	1.92	0.51
1:B:214:GLN:H	1:B:214:GLN:CD	2.19	0.51
2:C:39:LEU:HD13	2:C:141:LEU:HB3	1.93	0.51
2:C:173:TPO:HG21	2:C:270:PRO:HD3	1.93	0.50
2:D:49:HIS:CE1	2:D:60:LEU:HD11	2.46	0.50
1:A:491:VAL:HG11	1:A:494:ALA:HB2	1.93	0.50
2:D:302:ILE:O	2:D:303:LEU:HG	2.12	0.50
1:A:470:ASP:CG	2:C:228:ARG:HH22	2.19	0.50
1:B:491:VAL:HG22	1:B:494:ALA:HB2	1.93	0.49
1:B:196:LYS:O	1:B:503:ARG:HD3	2.14	0.48
1:A:359:SER:HB3	1:A:362:VAL:HG22	1.96	0.48
2:C:277:GLN:HG3	2:C:279:PRO:HD2	1.95	0.48
2:C:42:LEU:HD21	2:C:82:VAL:HG22	1.96	0.48
1:B:193:TYR:CG	1:B:207:SER:HB2	2.49	0.48
1:B:234:TYR:HB3	1:B:287:ARG:HB3	1.94	0.48
2:D:39:LEU:HB3	2:D:141:LEU:HD11	1.96	0.47
2:D:39:LEU:HD12	2:D:144:LEU:HD13	1.95	0.47
1:A:190:ARG:CZ	1:A:190:ARG:HA	2.44	0.47
1:A:223:ILE:HG23	1:A:279:TYR:CE1	2.49	0.47
2:D:42:LEU:HD23	2:D:85:VAL:CG1	2.43	0.47
1:B:186:GLN:O	1:B:187:VAL:HG22	2.14	0.47
2:D:298:THR:HG23	2:D:299:GLU:H	1.78	0.47
1:A:415:LEU:HD22	1:A:452:VAL:HG11	1.97	0.46
1:B:233:GLN:HB3	1:B:239:VAL:HG12	1.97	0.46
2:D:226:MET:HE1	2:D:232:VAL:CG2	2.45	0.46
1:A:312:ARG:HE	1:A:313:GLU:H	1.62	0.46
1:A:493:LEU:H	1:A:493:LEU:HD23	1.81	0.46
1:B:312:ARG:HG3	1:B:313:GLU:N	2.31	0.46
1:B:441:ALA:HB3	1:B:510:ASP:OD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:VAL:HA	1:B:510:ASP:HB2	1.96	0.46
2:D:286:HIS:CD2	2:D:287:LYS:H	2.33	0.46
1:A:311:LYS:HD2	1:A:319:GLU:OE1	2.16	0.46
1:A:406:LEU:O	1:A:407:LEU:HB2	2.14	0.46
1:A:437:ARG:NH2	4:A:601:SO4:O4	2.48	0.46
2:C:35:ALA:HB1	2:C:144:LEU:HD11	1.98	0.46
1:A:356:TYR:OH	1:A:383:SER:HB3	2.15	0.45
1:A:427:ALA:HB3	1:A:435:MET:HB3	1.97	0.45
1:A:491:VAL:CG1	1:A:494:ALA:HB2	2.46	0.45
1:B:197:VAL:HA	1:B:503:ARG:HD2	1.98	0.45
1:A:208:ARG:NH2	1:A:482:ASP:OD2	2.44	0.45
2:C:141:LEU:C	2:C:143:GLU:H	2.25	0.45
2:D:276:PRO:HG3	2:D:344:TYR:CG	2.52	0.45
2:C:138:ASN:O	2:C:142:VAL:HG23	2.17	0.45
2:C:226:MET:HE1	2:C:232:VAL:HG22	1.99	0.45
2:C:195:ALA:HB1	2:C:196:PRO:CD	2.44	0.44
1:B:322:ALA:O	1:B:326:ARG:HG3	2.18	0.44
1:B:520:VAL:HG13	1:B:527:ILE:HG13	2.00	0.44
2:C:56:GLU:O	2:C:59:GLU:HG3	2.18	0.44
2:C:226:MET:HE1	2:C:232:VAL:CG2	2.48	0.44
2:C:271:MET:HE1	2:C:339:LEU:HD21	2.00	0.44
1:A:263:PRO:O	1:A:264:PRO:C	2.60	0.44
2:D:189:VAL:O	2:D:214:THR:HA	2.17	0.44
1:A:337:GLN:HG2	1:A:364:ARG:HH12	1.83	0.43
1:A:312:ARG:HD2	1:A:312:ARG:HA	1.80	0.43
1:A:478:ASP:HB3	1:A:506:ASN:ND2	2.33	0.43
1:A:289:LEU:HA	1:A:293:MET:HE3	1.99	0.43
2:D:342:GLU:H	2:D:342:GLU:HG2	1.66	0.43
1:B:393:LEU:HD22	2:D:306:VAL:HG11	2.00	0.43
2:C:297:PHE:CB	2:C:304:GLU:HG3	2.49	0.43
2:D:301:ASP:OD2	2:D:305:LYS:HD3	2.19	0.43
1:A:199:LEU:HD23	2:D:162:ASN:HB2	2.01	0.43
2:D:190:ILE:HD11	2:D:217:MET:SD	2.58	0.43
1:B:410:ALA:O	1:B:413:TYR:HB3	2.19	0.42
1:A:457:CYS:HA	1:A:521:ILE:HG23	2.00	0.42
1:B:493:LEU:HB3	2:D:205:VAL:HG21	2.02	0.42
1:B:513:PRO:HD2	1:B:516:LEU:HD12	2.01	0.42
1:B:224:HIS:CG	1:B:225:PRO:HD2	2.55	0.42
2:D:57:LEU:HD22	2:D:89:ILE:HD13	2.01	0.42
2:C:39:LEU:HD12	2:C:144:LEU:HD13	2.01	0.42
2:D:195:ALA:HB1	2:D:196:PRO:CD	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:SER:O	1:A:285:GLN:HG2	2.20	0.42
1:A:520:VAL:HG13	1:A:527:ILE:HG13	2.02	0.42
1:A:380:VAL:HG22	1:A:404:SER:O	2.20	0.41
1:B:361:LEU:HD12	1:B:459:GLU:OE2	2.20	0.41
1:A:484:GLN:HG2	1:A:493:LEU:HG	2.02	0.41
1:B:445:LEU:HD22	2:D:223:PHE:CD1	2.55	0.41
1:B:187:VAL:HA	1:B:188:PRO:HD3	1.87	0.41
1:A:191:LYS:HB2	1:A:211:SER:HB3	2.02	0.41
2:D:276:PRO:HA	2:D:340:MET:SD	2.60	0.41
2:C:39:LEU:HD11	2:C:140:LEU:HD23	2.02	0.41
2:D:15:ILE:HG22	2:D:41:LEU:HD21	2.03	0.41
2:D:86:LEU:O	2:D:90:ARG:HG3	2.20	0.41
1:B:266:GLU:HG3	1:B:267:GLU:N	2.36	0.41
1:B:271:ASP:C	1:B:273:VAL:H	2.29	0.41
1:B:454:VAL:HG11	1:B:516:LEU:O	2.20	0.41
2:D:298:THR:HG23	2:D:299:GLU:N	2.36	0.41
1:A:329:GLN:HA	1:A:333:VAL:HG12	2.03	0.40
1:A:364:ARG:CZ	1:A:368:GLU:OE2	2.69	0.40
2:C:16:GLU:CD	2:C:16:GLU:H	2.29	0.40
1:A:223:ILE:HG23	1:A:279:TYR:HE1	1.85	0.40
1:B:218:ILE:N	1:B:219:PRO:HD3	2.37	0.40
2:D:265:LEU:HD23	2:D:321:ILE:HA	2.04	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	352/542 (65%)	313 (89%)	33 (9%)	6 (2%)	7	35
1	B	350/542 (65%)	306 (87%)	33 (9%)	11 (3%)	3	25
2	C	304/366 (83%)	282 (93%)	16 (5%)	6 (2%)	6	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	304/366 (83%)	283 (93%)	15 (5%)	6 (2%)	6	32
All	All	1310/1816 (72%)	1184 (90%)	97 (7%)	29 (2%)	5	30

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	PRO
1	A	410	ALA
1	B	219	PRO
1	B	408	ILE
2	C	29	ARG
2	D	278	PHE
1	A	193	TYR
1	A	487	ARG
1	B	264	PRO
1	B	272	LEU
1	B	492	ALA
2	C	195	ALA
2	C	210	ALA
2	D	195	ALA
2	D	210	ALA
1	A	265	ASN
1	B	187	VAL
1	A	212	LEU
1	B	214	GLN
1	B	220	SER
1	B	196	LYS
1	B	261	THR
2	C	212	ILE
2	D	212	ILE
1	B	489	GLU
2	C	142	VAL
2	D	302	ILE
2	C	302	ILE
2	D	142	VAL

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	310/460 (67%)	310 (100%)	0	100	100
1	B	308/460 (67%)	308 (100%)	0	100	100
2	C	263/312 (84%)	263 (100%)	0	100	100
2	D	263/312 (84%)	263 (100%)	0	100	100
All	All	1144/1544 (74%)	1144 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	GLN
1	A	255	GLN
1	A	329	GLN
1	A	337	GLN
1	A	398	HIS
1	A	497	GLN
1	A	499	HIS
1	B	205	GLN
1	B	233	GLN
1	B	274	ASN
1	B	337	GLN
1	B	451	ASN
2	C	97	HIS
2	C	158	HIS
2	C	160	HIS
2	C	162	ASN
2	D	160	HIS
2	D	260	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 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	TPO	D	173	2	8,10,11	3.10	1 (12%)	10,14,16	1.18	0
2	TPO	C	173	2	8,10,11	2.96	1 (12%)	10,14,16	1.12	1 (10%)
1	SEP	B	360	1	8,9,10	1.65	1 (12%)	7,12,14	1.34	1 (14%)
1	SEP	A	360	1	8,9,10	1.67	1 (12%)	7,12,14	1.25	1 (14%)

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	TPO	D	173	2	-	5/9/11/13	-
2	TPO	C	173	2	-	3/9/11/13	-
1	SEP	B	360	1	-	5/6/8/10	-
1	SEP	A	360	1	-	5/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	173	TPO	P-OG1	8.58	1.74	1.59
2	C	173	TPO	P-OG1	8.18	1.73	1.59
1	A	360	SEP	P-O1P	3.64	1.61	1.50
1	B	360	SEP	P-O1P	3.49	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	SEP	OG-CB-CA	2.57	110.64	108.14
1	A	360	SEP	OG-CB-CA	2.09	110.18	108.14
2	C	173	TPO	OG1-P-O1P	-2.07	101.97	109.33

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	360	SEP	N-CA-CB-OG
1	A	360	SEP	CB-OG-P-O1P
1	A	360	SEP	CB-OG-P-O2P
1	A	360	SEP	CB-OG-P-O3P
1	B	360	SEP	N-CA-CB-OG
1	B	360	SEP	CB-OG-P-O1P
1	B	360	SEP	CB-OG-P-O2P
1	B	360	SEP	CB-OG-P-O3P
2	C	173	TPO	O-C-CA-CB
2	D	173	TPO	O-C-CA-CB
1	A	360	SEP	CA-CB-OG-P
1	B	360	SEP	CA-CB-OG-P
2	C	173	TPO	CB-OG1-P-O3P
2	D	173	TPO	CB-OG1-P-O2P
2	C	173	TPO	CA-CB-OG1-P
2	D	173	TPO	CA-CB-OG1-P
2	D	173	TPO	CB-OG1-P-O3P
2	D	173	TPO	CB-OG1-P-O1P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	173	TPO	1	0
2	C	173	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
4	SO4	B	601	-	4,4,4	0.63	0	6,6,6	0.19	0
5	A1DBY	D	401	-	37,38,38	0.21	0	51,56,56	0.83	2 (3%)
4	SO4	A	601	-	4,4,4	0.68	0	6,6,6	0.13	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	A1DBY	D	401	-	-	9/20/45/45	0/5/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	401	A1DBY	C6-C7-C2	-2.64	109.80	113.56
5	D	401	A1DBY	C4-C3-C2	-2.42	110.10	113.56

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	401	A1DBY	C17-C16-N1-C2
5	D	401	A1DBY	C4-C5-N-C8
5	D	401	A1DBY	C9-C8-N-C5
5	D	401	A1DBY	O3-C16-N1-C2
5	D	401	A1DBY	C7-C2-N1-C16
5	D	401	A1DBY	C3-C2-N1-C16
5	D	401	A1DBY	C1-C2-N1-C16
5	D	401	A1DBY	O1-C8-N-C5
5	D	401	A1DBY	C-C5-N-C8

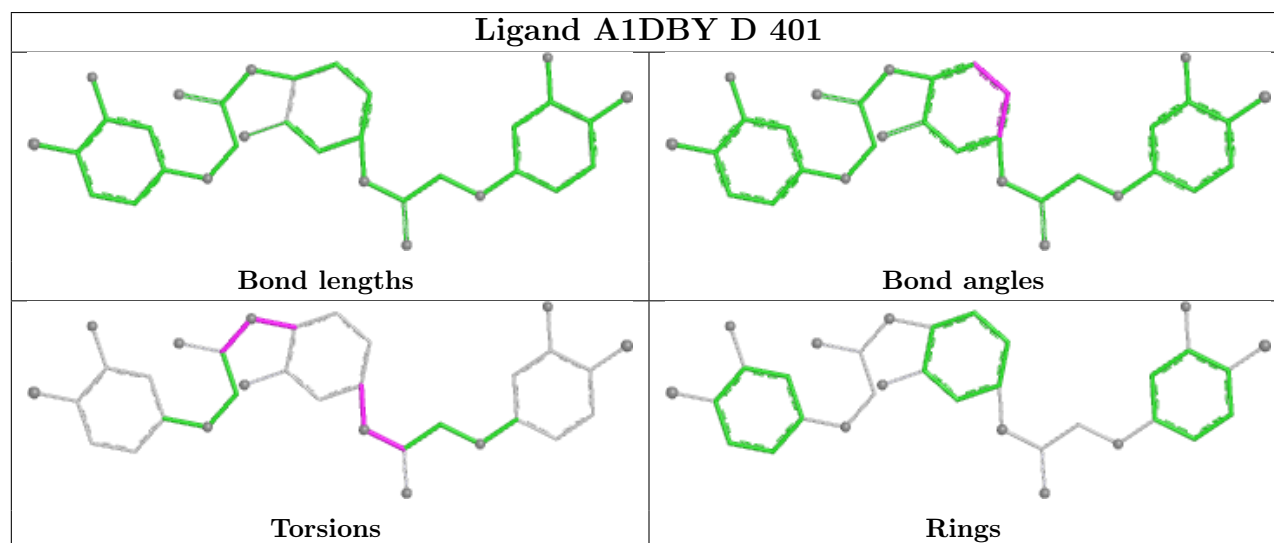
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	354/542 (65%)	0.04	5 (1%)	73 48	22, 66, 122, 148	0
1	B	352/542 (64%)	0.01	6 (1%)	69 43	28, 64, 127, 161	0
2	C	310/366 (84%)	0.06	5 (1%)	70 45	27, 68, 123, 143	0
2	D	310/366 (84%)	-0.08	6 (1%)	66 41	24, 54, 103, 139	0
3	F	0/16	-	-	-	-	-
All	All	1326/1832 (72%)	0.01	22 (1%)	69 43	22, 64, 121, 161	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	213	THR	3.3
1	A	212	LEU	3.2
1	B	218	ILE	2.8
1	A	190	ARG	2.8
1	B	269	SER	2.7
2	D	277	GLN	2.6
2	D	286	HIS	2.5
1	B	188	PRO	2.5
2	C	122	PHE	2.4
1	A	262	THR	2.4
1	B	265	ASN	2.3
2	D	98	GLY	2.3
2	C	47	THR	2.3
2	C	51	TRP	2.3
1	B	215	PHE	2.3
2	D	75	GLU	2.3
1	B	264	PRO	2.3
2	D	278	PHE	2.2
1	A	193	TYR	2.2
2	D	279	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	91	GLU	2.1
2	C	13	GLU	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
1	SEP	B	360	10/11	0.90	0.09	58,69,111,120	0
1	SEP	A	360	10/11	0.92	0.08	65,83,100,121	0
2	TPO	C	173	11/12	0.92	0.11	46,56,97,105	0
2	TPO	D	173	11/12	0.94	0.09	21,39,78,94	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

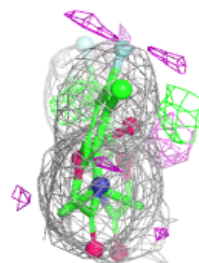
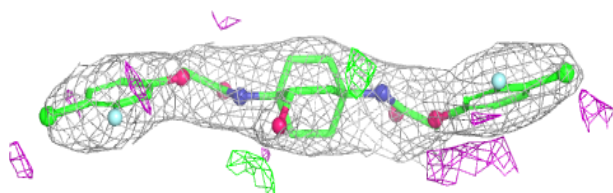
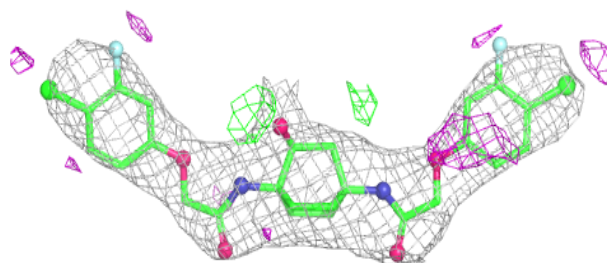
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	A	601	5/5	0.95	0.08	63,71,83,85	0
5	A1DBY	D	401	35/35	0.95	0.11	32,47,77,96	0
4	SO4	B	601	5/5	0.99	0.05	61,71,81,88	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1DBY D 401:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.