



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:34 PM UTC

PDB ID : 5WH1 / pdb_00005wh1
Title : Apo form of the C-terminal region of human Transcription Factor IIB
Authors : Bratkowski, M.A.; Liu, X.
Deposited on : 2017-07-14
Resolution : 3.39 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

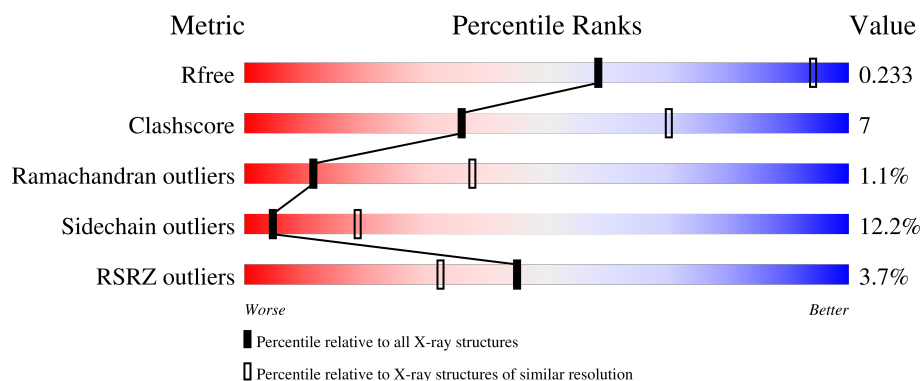
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	211	6% 67% 25% ...
1	B	211	6% 71% 24% 5%
1	C	211	2% 74% 21% .
1	D	211	% 73% 22% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6640 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.

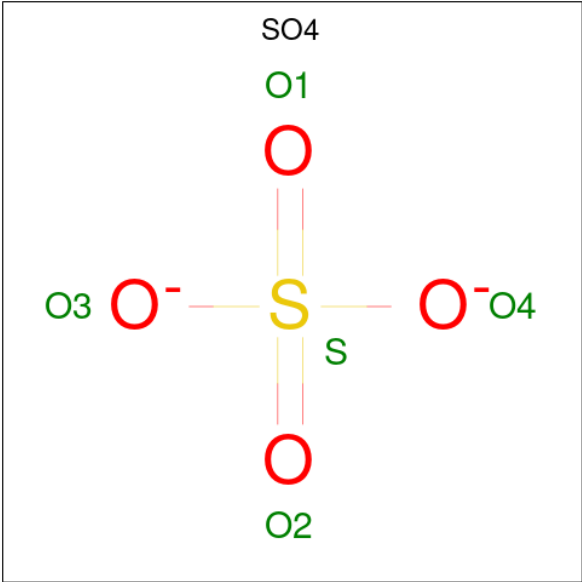
- Molecule 1 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1605	1009	287	297	12			
1	B	210	Total	C	N	O	S	0	0	0
			1635	1028	291	303	13			
1	C	210	Total	C	N	O	S	0	0	0
			1635	1028	291	303	13			
1	D	210	Total	C	N	O	S	0	0	0
			1635	1028	291	303	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	SER	-	expression tag	UNP Q00403
B	106	SER	-	expression tag	UNP Q00403
C	106	SER	-	expression tag	UNP Q00403
D	106	SER	-	expression tag	UNP Q00403

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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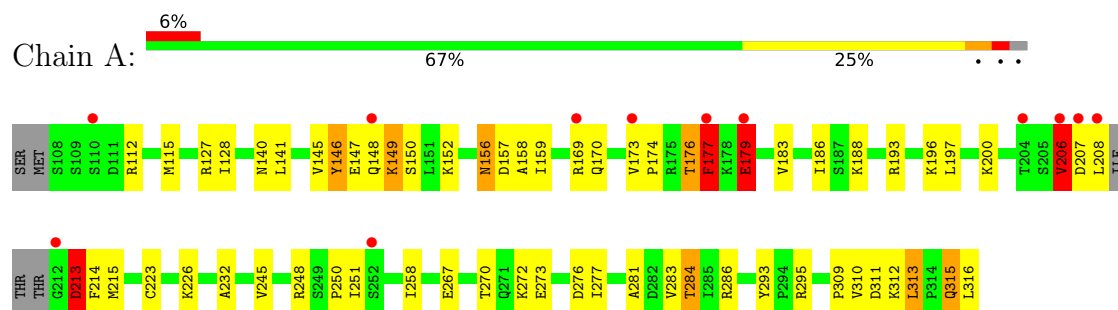
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

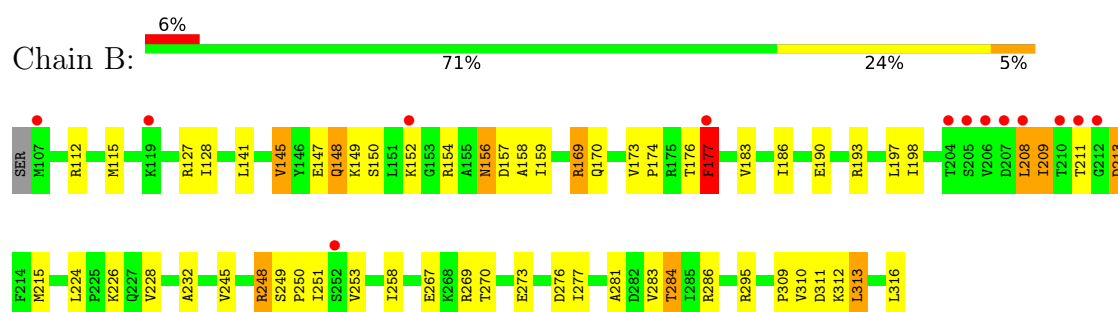
3 Residue-property plots [i](#)

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.

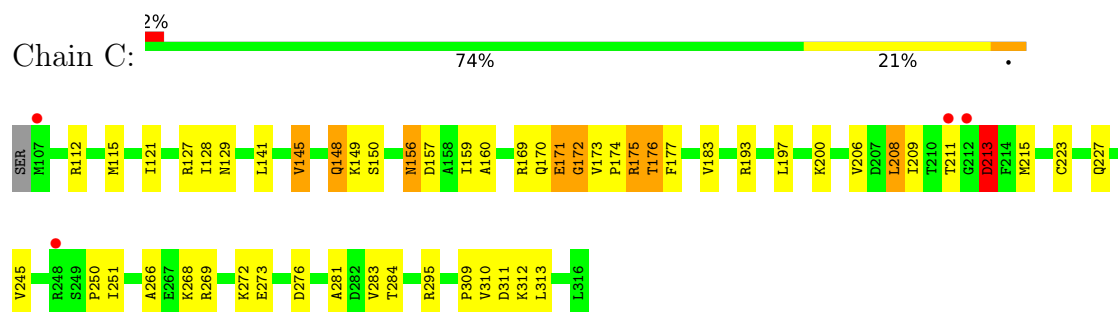
• Molecule 1: Transcription initiation factor IIB



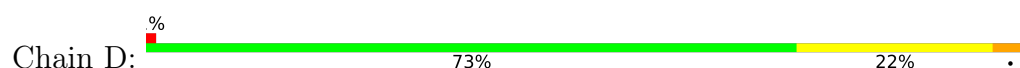
• Molecule 1: Transcription initiation factor IIB

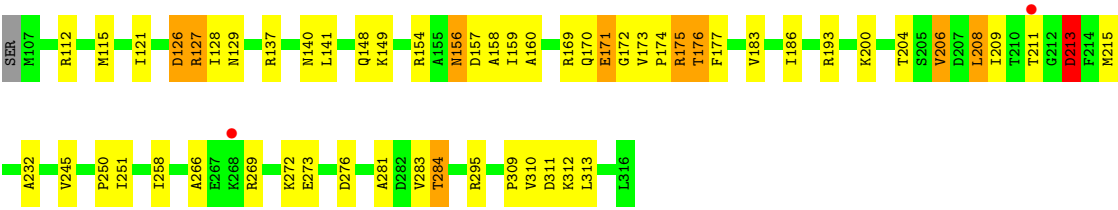


• Molecule 1: Transcription initiation factor IIB



• Molecule 1: Transcription initiation factor IIB





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.17Å 126.46Å 158.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 3.39 49.73 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.73-3.39) 99.6 (49.73-3.39)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.194 , 0.214 0.218 , 0.233	Depositor DCC
R_{free} test set	1511 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	92.4	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 85.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6640	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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

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	0.86	2/1628 (0.1%)	1.57	18/2191 (0.8%)
1	B	0.86	0/1659	1.59	20/2235 (0.9%)
1	C	0.85	1/1659 (0.1%)	1.57	18/2235 (0.8%)
1	D	0.83	0/1659	1.58	18/2235 (0.8%)
All	All	0.85	3/6605 (0.0%)	1.58	74/8896 (0.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	215	MET	SD-CE	-6.75	1.62	1.79
1	A	173	VAL	CA-C	5.99	1.59	1.52
1	A	206	VAL	C-N	5.20	1.40	1.33

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	126	ASP	CA-CB-CG	11.39	123.99	112.60
1	B	213	ASP	N-CA-C	-9.84	99.59	111.69
1	C	213	ASP	N-CA-C	-9.51	99.99	111.69
1	D	213	ASP	N-CA-C	-9.42	100.10	111.69
1	A	213	ASP	N-CA-C	-9.18	100.39	111.69
1	D	213	ASP	CA-C-N	8.33	131.27	120.44
1	D	213	ASP	C-N-CA	8.33	131.27	120.44
1	B	174	PRO	N-CA-C	8.17	123.30	111.13
1	C	213	ASP	CA-C-N	8.05	130.91	120.44
1	C	213	ASP	C-N-CA	8.05	130.91	120.44
1	B	213	ASP	CA-C-N	7.71	130.61	120.28
1	B	213	ASP	C-N-CA	7.71	130.61	120.28
1	A	148	GLN	N-CA-C	7.66	120.68	107.28
1	A	213	ASP	CA-C-N	7.61	130.48	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	ASP	C-N-CA	7.61	130.48	120.28
1	A	179	GLU	CB-CG-CD	7.24	124.90	112.60
1	A	177	PHE	CA-CB-CG	6.88	120.69	113.80
1	B	177	PHE	CA-CB-CG	6.45	120.25	113.80
1	B	174	PRO	CA-C-N	6.36	133.69	121.54
1	B	174	PRO	C-N-CA	6.36	133.69	121.54
1	C	156	ASN	CA-C-N	6.24	128.56	120.44
1	C	156	ASN	C-N-CA	6.24	128.56	120.44
1	D	156	ASN	CA-C-N	6.17	128.46	120.44
1	D	156	ASN	C-N-CA	6.17	128.46	120.44
1	A	156	ASN	CA-C-N	6.10	128.37	120.44
1	A	156	ASN	C-N-CA	6.10	128.37	120.44
1	B	276	ASP	CA-CB-CG	6.09	118.69	112.60
1	D	276	ASP	CA-CB-CG	6.07	118.67	112.60
1	B	173	VAL	CB-CA-C	6.00	116.89	110.53
1	C	157	ASP	CA-CB-CG	5.98	118.58	112.60
1	B	145	VAL	N-CA-C	5.95	116.72	111.90
1	A	169	ARG	CA-C-N	5.93	128.22	120.28
1	A	169	ARG	C-N-CA	5.93	128.22	120.28
1	C	171	GLU	CB-CG-CD	5.91	122.65	112.60
1	D	177	PHE	CA-CB-CG	-5.88	107.92	113.80
1	A	145	VAL	N-CA-C	5.88	116.66	111.90
1	C	173	VAL	N-CA-CB	5.88	118.67	111.21
1	D	173	VAL	N-CA-CB	5.87	118.66	111.21
1	B	156	ASN	CA-C-N	5.84	128.42	120.54
1	B	156	ASN	C-N-CA	5.84	128.42	120.54
1	C	177	PHE	CA-CB-CG	-5.82	107.98	113.80
1	A	276	ASP	CA-CB-CG	5.76	118.36	112.60
1	D	169	ARG	CA-C-N	5.72	128.26	120.54
1	D	169	ARG	C-N-CA	5.72	128.26	120.54
1	C	276	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	169	ARG	CA-C-N	5.68	127.89	120.28
1	B	169	ARG	C-N-CA	5.68	127.89	120.28
1	C	145	VAL	N-CA-C	5.64	116.47	111.90
1	C	169	ARG	CA-C-N	5.57	128.05	120.54
1	C	169	ARG	C-N-CA	5.57	128.05	120.54
1	A	140	ASN	CA-CB-CG	5.50	118.10	112.60
1	A	174	PRO	CA-C-N	5.50	130.21	122.46
1	A	174	PRO	C-N-CA	5.50	130.21	122.46
1	D	157	ASP	CA-CB-CG	5.47	118.07	112.60
1	C	149	LYS	CA-C-N	5.46	127.60	120.28
1	C	149	LYS	C-N-CA	5.46	127.60	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	157	ASP	CA-CB-CG	5.43	118.03	112.60
1	B	149	LYS	CA-C-N	5.43	127.55	120.28
1	B	149	LYS	C-N-CA	5.43	127.55	120.28
1	B	173	VAL	N-CA-CB	5.37	118.03	111.21
1	A	149	LYS	CA-C-N	5.34	127.43	120.28
1	A	149	LYS	C-N-CA	5.34	127.43	120.28
1	D	171	GLU	CB-CG-CD	5.32	121.65	112.60
1	B	147	GLU	CB-CG-CD	5.24	121.50	112.60
1	D	176	THR	N-CA-C	5.16	118.53	110.32
1	D	149	LYS	CA-C-N	5.14	127.17	120.28
1	D	149	LYS	C-N-CA	5.14	127.17	120.28
1	D	140	ASN	CA-C-N	5.09	127.10	120.28
1	D	140	ASN	C-N-CA	5.09	127.10	120.28
1	C	172	GLY	CA-C-N	-5.07	118.38	123.04
1	C	172	GLY	C-N-CA	-5.07	118.38	123.04
1	C	176	THR	N-CA-C	5.01	118.28	110.32
1	B	190	GLU	CB-CG-CD	5.00	121.10	112.60

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	1605	0	1654	30	0
1	B	1635	0	1689	33	0
1	C	1635	0	1689	22	0
1	D	1635	0	1689	27	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
2	C	40	0	0	0	0
2	D	40	0	0	0	0
All	All	6640	0	6721	98	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 7.

All (98) 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:208:LEU:C	1:A:208:LEU:HD23	2.14	0.72
1:B:277:ILE:HD11	1:C:206:VAL:HG12	1.71	0.72
1:D:172:GLY:CA	1:D:251:ILE:HD13	2.22	0.70
1:B:245:VAL:HG22	1:B:248:ARG:HG3	1.73	0.69
1:C:281:ALA:O	1:C:284:THR:HG22	1.93	0.68
1:A:176:THR:HA	1:A:179:GLU:HG2	1.77	0.67
1:B:177:PHE:N	1:B:177:PHE:CD2	2.62	0.66
1:A:208:LEU:H	1:A:213:ASP:HB2	1.61	0.65
1:C:172:GLY:CA	1:C:251:ILE:HD13	2.28	0.63
1:A:177:PHE:N	1:A:177:PHE:CD2	2.66	0.62
1:D:172:GLY:HA2	1:D:251:ILE:HD13	1.83	0.61
1:B:208:LEU:HD23	1:B:209:ILE:HG13	1.84	0.59
1:A:273:GLU:HB2	1:D:206:VAL:HG21	1.85	0.59
1:A:193:ARG:HA	1:A:196:LYS:HE2	1.86	0.58
1:C:172:GLY:HA2	1:C:251:ILE:HD13	1.87	0.55
1:B:127:ARG:HD3	1:B:183:VAL:HG13	1.88	0.55
1:B:277:ILE:HD11	1:C:206:VAL:CG1	2.38	0.53
1:C:193:ARG:O	1:C:197:LEU:HD13	2.08	0.53
1:B:177:PHE:N	1:B:177:PHE:HD2	2.06	0.52
1:D:127:ARG:HG2	1:D:127:ARG:HH21	1.74	0.52
1:A:207:ASP:HB3	1:A:214:PHE:CZ	2.44	0.52
1:B:245:VAL:HG22	1:B:248:ARG:CG	2.40	0.52
1:A:309:PRO:HG2	1:A:312:LYS:HB2	1.92	0.51
1:C:150:SER:HB2	1:C:197:LEU:HD23	1.92	0.50
1:D:309:PRO:HG2	1:D:312:LYS:HB2	1.93	0.50
1:A:273:GLU:CD	1:C:269:ARG:HH22	2.19	0.50
1:B:309:PRO:HG2	1:B:312:LYS:HB2	1.93	0.50
1:C:145:VAL:O	1:C:148:GLN:HB2	2.12	0.49
1:B:270:THR:HG21	1:D:266:ALA:O	2.11	0.49
1:A:223:CYS:SG	1:C:223:CYS:HB2	2.53	0.49
1:A:277:ILE:O	1:D:137:ARG:NH2	2.46	0.49
1:D:215:MET:HE1	1:D:258:ILE:HG13	1.95	0.49
1:A:267:GLU:HG3	1:C:273:GLU:HG3	1.95	0.49
1:A:150:SER:HB3	1:A:197:LEU:HD22	1.94	0.49
1:B:215:MET:HE1	1:B:232:ALA:CB	2.43	0.49
1:D:172:GLY:HA3	1:D:251:ILE:HD13	1.92	0.48
1:A:177:PHE:N	1:A:177:PHE:HD2	2.10	0.48
1:A:215:MET:HE1	1:A:232:ALA:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:PRO:HG2	1:C:312:LYS:HB2	1.95	0.48
1:A:215:MET:HE1	1:A:258:ILE:HG13	1.95	0.47
1:B:245:VAL:O	1:B:245:VAL:HG13	2.14	0.47
1:D:127:ARG:HG2	1:D:127:ARG:NH2	2.29	0.47
1:A:208:LEU:C	1:A:208:LEU:CD2	2.86	0.47
1:D:172:GLY:HA2	1:D:251:ILE:CD1	2.44	0.47
1:D:281:ALA:HB3	1:D:284:THR:HG23	1.96	0.46
1:D:208:LEU:HD23	1:D:213:ASP:HB3	1.97	0.46
1:A:206:VAL:HB	1:A:207:ASP:H	1.65	0.46
1:B:156:ASN:HA	1:B:159:ILE:HD12	1.98	0.46
1:D:215:MET:HE1	1:D:232:ALA:CB	2.46	0.45
1:A:156:ASN:HA	1:A:159:ILE:HD12	1.99	0.45
1:B:154:ARG:HH22	1:B:193:ARG:HH21	1.65	0.44
1:C:227:GLN:HG3	1:D:204:THR:HG22	1.99	0.44
1:A:146:TYR:CE1	1:A:147:GLU:HG3	2.52	0.44
1:C:208:LEU:HD23	1:C:213:ASP:HB3	1.99	0.44
1:A:313:LEU:HD12	1:A:313:LEU:HA	1.92	0.44
1:B:215:MET:CE	1:B:232:ALA:HB3	2.48	0.44
1:B:281:ALA:HB3	1:B:284:THR:HG23	2.00	0.43
1:B:313:LEU:HD12	1:B:313:LEU:HA	1.92	0.43
1:C:128:ILE:HG23	1:C:183:VAL:HG11	2.00	0.43
1:A:215:MET:CE	1:A:232:ALA:HB3	2.48	0.43
1:B:215:MET:HE1	1:B:258:ILE:HG13	2.00	0.43
1:C:172:GLY:HA2	1:C:251:ILE:CD1	2.48	0.43
1:B:269:ARG:HE	1:D:269:ARG:NH2	2.16	0.43
1:B:250:PRO:HG2	1:B:251:ILE:HD12	2.01	0.43
1:B:245:VAL:HG22	1:B:248:ARG:CB	2.48	0.43
1:D:154:ARG:HH22	1:D:193:ARG:HH21	1.67	0.43
1:A:158:ALA:HB2	1:A:186:ILE:HG21	2.01	0.42
1:C:121:ILE:HG13	1:C:160:ALA:HB1	2.01	0.42
1:B:128:ILE:HG23	1:B:183:VAL:HG21	2.00	0.42
1:B:273:GLU:CD	1:D:269:ARG:HH22	2.28	0.42
1:D:121:ILE:HG13	1:D:160:ALA:HB1	2.02	0.42
1:C:156:ASN:HA	1:C:159:ILE:HD12	2.02	0.42
1:D:156:ASN:HA	1:D:159:ILE:HD12	2.02	0.42
1:D:174:PRO:O	1:D:175:ARG:HD3	2.19	0.42
1:A:208:LEU:HD23	1:A:208:LEU:O	2.19	0.41
1:A:270:THR:HG21	1:C:266:ALA:O	2.20	0.41
1:B:245:VAL:HG21	1:B:253:VAL:HG22	2.02	0.41
1:D:215:MET:CE	1:D:232:ALA:HB3	2.50	0.41
1:B:145:VAL:HG11	1:B:198:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ARG:HH12	1:C:128:ILE:HA	1.84	0.41
1:B:215:MET:HE1	1:B:232:ALA:HB1	2.02	0.41
1:B:286:ARG:HG2	1:B:316:LEU:HB3	2.02	0.41
1:C:174:PRO:O	1:C:175:ARG:HD3	2.20	0.41
1:D:127:ARG:HH21	1:D:127:ARG:CG	2.32	0.41
1:A:286:ARG:HG2	1:A:316:LEU:HB3	2.01	0.41
1:A:128:ILE:HG23	1:A:183:VAL:HG21	2.03	0.41
1:A:250:PRO:HG2	1:A:251:ILE:HD12	2.03	0.41
1:A:293:TYR:CZ	1:A:315:GLN:HG3	2.56	0.41
1:D:158:ALA:HB2	1:D:186:ILE:HG21	2.01	0.41
1:B:150:SER:HB2	1:B:197:LEU:HD22	2.02	0.41
1:B:224:LEU:HD22	1:B:228:VAL:HG11	2.03	0.41
1:B:145:VAL:O	1:B:148:GLN:HB2	2.20	0.41
1:C:250:PRO:HG2	1:C:251:ILE:HD12	2.02	0.41
1:B:158:ALA:HB2	1:B:186:ILE:HG21	2.03	0.41
1:D:250:PRO:HG2	1:D:251:ILE:HD12	2.02	0.40
1:A:281:ALA:HB3	1:A:284:THR:HG23	2.04	0.40
1:B:267:GLU:HG3	1:D:273:GLU:HG3	2.03	0.40
1:D:128:ILE:HG23	1:D:183:VAL:HG11	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	202/211 (96%)	192 (95%)	7 (4%)	3 (2%)	8	30
1	B	208/211 (99%)	197 (95%)	9 (4%)	2 (1%)	12	40
1	C	208/211 (99%)	199 (96%)	7 (3%)	2 (1%)	12	40
1	D	208/211 (99%)	200 (96%)	6 (3%)	2 (1%)	12	40
All	All	826/844 (98%)	788 (95%)	29 (4%)	9 (1%)	11	38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	VAL
1	B	148	GLN
1	B	211	THR
1	C	148	GLN
1	C	211	THR
1	D	148	GLN
1	D	211	THR
1	A	146	TYR
1	A	149	LYS

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	175/180 (97%)	151 (86%)	24 (14%)	3	14
1	B	179/180 (99%)	160 (89%)	19 (11%)	6	23
1	C	179/180 (99%)	158 (88%)	21 (12%)	5	20
1	D	179/180 (99%)	156 (87%)	23 (13%)	4	17
All	All	712/720 (99%)	625 (88%)	87 (12%)	5	19

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ARG
1	A	115	MET
1	A	127	ARG
1	A	141	LEU
1	A	152	LYS
1	A	170	GLN
1	A	176	THR
1	A	177	PHE
1	A	179	GLU
1	A	188	LYS
1	A	200	LYS

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Mol	Chain	Res	Type
1	A	206	VAL
1	A	213	ASP
1	A	226	LYS
1	A	245	VAL
1	A	248	ARG
1	A	272	LYS
1	A	283	VAL
1	A	284	THR
1	A	295	ARG
1	A	310	VAL
1	A	311	ASP
1	A	313	LEU
1	A	315	GLN
1	B	112	ARG
1	B	115	MET
1	B	141	LEU
1	B	152	LYS
1	B	170	GLN
1	B	176	THR
1	B	177	PHE
1	B	208	LEU
1	B	209	ILE
1	B	213	ASP
1	B	226	LYS
1	B	248	ARG
1	B	249	SER
1	B	283	VAL
1	B	284	THR
1	B	295	ARG
1	B	310	VAL
1	B	311	ASP
1	B	313	LEU
1	C	112	ARG
1	C	115	MET
1	C	127	ARG
1	C	129	ASN
1	C	141	LEU
1	C	170	GLN
1	C	171	GLU
1	C	175	ARG
1	C	176	THR
1	C	200	LYS

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Mol	Chain	Res	Type
1	C	208	LEU
1	C	209	ILE
1	C	213	ASP
1	C	245	VAL
1	C	268	LYS
1	C	272	LYS
1	C	283	VAL
1	C	295	ARG
1	C	310	VAL
1	C	311	ASP
1	C	313	LEU
1	D	112	ARG
1	D	115	MET
1	D	126	ASP
1	D	127	ARG
1	D	129	ASN
1	D	141	LEU
1	D	170	GLN
1	D	171	GLU
1	D	175	ARG
1	D	176	THR
1	D	200	LYS
1	D	206	VAL
1	D	208	LEU
1	D	209	ILE
1	D	213	ASP
1	D	245	VAL
1	D	272	LYS
1	D	283	VAL
1	D	284	THR
1	D	295	ARG
1	D	310	VAL
1	D	311	ASP
1	D	313	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	144	GLN
1	A	148	GLN
1	A	221	ASN

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Mol	Chain	Res	Type
1	A	227	GLN
1	B	139	ASN
1	B	271	GLN
1	C	129	ASN
1	C	139	ASN
1	C	140	ASN
1	D	139	ASN
1	D	140	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

26 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	B	402	-	4,4,4	0.36	0	6,6,6	0.38	0
2	SO4	A	402	-	4,4,4	0.25	0	6,6,6	0.23	0
2	SO4	C	408	-	4,4,4	0.27	0	6,6,6	0.12	0
2	SO4	D	403	-	4,4,4	0.30	0	6,6,6	0.10	0
2	SO4	C	402	-	4,4,4	0.27	0	6,6,6	0.22	0
2	SO4	B	401	-	4,4,4	0.28	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	403	-	4,4,4	0.23	0	6,6,6	0.20	0
2	SO4	D	406	-	4,4,4	0.36	0	6,6,6	0.19	0
2	SO4	B	405	-	4,4,4	0.34	0	6,6,6	0.22	0
2	SO4	D	401	-	4,4,4	0.48	0	6,6,6	0.29	0
2	SO4	C	405	-	4,4,4	0.26	0	6,6,6	0.26	0
2	SO4	C	403	-	4,4,4	0.32	0	6,6,6	0.27	0
2	SO4	A	403	-	4,4,4	0.11	0	6,6,6	0.52	0
2	SO4	C	406	-	4,4,4	0.33	0	6,6,6	0.11	0
2	SO4	D	404	-	4,4,4	0.29	0	6,6,6	0.08	0
2	SO4	C	401	-	4,4,4	0.21	0	6,6,6	0.28	0
2	SO4	A	405	-	4,4,4	0.21	0	6,6,6	0.37	0
2	SO4	D	407	-	4,4,4	0.34	0	6,6,6	0.18	0
2	SO4	A	401	-	4,4,4	0.32	0	6,6,6	0.21	0
2	SO4	D	402	-	4,4,4	0.20	0	6,6,6	0.25	0
2	SO4	A	404	-	4,4,4	0.33	0	6,6,6	0.16	0
2	SO4	C	407	-	4,4,4	0.23	0	6,6,6	0.24	0
2	SO4	C	404	-	4,4,4	0.24	0	6,6,6	0.20	0
2	SO4	B	404	-	4,4,4	0.19	0	6,6,6	0.27	0
2	SO4	D	408	-	4,4,4	0.29	0	6,6,6	0.23	0
2	SO4	D	405	-	4,4,4	0.30	0	6,6,6	0.17	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

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	206/211 (97%)	0.39	12 (5%)	29 22	68, 107, 163, 200	0
1	B	210/211 (99%)	0.35	13 (6%)	26 21	68, 106, 153, 169	0
1	C	210/211 (99%)	0.02	4 (1%)	66 51	69, 91, 122, 144	0
1	D	210/211 (99%)	0.03	2 (0%)	79 66	71, 91, 125, 145	0
All	All	836/844 (99%)	0.20	31 (3%)	45 32	68, 96, 150, 200	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	GLY	5.0
1	A	208	LEU	4.5
1	B	204	THR	4.3
1	B	107	MET	3.8
1	A	179	GLU	3.7
1	B	206	VAL	3.6
1	B	177	PHE	3.5
1	A	169	ARG	3.4
1	D	211	THR	3.3
1	A	204	THR	3.0
1	D	268	LYS	3.0
1	B	211	THR	2.9
1	B	252	SER	2.8
1	A	148	GLN	2.8
1	A	110	SER	2.8
1	B	210	THR	2.6
1	C	211	THR	2.6
1	B	208	LEU	2.6
1	B	205	SER	2.5
1	C	107	MET	2.5
1	A	173	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	248	ARG	2.4
1	A	207	ASP	2.4
1	A	252	SER	2.3
1	B	119	LYS	2.3
1	A	177	PHE	2.3
1	B	207	ASP	2.3
1	B	212	GLY	2.2
1	B	152	LYS	2.2
1	C	212	GLY	2.1
1	A	206	VAL	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
2	SO4	C	408	5/5	0.41	0.12	194,194,195,195	0
2	SO4	D	406	5/5	0.43	0.18	183,183,184,185	0
2	SO4	B	405	5/5	0.49	0.17	172,173,173,174	0
2	SO4	D	404	5/5	0.62	0.11	180,182,183,183	0
2	SO4	A	401	5/5	0.66	0.17	176,176,178,179	0
2	SO4	A	404	5/5	0.66	0.21	162,164,164,164	0
2	SO4	A	402	5/5	0.68	0.21	158,160,161,162	0
2	SO4	D	405	5/5	0.70	0.15	163,164,165,167	0
2	SO4	C	403	5/5	0.70	0.22	156,157,159,160	0
2	SO4	A	405	5/5	0.72	0.13	150,153,153,154	0
2	SO4	D	408	5/5	0.72	0.15	181,182,183,185	0
2	SO4	C	404	5/5	0.75	0.18	180,180,181,182	0
2	SO4	B	401	5/5	0.76	0.22	157,157,159,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	403	5/5	0.79	0.23	154,156,157,157	0
2	SO4	B	404	5/5	0.79	0.15	150,151,153,153	0
2	SO4	C	407	5/5	0.80	0.12	180,182,183,185	0
2	SO4	C	406	5/5	0.80	0.21	151,153,154,155	0
2	SO4	C	405	5/5	0.84	0.14	153,154,156,156	0
2	SO4	D	407	5/5	0.86	0.17	155,157,159,159	0
2	SO4	D	403	5/5	0.89	0.12	158,160,161,161	0
2	SO4	D	402	5/5	0.91	0.15	132,133,134,135	0
2	SO4	C	401	5/5	0.92	0.09	107,107,107,108	0
2	SO4	C	402	5/5	0.93	0.13	119,122,123,126	0
2	SO4	B	402	5/5	0.93	0.09	104,106,107,108	0
2	SO4	A	403	5/5	0.95	0.12	100,100,100,101	0
2	SO4	D	401	5/5	0.96	0.07	103,104,106,106	0

6.5 Other polymers [i](#)

There are no such residues in this entry.