



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:18 PM UTC

PDB ID : 3IAV / pdb_00003iav
Title : Propionyl-CoA Carboxylase Beta Subunit, D422V
Authors : Diacovich, L.; Arabolaza, A.; Shillito, E.M.; Lin, T.-W.; Mitchell, D.L.; Pham, H.; Melgar, M.M.
Deposited on : 2009-07-14
Resolution : 1.75 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

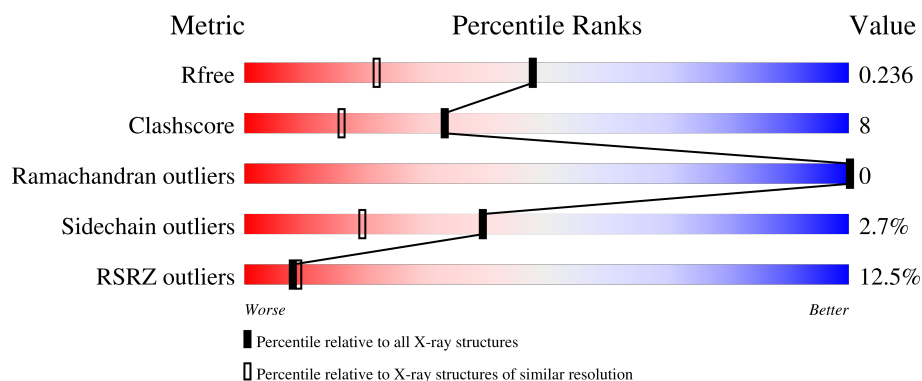
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	530	12% 81% 16% ..
1	B	530	13% 82% 15% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8254 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.

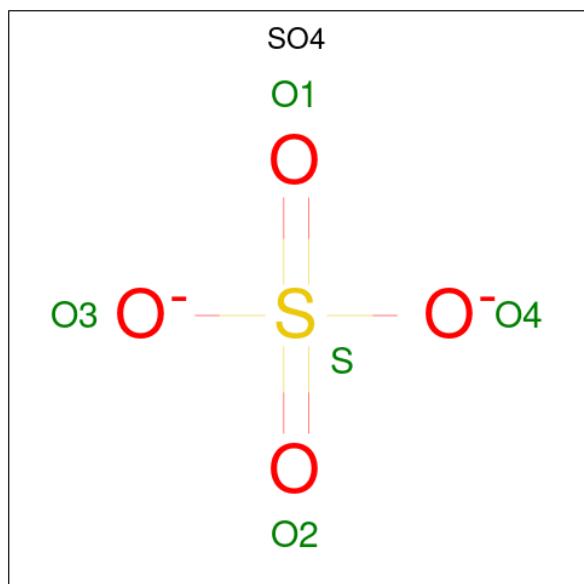
- Molecule 1 is a protein called Propionyl-CoA carboxylase complex B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			3952	2482	698	759	13			
1	B	521	Total	C	N	O	S	0	0	0
			3952	2482	698	759	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	VAL	ASP	engineered mutation	UNP Q9X4K7
B	422	VAL	ASP	engineered mutation	UNP Q9X4K7

- 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		

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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		

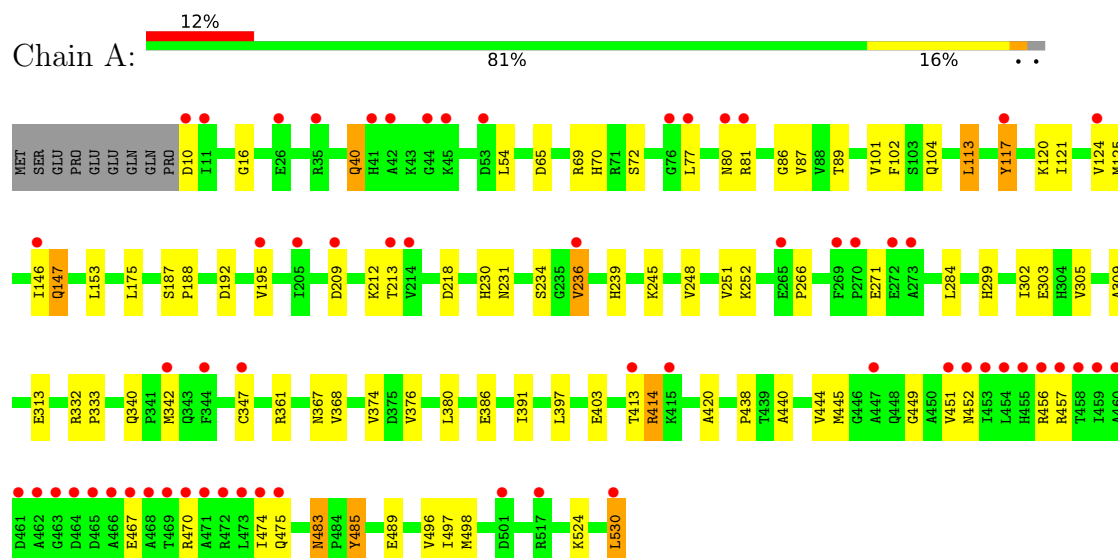
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	162	Total	O	0	0
			162	162		
3	B	158	Total	O	0	0
			158	158		

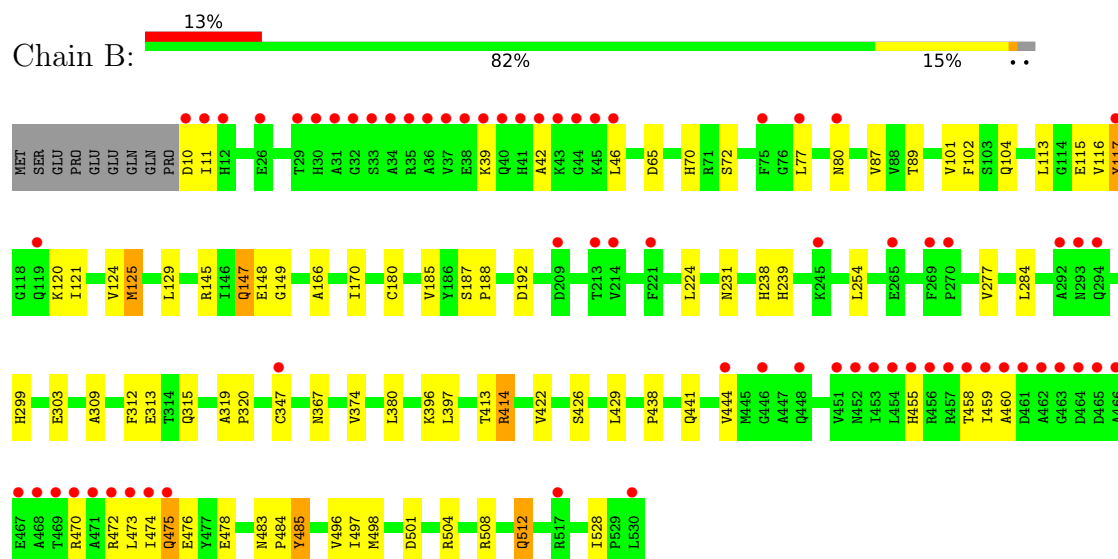
3 Residue-property plots [i](#)

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: Propionyl-CoA carboxylase complex B subunit



- Molecule 1: Propionyl-CoA carboxylase complex B subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	171.53Å 171.53Å 75.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.75 50.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	89.2 (50.00-1.75) 89.2 (50.00-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 1.75Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.233 0.221 , 0.236	Depositor DCC
R_{free} test set	6241 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 25.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8254	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.99% 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	0.40	0/4032	0.90	10/5477 (0.2%)
1	B	0.42	1/4032 (0.0%)	0.93	14/5477 (0.3%)
All	All	0.41	1/8064 (0.0%)	0.91	24/10954 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	VAL	C-N	-7.57	1.23	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	VAL	N-CA-C	8.11	119.53	108.17
1	A	413	THR	N-CA-C	-7.49	101.58	111.24
1	A	413	THR	CB-CA-C	7.44	123.14	110.86
1	A	192	ASP	N-CA-C	7.22	119.23	111.36
1	B	374	VAL	N-CA-C	7.08	118.09	108.17
1	B	413	THR	N-CA-C	6.70	118.37	111.14
1	B	192	ASP	N-CA-C	6.62	118.58	111.36
1	B	460	ALA	N-CA-C	-6.54	103.77	111.03
1	A	496	VAL	N-CA-C	-6.30	98.80	107.99
1	B	414	ARG	O-C-N	-5.97	114.66	122.59
1	B	367	ASN	N-CA-C	5.96	119.86	112.24
1	B	498	MET	N-CA-C	-5.82	102.43	109.83
1	B	116	VAL	CA-C-N	5.78	128.60	120.28
1	B	116	VAL	C-N-CA	5.78	128.60	120.28
1	B	496	VAL	N-CA-C	-5.74	99.47	107.80
1	B	414	ARG	N-CA-C	5.72	122.99	110.80
1	B	115	GLU	N-CA-C	5.65	117.13	110.97
1	B	180	CYS	N-CA-C	-5.55	97.97	107.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	485	TYR	N-CA-C	5.48	118.18	111.82
1	A	485	TYR	N-CA-C	5.17	118.74	112.23
1	A	414	ARG	N-CA-C	5.13	121.72	110.80
1	A	367	ASN	N-CA-C	5.10	118.76	112.24
1	A	524	LYS	N-CA-C	-5.09	105.81	111.36
1	A	498	MET	N-CA-C	-5.01	103.47	109.83

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	3952	0	3885	67	0
1	B	3952	0	3885	62	0
2	A	25	0	0	0	0
2	B	5	0	0	0	0
3	A	162	0	0	1	0
3	B	158	0	0	0	0
All	All	8254	0	7770	123	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 (123) 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:87:VAL:HB	1:A:117:TYR:CE1	1.69	1.27
1:A:104:GLN:HG2	1:A:117:TYR:OH	1.46	1.13
1:A:104:GLN:HG2	1:A:117:TYR:HH	1.05	1.11
1:B:104:GLN:HG2	1:B:117:TYR:OH	1.60	1.01
1:A:104:GLN:CG	1:A:117:TYR:OH	2.22	0.87
1:B:187:SER:HB3	1:B:188:PRO:HD3	1.58	0.86
1:A:117:TYR:CD2	1:A:117:TYR:O	2.30	0.84
1:B:117:TYR:HE1	1:B:121:ILE:HD11	1.39	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLN:NE2	1:A:147:GLN:H	1.78	0.81
1:A:146:ILE:HD12	1:A:146:ILE:H	1.45	0.81
1:B:104:GLN:CG	1:B:117:TYR:OH	2.28	0.81
1:B:117:TYR:HD1	1:B:117:TYR:C	1.89	0.80
1:B:483:ASN:HD22	1:B:485:TYR:H	1.32	0.77
1:A:117:TYR:CD2	1:A:117:TYR:C	2.63	0.74
1:B:117:TYR:C	1:B:117:TYR:CD1	2.60	0.74
1:B:121:ILE:HG22	1:B:125:MET:CE	2.18	0.74
1:A:147:GLN:H	1:A:147:GLN:HE21	1.35	0.74
1:A:485:TYR:O	1:A:489:GLU:HG3	1.88	0.73
1:B:117:TYR:CE1	1:B:121:ILE:HD11	2.24	0.71
1:A:483:ASN:HD22	1:A:485:TYR:H	1.36	0.71
1:B:117:TYR:HD1	1:B:117:TYR:O	1.74	0.71
1:A:187:SER:HB3	1:A:188:PRO:HD3	1.72	0.70
1:A:87:VAL:HB	1:A:117:TYR:CD1	2.24	0.70
1:B:10:ASP:CG	1:B:11:ILE:H	2.02	0.68
1:B:117:TYR:CD1	1:B:117:TYR:O	2.47	0.67
1:B:70:HIS:HD2	1:B:72:SER:H	1.44	0.65
1:A:451:VAL:HG21	1:A:474:ILE:HG12	1.79	0.65
1:A:248:VAL:O	1:A:251:VAL:HG22	1.96	0.65
1:B:299:HIS:HE1	1:B:313:GLU:OE2	1.79	0.64
1:A:70:HIS:HD2	1:A:72:SER:H	1.47	0.63
1:B:121:ILE:HG22	1:B:125:MET:HE1	1.80	0.63
1:B:147:GLN:NE2	1:B:147:GLN:H	1.95	0.63
1:A:87:VAL:HB	1:A:117:TYR:CZ	2.32	0.63
1:A:456:ARG:HH21	1:A:457:ARG:HD2	1.65	0.62
1:B:121:ILE:HG22	1:B:125:MET:HE3	1.82	0.61
1:A:113:LEU:HD22	1:A:117:TYR:CE2	2.35	0.61
1:A:87:VAL:CB	1:A:117:TYR:CE1	2.64	0.60
1:A:113:LEU:HD22	1:A:117:TYR:CD2	2.37	0.60
1:B:87:VAL:HB	1:B:117:TYR:CZ	2.37	0.59
1:B:231:ASN:HD21	1:B:239:HIS:N	2.01	0.58
1:A:89:THR:HB	1:A:124:VAL:HG21	1.87	0.56
1:A:299:HIS:HE1	1:A:313:GLU:OE2	1.88	0.56
1:B:65:ASP:HB2	1:B:120:LYS:HE3	1.86	0.56
1:B:147:GLN:H	1:B:147:GLN:HE21	1.52	0.56
1:A:361:ARG:HD2	1:A:403:GLU:OE2	2.05	0.56
1:A:89:THR:HB	1:A:124:VAL:CG2	2.36	0.56
1:A:69:ARG:HD3	1:A:81:ARG:O	2.06	0.56
1:A:445:MET:HE2	1:A:449:GLY:HA3	1.87	0.55
1:B:70:HIS:HE1	1:B:80:ASN:O	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:VAL:HB	1:B:117:TYR:CE2	2.42	0.54
1:B:125:MET:O	1:B:129:LEU:HD23	2.08	0.54
1:B:455:HIS:HB3	1:B:458:THR:CG2	2.38	0.54
1:A:65:ASP:HB2	1:A:120:LYS:HE3	1.90	0.53
1:B:129:LEU:HD22	1:B:170:ILE:HD11	1.90	0.53
1:B:121:ILE:CG2	1:B:125:MET:HE1	2.38	0.53
1:A:117:TYR:C	1:A:117:TYR:HD2	2.12	0.52
1:B:426:SER:OG	1:B:429:LEU:HD13	2.10	0.52
1:A:231:ASN:HD21	1:A:239:HIS:N	2.08	0.52
1:A:209:ASP:O	1:A:213:THR:HG23	2.11	0.51
1:A:391:ILE:HG12	1:B:185:VAL:HG21	1.93	0.51
1:A:86:GLY:O	1:A:117:TYR:HE1	1.95	0.50
1:B:438:PRO:HD3	1:B:497:ILE:O	2.11	0.50
1:A:230:HIS:HB3	1:A:236:VAL:HG22	1.94	0.50
1:B:117:TYR:HE1	1:B:121:ILE:CD1	2.20	0.50
1:A:153:LEU:HD11	1:B:444:VAL:HA	1.93	0.49
1:A:414:ARG:HA	1:A:440:ALA:HA	1.92	0.49
1:A:234:SER:OG	1:A:236:VAL:HG13	2.11	0.49
1:B:121:ILE:CG2	1:B:125:MET:CE	2.89	0.48
1:B:455:HIS:HB3	1:B:458:THR:HG22	1.94	0.48
1:B:277:VAL:HG13	1:B:277:VAL:O	2.12	0.48
1:B:347:CYS:SG	1:B:380:LEU:HB2	2.54	0.48
1:A:101:VAL:HG22	1:A:102:PHE:N	2.29	0.48
1:B:422:VAL:HG12	1:B:429:LEU:HD11	1.96	0.47
1:B:89:THR:HB	1:B:124:VAL:HG11	1.97	0.47
1:B:187:SER:HB3	1:B:188:PRO:CD	2.39	0.47
1:A:347:CYS:SG	1:A:380:LEU:HD13	2.55	0.47
1:A:530:LEU:HG	1:B:396:LYS:HD3	1.97	0.47
1:A:10:ASP:O	1:A:16:GLY:HA3	2.15	0.46
1:A:146:ILE:H	1:A:146:ILE:CD1	2.20	0.46
1:B:459:ILE:HD13	1:B:470:ARG:HH21	1.80	0.46
1:B:474:ILE:O	1:B:478:GLU:HG3	2.15	0.46
1:A:302:ILE:O	1:A:305:VAL:HG22	2.16	0.46
1:B:113:LEU:C	1:B:113:LEU:HD23	2.41	0.46
1:A:376:VAL:HG21	1:A:420:ALA:HB1	1.98	0.45
1:B:101:VAL:HG22	1:B:102:PHE:N	2.30	0.45
1:A:147:GLN:HE21	1:A:147:GLN:N	2.10	0.45
1:B:46:LEU:HD12	1:B:46:LEU:N	2.32	0.45
1:B:472:ARG:O	1:B:476:GLU:HG3	2.17	0.45
1:B:254:LEU:HD13	1:B:312:PHE:HE2	1.82	0.45
1:A:87:VAL:CB	1:A:117:TYR:CD1	2.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:GLN:HE21	1:B:512:GLN:HB3	1.62	0.44
1:B:504:ARG:NH1	1:B:508:ARG:HD2	2.32	0.44
1:A:438:PRO:HD3	1:A:497:ILE:O	2.17	0.43
1:A:271:GLU:O	1:A:271:GLU:HG3	2.17	0.43
1:A:467:GLU:CD	1:A:470:ARG:HH12	2.26	0.43
1:A:248:VAL:HG12	1:A:252:LYS:HE3	2.00	0.43
1:A:54:LEU:HD21	1:A:245:LYS:HA	2.00	0.43
1:A:212:LYS:HD3	1:A:218:ASP:OD1	2.19	0.43
1:B:39:LYS:O	1:B:42:ALA:HB3	2.19	0.43
1:A:340:GLN:CD	1:A:342:MET:HG2	2.44	0.42
1:B:319:ALA:N	1:B:320:PRO:HD3	2.34	0.42
1:A:452:ASN:O	1:A:456:ARG:HB2	2.20	0.42
1:B:145:ARG:HD2	1:B:148:GLU:OE2	2.20	0.42
1:A:266:PRO:CG	1:A:368:VAL:HG22	2.49	0.42
1:B:129:LEU:HD21	1:B:166:ALA:HB2	2.01	0.42
1:A:303:GLU:O	1:A:309:ALA:HA	2.20	0.42
1:A:40:GLN:HE21	1:A:40:GLN:HA	1.84	0.42
1:B:10:ASP:CG	1:B:11:ILE:N	2.73	0.41
1:A:444:VAL:HG13	1:B:149:GLY:C	2.44	0.41
1:A:101:VAL:CG2	1:A:102:PHE:N	2.83	0.41
1:A:121:ILE:O	1:A:125:MET:HG3	2.20	0.41
1:A:386:GLU:HG3	1:B:224:LEU:HD11	2.02	0.41
1:A:451:VAL:HG21	1:A:474:ILE:CG1	2.49	0.41
1:A:332:ARG:HA	1:A:333:PRO:HD3	1.95	0.41
1:B:231:ASN:HD21	1:B:239:HIS:CA	2.33	0.41
1:B:238:HIS:HA	1:B:315:GLN:HG2	2.03	0.41
1:B:414:ARG:O	1:B:441:GLN:N	2.52	0.41
1:A:361:ARG:NH2	1:B:528:ILE:HG22	2.36	0.41
1:A:444:VAL:HG22	3:A:618:HOH:O	2.21	0.40
1:B:303:GLU:O	1:B:309:ALA:HA	2.21	0.40
1:A:70:HIS:HE1	1:A:80:ASN:O	2.04	0.40
1:A:175:LEU:HD12	1:A:195:VAL:HG13	2.03	0.40
1:B:475:GLN:HE21	1:B:475:GLN:HB3	1.59	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	519/530 (98%)	502 (97%)	17 (3%)	0	100	100
1	B	519/530 (98%)	503 (97%)	16 (3%)	0	100	100
All	All	1038/1060 (98%)	1005 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	412/421 (98%)	401 (97%)	11 (3%)	39	19
1	B	412/421 (98%)	401 (97%)	11 (3%)	39	19
All	All	824/842 (98%)	802 (97%)	22 (3%)	39	19

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	77	LEU
1	A	113	LEU
1	A	117	TYR
1	A	147	GLN
1	A	236	VAL
1	A	284	LEU
1	A	397	LEU

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Mol	Chain	Res	Type
1	A	475	GLN
1	A	483	ASN
1	A	530	LEU
1	B	77	LEU
1	B	117	TYR
1	B	125	MET
1	B	147	GLN
1	B	284	LEU
1	B	397	LEU
1	B	473	LEU
1	B	475	GLN
1	B	484	PRO
1	B	501	ASP
1	B	512	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	40	GLN
1	A	70	HIS
1	A	74	ASN
1	A	80	ASN
1	A	119	GLN
1	A	147	GLN
1	A	163	ASN
1	A	199	GLN
1	A	231	ASN
1	A	299	HIS
1	A	367	ASN
1	A	448	GLN
1	A	475	GLN
1	A	483	ASN
1	A	512	GLN
1	B	40	GLN
1	B	70	HIS
1	B	74	ASN
1	B	119	GLN
1	B	147	GLN
1	B	163	ASN
1	B	199	GLN
1	B	231	ASN

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Mol	Chain	Res	Type
1	B	299	HIS
1	B	455	HIS
1	B	475	GLN
1	B	483	ASN
1	B	512	GLN
1	B	527	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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	535	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	B	531	-	4,4,4	0.38	0	6,6,6	0.08	0
2	SO4	A	534	-	4,4,4	0.40	0	6,6,6	0.09	0
2	SO4	A	533	-	4,4,4	0.35	0	6,6,6	0.11	0
2	SO4	A	532	-	4,4,4	0.46	0	6,6,6	0.09	0
2	SO4	A	531	-	4,4,4	0.45	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	521/530 (98%)	0.73	61 (11%) 9 10	11, 18, 41, 102	0
1	B	521/530 (98%)	0.65	69 (13%) 7 8	11, 17, 45, 89	0
All	All	1042/1060 (98%)	0.69	130 (12%) 8 9	11, 17, 45, 102	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	ALA	10.0
1	B	44	GLY	10.0
1	A	117	TYR	9.8
1	A	462	ALA	9.6
1	B	462	ALA	8.9
1	A	459	ILE	8.8
1	B	459	ILE	8.7
1	A	463	GLY	8.2
1	A	458	THR	8.2
1	B	458	THR	7.7
1	A	466	ALA	7.4
1	B	117	TYR	7.2
1	B	463	GLY	6.9
1	A	468	ALA	6.7
1	A	471	ALA	6.6
1	B	468	ALA	6.5
1	B	37	VAL	6.5
1	B	466	ALA	6.3
1	A	469	THR	6.2
1	A	269	PHE	6.0
1	A	454	LEU	5.8
1	A	465	ASP	5.7
1	A	461	ASP	5.6
1	B	465	ASP	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	467	GLU	5.5
1	B	31	ALA	5.5
1	B	32	GLY	5.5
1	A	10	ASP	5.4
1	B	460	ALA	5.3
1	A	453	ILE	5.3
1	A	347	CYS	5.2
1	B	464	ASP	5.0
1	B	457	ARG	5.0
1	A	473	LEU	4.8
1	B	469	THR	4.8
1	A	457	ARG	4.7
1	A	474	ILE	4.5
1	B	461	ASP	4.5
1	B	456	ARG	4.5
1	A	464	ASP	4.4
1	B	11	ILE	4.4
1	B	41	HIS	4.3
1	A	470	ARG	4.2
1	B	34	ALA	4.2
1	B	39	LYS	4.2
1	B	269	PHE	4.2
1	B	347	CYS	4.1
1	B	43	LYS	4.1
1	B	42	ALA	4.0
1	B	38	GLU	4.0
1	A	517	ARG	4.0
1	A	455	HIS	4.0
1	A	41	HIS	3.9
1	B	36	ALA	3.9
1	B	35	ARG	3.9
1	B	530	LEU	3.9
1	A	530	LEU	3.8
1	B	30	HIS	3.8
1	A	456	ARG	3.8
1	A	11	ILE	3.7
1	B	33	SER	3.7
1	B	517	ARG	3.7
1	B	10	ASP	3.6
1	B	213	THR	3.6
1	A	35	ARG	3.6
1	A	272	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	451	VAL	3.5
1	B	471	ALA	3.5
1	B	209	ASP	3.4
1	A	467	GLU	3.4
1	A	77	LEU	3.4
1	B	470	ARG	3.4
1	A	344	PHE	3.3
1	B	451	VAL	3.3
1	A	452	ASN	3.3
1	B	453	ILE	3.2
1	A	472	ARG	3.2
1	B	293	ASN	3.1
1	A	475	GLN	3.1
1	A	44	GLY	3.0
1	A	213	THR	3.0
1	B	265	GLU	2.9
1	B	45	LYS	2.8
1	B	245	LYS	2.8
1	B	46	LEU	2.8
1	B	452	ASN	2.8
1	A	342	MET	2.7
1	B	472	ARG	2.7
1	A	447	ALA	2.7
1	A	265	GLU	2.6
1	A	413	THR	2.6
1	B	454	LEU	2.6
1	B	40	GLN	2.6
1	B	455	HIS	2.6
1	B	80	ASN	2.6
1	B	294	GLN	2.5
1	B	77	LEU	2.5
1	A	80	ASN	2.4
1	A	124	VAL	2.4
1	B	214	VAL	2.4
1	B	221	PHE	2.4
1	A	53	ASP	2.4
1	A	26	GLU	2.3
1	B	75	PHE	2.3
1	A	195	VAL	2.3
1	B	444	VAL	2.3
1	B	26	GLU	2.3
1	A	415	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	473	LEU	2.3
1	A	146	ILE	2.3
1	B	475	GLN	2.2
1	B	12	HIS	2.2
1	B	270	PRO	2.2
1	B	292	ALA	2.2
1	A	205	ILE	2.2
1	B	119	GLN	2.2
1	B	474	ILE	2.2
1	A	270	PRO	2.1
1	A	42	ALA	2.1
1	A	214	VAL	2.1
1	A	273	ALA	2.1
1	B	448	GLN	2.1
1	A	81	ARG	2.1
1	B	29	THR	2.1
1	A	209	ASP	2.1
1	A	501	ASP	2.1
1	A	45	LYS	2.1
1	A	76	GLY	2.0
1	B	446	GLY	2.0
1	A	236	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	A	532	5/5	0.14	0.26	63,64,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	531	5/5	0.90	0.11	41,42,42,43	0
2	SO4	A	533	5/5	0.94	0.16	30,31,34,34	0
2	SO4	A	534	5/5	0.95	0.09	36,37,39,40	0
2	SO4	A	535	5/5	0.96	0.09	26,28,29,31	0
2	SO4	B	531	5/5	0.97	0.07	25,29,30,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.