



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:04 AM UTC

PDB ID : 2BUH / pdb_00002buh
Title : E. COLI BETA-KETOACYL (ACYL CARRIER PROTEIN) SYNTHASE I,
120 K
Authors : Olsen, J.G.; Von Wettstein-Knowles, P.; Henriksen, A.
Deposited on : 2005-06-13
Resolution : 1.90 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
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

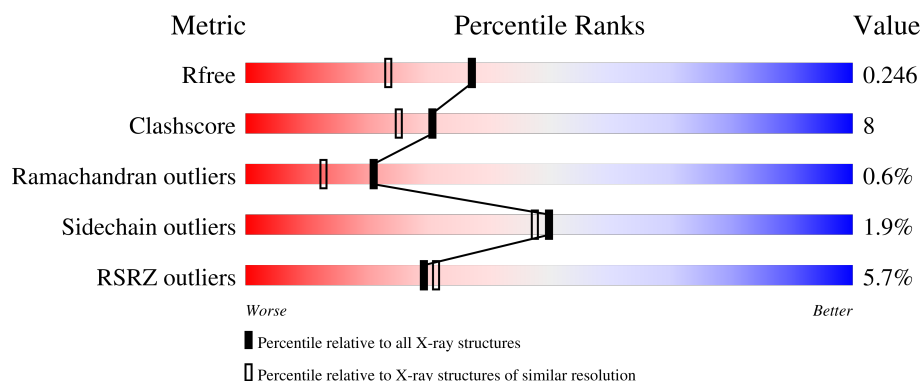
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	406	3% 83% 15% .
1	B	406	9% 83% 15% .
1	C	406	7% 79% 19% .
1	D	406	4% 88% 10% .

2 Entry composition [i](#)

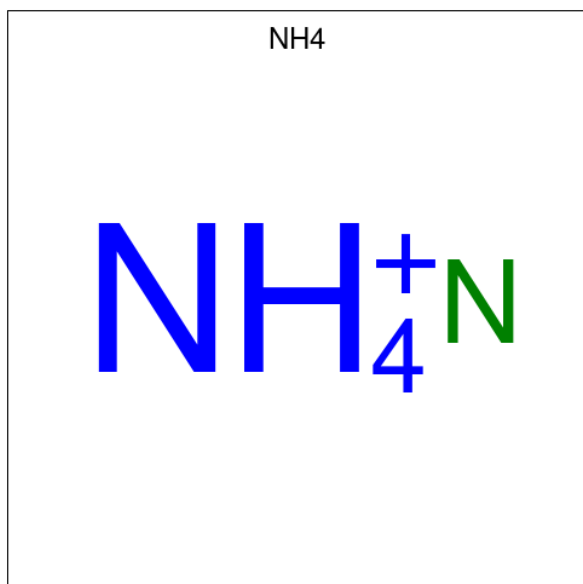
There are 3 unique types of molecules in this entry. The entry contains 12825 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			2981	1853	519	586	23			
1	B	406	Total	C	N	O	S	0	0	0
			2981	1853	519	586	23			
1	C	406	Total	C	N	O	S	0	0	0
			2981	1853	519	586	23			
1	D	406	Total	C	N	O	S	0	0	0
			2981	1853	519	586	23			

- Molecule 2 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	N	0	0
			1	1		
2	B	1	Total	N	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total N 1 1	0	0
2	D	1	Total N 1 1	0	0

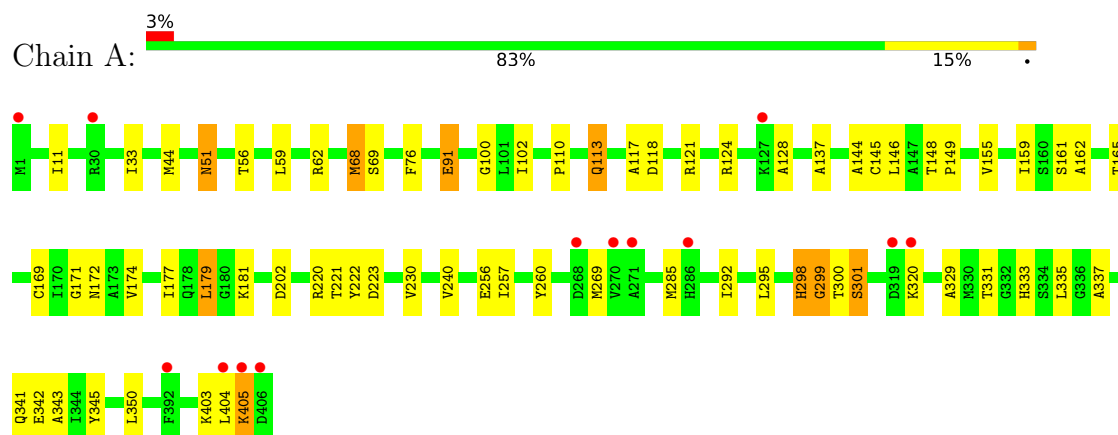
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	256	Total O 256 256	0	0
3	B	196	Total O 196 196	0	0
3	C	191	Total O 191 191	0	0
3	D	254	Total O 254 254	0	0

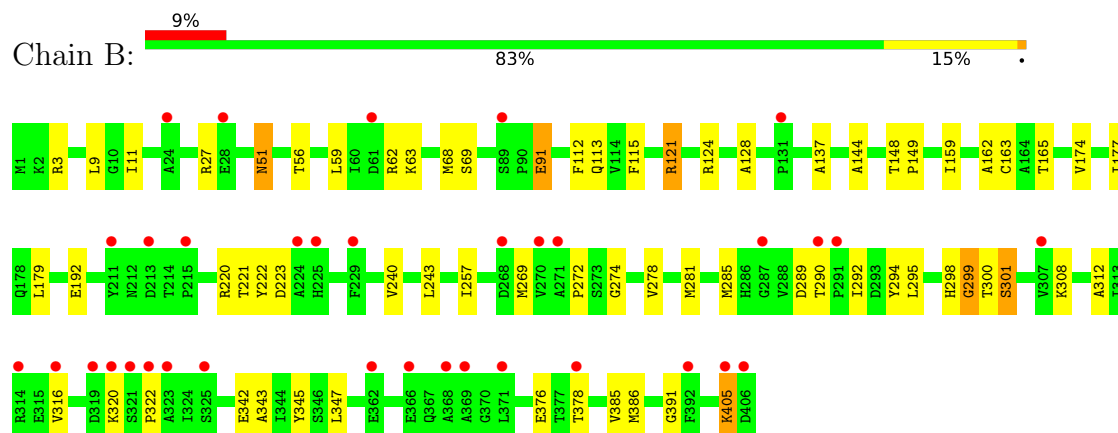
3 Residue-property plots

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.

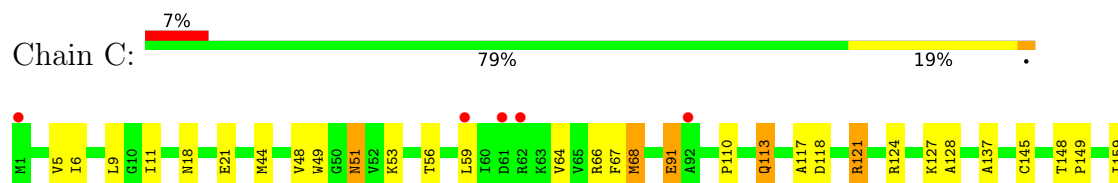
• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I

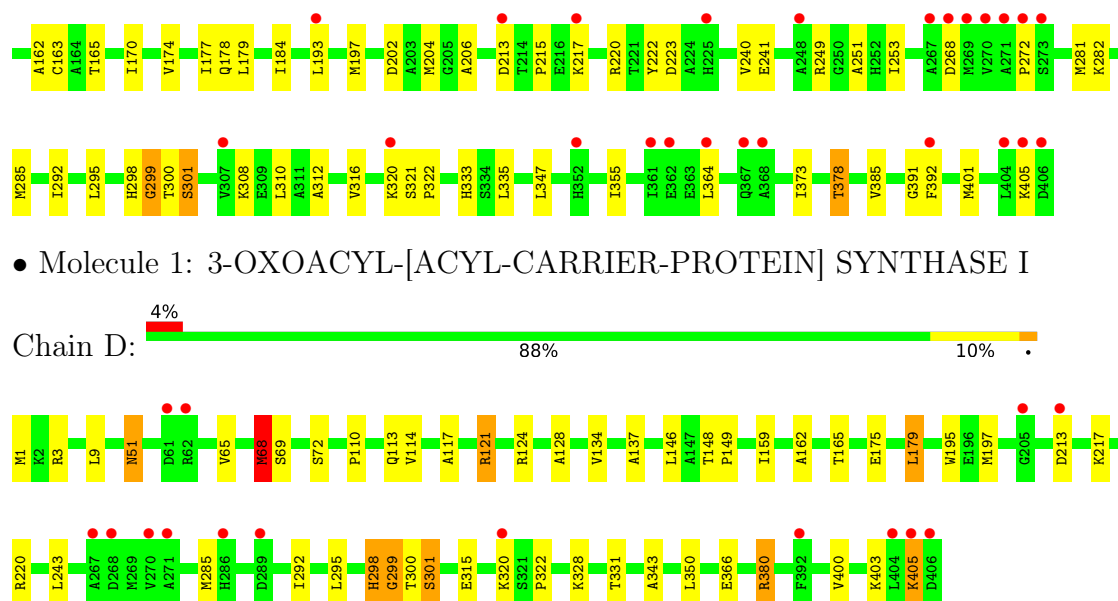


• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I

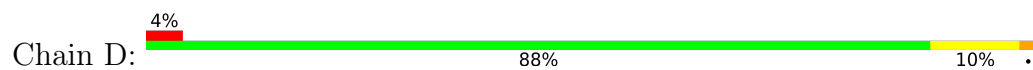


• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I





● Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.12Å 139.43Å 212.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.73 – 1.90 29.73 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.5 (29.73-1.90) 89.6 (29.73-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.256 0.204 , 0.246	Depositor DCC
R_{free} test set	6276 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12825	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: NH4

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	0/3029	0.90	8/4090 (0.2%)
1	B	0.38	0/3029	0.85	5/4090 (0.1%)
1	C	0.37	0/3029	0.84	4/4090 (0.1%)
1	D	0.41	0/3029	0.90	7/4090 (0.2%)
All	All	0.39	0/12116	0.87	24/16360 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	MET	N-CA-C	7.59	122.20	109.76
1	A	68	MET	N-CA-C	7.36	121.83	109.76
1	A	331	THR	N-CA-C	7.17	122.12	113.23
1	C	68	MET	N-CA-C	6.88	120.88	109.95
1	D	243	LEU	N-CA-C	6.80	119.27	111.11
1	D	68	MET	N-CA-C	6.62	120.83	110.17
1	A	298	HIS	N-CA-C	-6.56	104.21	111.36
1	D	298	HIS	N-CA-C	-6.44	104.19	111.14
1	D	343	ALA	N-CA-C	-6.41	104.38	111.36
1	A	69	SER	N-CA-C	-6.38	101.02	110.46
1	A	343	ALA	N-CA-C	-6.14	104.67	111.36
1	D	331	THR	N-CA-C	5.76	120.38	113.23
1	A	113	GLN	N-CA-C	-5.63	105.06	111.14
1	B	162	ALA	CB-CA-C	-5.62	110.08	116.54
1	A	162	ALA	CB-CA-C	-5.58	110.12	116.54
1	C	11	ILE	N-CA-C	5.45	115.40	107.88
1	C	113	GLN	N-CA-C	-5.34	105.54	111.36
1	C	162	ALA	CB-CA-C	-5.34	110.40	116.54
1	D	69	SER	N-CA-C	-5.29	102.19	110.17
1	D	162	ALA	CB-CA-C	-5.28	110.47	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	ILE	N-CA-C	5.26	115.13	107.88
1	B	243	LEU	N-CA-C	5.23	117.40	111.02
1	B	69	SER	N-CA-C	-5.22	102.74	110.46
1	B	11	ILE	N-CA-C	5.07	114.55	108.06

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	2981	0	2939	51	0
1	B	2981	0	2939	53	0
1	C	2981	0	2939	63	0
1	D	2981	0	2939	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	256	0	0	2	0
3	B	196	0	0	2	0
3	C	191	0	0	4	0
3	D	254	0	0	3	0
All	All	12825	0	11756	197	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 (197) 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:110:PRO:HG3	1:B:113:GLN:HE22	1.29	0.96
1:B:285:MET:HE2	1:B:386:MET:HE1	1.45	0.95
1:A:405:LYS:HD2	1:A:405:LYS:H	1.33	0.93
1:B:51:ASN:H	1:B:51:ASN:HD22	1.19	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:ASN:H	1:D:51:ASN:HD22	1.17	0.90
1:C:405:LYS:HD2	1:C:405:LYS:H	1.34	0.89
1:A:51:ASN:H	1:A:51:ASN:HD22	1.15	0.88
1:B:285:MET:HE1	1:B:316:VAL:HG11	1.61	0.82
1:B:3:ARG:HH22	1:B:405:LYS:HZ1	1.30	0.80
1:D:285:MET:HE2	1:D:285:MET:HA	1.65	0.79
1:D:285:MET:HE3	1:D:400:VAL:HG21	1.63	0.79
1:C:204:MET:HE2	1:C:206:ALA:HB2	1.66	0.78
1:C:148:THR:HB	1:C:149:PRO:HD3	1.66	0.78
1:B:124:ARG:HB2	1:B:128:ALA:HB2	1.66	0.77
1:D:380:ARG:HD3	3:D:2244:HOH:O	1.87	0.74
1:C:282:LYS:HA	1:C:285:MET:HE2	1.68	0.73
1:B:148:THR:HB	1:B:149:PRO:HD3	1.69	0.73
1:C:177:ILE:HD12	1:C:240:VAL:HG12	1.71	0.72
1:D:148:THR:HB	1:D:149:PRO:HD3	1.71	0.72
1:A:148:THR:HB	1:A:149:PRO:HD3	1.71	0.71
1:C:124:ARG:HB2	1:C:128:ALA:HB2	1.73	0.71
1:A:405:LYS:H	1:A:405:LYS:CD	1.97	0.71
1:C:110:PRO:HG3	1:D:113:GLN:HE22	1.55	0.70
1:B:51:ASN:HD22	1:B:51:ASN:N	1.88	0.68
1:A:405:LYS:HD2	1:A:405:LYS:N	2.08	0.67
1:A:51:ASN:HD22	1:A:51:ASN:N	1.89	0.66
1:B:62:ARG:HH21	1:B:63:LYS:HE3	1.62	0.65
1:C:56:THR:HA	1:C:59:LEU:HD12	1.78	0.65
1:A:177:ILE:HD12	1:A:240:VAL:HG12	1.80	0.64
1:B:376:GLU:O	1:B:378:THR:HG23	1.97	0.64
1:A:113:GLN:OE1	1:B:113:GLN:HG3	1.97	0.64
1:B:51:ASN:H	1:B:51:ASN:ND2	1.95	0.64
1:C:217:LYS:HB3	1:C:220:ARG:HH21	1.61	0.64
1:A:320:LYS:O	1:A:320:LYS:HD2	1.98	0.63
1:D:285:MET:CE	1:D:292:ILE:HD11	2.29	0.63
1:B:177:ILE:HD12	1:B:240:VAL:HG12	1.79	0.62
1:D:68:MET:HB3	1:D:72:SER:HB2	1.81	0.62
1:C:292:ILE:O	1:C:322:PRO:HB3	2.00	0.62
1:C:110:PRO:HG3	1:D:113:GLN:NE2	2.15	0.60
1:A:113:GLN:HG3	1:A:137:ALA:HB1	1.84	0.60
1:A:285:MET:SD	1:A:292:ILE:HD11	2.41	0.60
1:D:3:ARG:HH22	1:D:405:LYS:NZ	2.00	0.60
1:D:51:ASN:HD22	1:D:51:ASN:N	1.94	0.59
1:D:300:THR:HG22	1:D:328:LYS:HE2	1.84	0.59
1:C:51:ASN:HD21	1:C:53:LYS:HE3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:VAL:HG12	1:C:68:MET:HE3	1.85	0.59
1:C:272:PRO:HG2	1:C:308:LYS:HG3	1.84	0.59
1:A:118:ASP:OD2	1:B:121:ARG:NH2	2.30	0.58
1:B:3:ARG:HH22	1:B:405:LYS:NZ	2.00	0.58
1:C:51:ASN:HD22	1:C:51:ASN:H	1.51	0.58
1:C:110:PRO:HG2	1:C:197:MET:HB2	1.85	0.58
1:D:217:LYS:HB3	1:D:220:ARG:HH21	1.69	0.58
1:C:51:ASN:HD22	1:C:51:ASN:N	2.01	0.57
1:A:337:ALA:O	1:A:341:GLN:HG3	2.04	0.57
1:B:285:MET:CE	1:B:386:MET:HE1	2.27	0.57
1:D:124:ARG:HB2	1:D:128:ALA:HB2	1.86	0.57
1:B:91:GLU:H	1:B:91:GLU:CD	2.12	0.57
1:B:220:ARG:HD3	1:B:223:ASP:OD2	2.04	0.56
1:C:320:LYS:HD2	1:C:320:LYS:O	2.05	0.56
1:A:33:ILE:HD12	1:A:230:VAL:HG11	1.87	0.56
1:C:159:ILE:O	1:C:165:THR:HG23	2.05	0.56
1:D:117:ALA:O	1:D:121:ARG:HD2	2.05	0.55
1:C:6:ILE:HD13	1:C:347:LEU:HD11	1.89	0.54
1:C:364:LEU:HD11	1:C:373:ILE:HD12	1.89	0.54
1:C:174:VAL:O	1:C:178:GLN:HG3	2.07	0.54
1:A:91:GLU:H	1:A:91:GLU:CD	2.16	0.53
1:A:144:ALA:C	1:B:269:MET:HE1	2.33	0.53
1:D:68:MET:HB3	1:D:72:SER:CB	2.39	0.53
1:D:65:VAL:HA	1:D:68:MET:HG3	1.91	0.53
1:D:300:THR:O	1:D:301:SER:HB3	2.07	0.53
1:A:329:ALA:HB3	3:A:2228:HOH:O	2.08	0.53
1:D:51:ASN:H	1:D:51:ASN:ND2	1.96	0.53
1:A:179:LEU:HD13	1:B:179:LEU:HD21	1.91	0.52
1:A:56:THR:HA	1:A:59:LEU:HD12	1.91	0.52
1:B:174:VAL:HG21	1:B:257:ILE:HG21	1.91	0.52
1:B:300:THR:O	1:B:301:SER:HB3	2.10	0.51
1:C:184:ILE:HG12	1:C:241:GLU:HG3	1.92	0.51
1:A:220:ARG:HD3	1:A:223:ASP:OD2	2.09	0.51
1:A:44:MET:HE3	1:A:202:ASP:HB2	1.92	0.51
1:D:285:MET:HE1	1:D:292:ILE:HD11	1.93	0.50
1:A:124:ARG:HB2	1:A:128:ALA:HB2	1.91	0.50
1:C:49:TRP:CE3	1:C:193:LEU:HG	2.46	0.50
1:A:295:LEU:C	1:A:295:LEU:HD23	2.37	0.50
1:A:350:LEU:HD11	1:A:403:LYS:HG3	1.94	0.50
1:B:177:ILE:CD1	1:B:240:VAL:HG12	2.41	0.50
1:B:320:LYS:O	1:B:320:LYS:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ASN:H	1:A:51:ASN:ND2	1.94	0.50
1:B:292:ILE:O	1:B:322:PRO:HB3	2.13	0.49
1:A:161:SER:OG	1:A:165:THR:HA	2.13	0.49
1:B:281:MET:HB3	1:B:285:MET:CE	2.42	0.49
1:D:159:ILE:O	1:D:165:THR:HG23	2.13	0.49
1:C:91:GLU:CD	1:C:91:GLU:H	2.20	0.48
1:B:295:LEU:C	1:B:295:LEU:HD23	2.38	0.48
1:C:320:LYS:NZ	3:C:2157:HOH:O	2.46	0.48
1:B:56:THR:HA	1:B:59:LEU:HD12	1.94	0.48
1:C:355:ILE:HB	1:C:378:THR:HG23	1.96	0.48
1:A:68:MET:HE1	1:A:76:PHE:HB2	1.96	0.48
1:C:48:VAL:HG12	1:C:215:PRO:HB3	1.95	0.48
1:D:1:MET:O	1:D:1:MET:HE3	2.14	0.48
1:C:320:LYS:HG2	3:C:2064:HOH:O	2.14	0.48
1:C:113:GLN:HG3	1:C:137:ALA:HB1	1.94	0.48
1:C:285:MET:HE1	1:C:316:VAL:HG13	1.96	0.48
1:D:110:PRO:O	1:D:114:VAL:HG23	2.13	0.47
1:D:134:VAL:HB	3:D:2113:HOH:O	2.13	0.47
1:A:342:GLU:HA	1:A:345:TYR:CD2	2.50	0.47
1:B:9:LEU:C	1:B:9:LEU:HD12	2.40	0.47
1:C:18:ASN:OD1	1:C:21:GLU:HG3	2.15	0.47
1:C:113:GLN:OE1	1:D:113:GLN:HG3	2.13	0.47
1:C:66:ARG:HD2	3:C:2043:HOH:O	2.15	0.47
1:C:321:SER:HB3	3:C:2176:HOH:O	2.15	0.47
1:A:118:ASP:CG	1:B:121:ARG:HH22	2.19	0.47
1:C:300:THR:O	1:C:301:SER:HB3	2.15	0.47
1:B:281:MET:C	1:B:285:MET:HE3	2.41	0.46
1:B:298:HIS:O	1:B:299:GLY:C	2.59	0.46
1:C:56:THR:HA	1:C:59:LEU:CD1	2.44	0.46
1:A:117:ALA:O	1:A:121:ARG:CD	2.63	0.46
1:B:112:PHE:HA	1:B:115:PHE:HB3	1.97	0.46
1:D:350:LEU:HD11	1:D:403:LYS:HG3	1.97	0.46
1:C:170:ILE:O	1:C:174:VAL:HG23	2.16	0.46
1:D:110:PRO:HG2	1:D:197:MET:HB2	1.98	0.45
1:C:295:LEU:HD23	1:C:295:LEU:C	2.41	0.45
1:A:298:HIS:O	1:A:299:GLY:C	2.60	0.45
1:B:159:ILE:O	1:B:165:THR:HG23	2.16	0.45
1:C:177:ILE:CD1	1:C:240:VAL:HG12	2.44	0.45
1:C:66:ARG:HG3	1:C:67:PHE:CD1	2.51	0.45
1:C:117:ALA:O	1:C:121:ARG:CD	2.64	0.45
1:A:269:MET:HE1	1:B:144:ALA:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ILE:H	1:B:320:LYS:NZ	2.15	0.45
1:C:281:MET:O	1:C:285:MET:HG3	2.16	0.45
1:B:292:ILE:H	1:B:320:LYS:HZ3	1.64	0.44
1:B:342:GLU:HA	1:B:345:TYR:CD2	2.52	0.44
1:C:6:ILE:CD1	1:C:347:LEU:HD11	2.48	0.44
1:D:295:LEU:C	1:D:295:LEU:HD23	2.42	0.44
1:C:118:ASP:CG	1:D:121:ARG:HH22	2.23	0.44
1:B:272:PRO:HG2	1:B:308:LYS:HG3	1.98	0.44
1:C:163:CYS:SG	1:C:391:GLY:HA2	2.58	0.44
1:A:159:ILE:HD12	1:A:169:CYS:HA	1.98	0.44
1:A:221:THR:O	1:A:222:TYR:HB2	2.18	0.44
1:B:27:ARG:NH1	3:B:2013:HOH:O	2.50	0.44
1:D:300:THR:O	1:D:301:SER:CB	2.65	0.44
1:C:220:ARG:HD3	1:C:223:ASP:OD2	2.17	0.44
1:C:312:ALA:O	1:C:316:VAL:HG23	2.18	0.44
1:B:221:THR:O	1:B:222:TYR:HB2	2.18	0.43
1:A:146:LEU:C	1:A:149:PRO:HD2	2.42	0.43
1:C:121:ARG:HD2	1:D:195:TRP:HH2	1.83	0.43
1:A:100:GLY:HA3	1:A:155:VAL:HG22	1.99	0.43
1:A:145:CYS:O	1:A:149:PRO:HG2	2.18	0.43
1:B:163:CYS:SG	1:B:391:GLY:HA2	2.58	0.43
1:C:124:ARG:CB	1:C:128:ALA:HB2	2.46	0.43
1:C:145:CYS:O	1:C:149:PRO:HG2	2.18	0.43
1:A:174:VAL:HG21	1:A:257:ILE:HG21	2.00	0.43
1:A:256:GLU:HB2	1:A:404:LEU:HD11	2.01	0.43
1:D:113:GLN:CD	1:D:137:ALA:HB1	2.44	0.43
1:A:102:ILE:HD13	1:A:172:ASN:HD22	1.84	0.43
1:A:113:GLN:CG	1:A:137:ALA:HB1	2.48	0.43
1:B:289:ASP:OD1	1:B:290:THR:HG23	2.19	0.43
1:B:300:THR:O	1:B:301:SER:CB	2.67	0.43
1:B:62:ARG:NH2	1:B:63:LYS:HE3	2.32	0.43
1:D:117:ALA:O	1:D:121:ARG:CD	2.67	0.43
1:C:385:VAL:HG23	1:C:401:MET:HE3	2.01	0.43
1:C:124:ARG:O	1:C:127:LYS:HE3	2.20	0.42
1:D:179:LEU:HD12	1:D:179:LEU:HA	1.91	0.42
1:D:292:ILE:O	1:D:322:PRO:HB3	2.19	0.42
1:D:298:HIS:O	1:D:299:GLY:C	2.62	0.42
1:A:171:GLY:HA3	1:A:260:TYR:CZ	2.54	0.42
1:B:274:GLY:O	1:B:278:VAL:HG23	2.19	0.42
1:C:222:TYR:CD1	1:C:310:LEU:HD11	2.55	0.42
1:A:62:ARG:HG3	3:A:2065:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:THR:O	1:A:301:SER:HB3	2.19	0.42
1:B:294:TYR:HB3	1:B:385:VAL:HG12	2.02	0.42
1:B:312:ALA:O	1:B:316:VAL:HG23	2.19	0.42
1:D:3:ARG:HH22	1:D:405:LYS:HZ2	1.66	0.42
1:C:333:HIS:CE1	1:C:335:LEU:HA	2.54	0.42
1:A:350:LEU:O	1:A:403:LYS:HE2	2.19	0.41
1:C:113:GLN:CG	1:C:137:ALA:HB1	2.50	0.41
1:C:249:ARG:CZ	1:C:251:ALA:HB2	2.51	0.41
1:A:179:LEU:HD12	1:A:179:LEU:HA	1.91	0.41
1:C:44:MET:HE3	1:C:202:ASP:HB2	2.02	0.41
1:A:300:THR:O	1:A:301:SER:CB	2.69	0.41
1:C:300:THR:O	1:C:301:SER:CB	2.68	0.41
1:B:192:GLU:HG2	3:B:2113:HOH:O	2.20	0.41
1:C:5:VAL:HB	1:C:253:ILE:HG23	2.03	0.41
1:C:298:HIS:O	1:C:299:GLY:C	2.63	0.41
1:D:113:GLN:HG2	1:D:137:ALA:HB1	2.02	0.41
1:D:175:GLU:O	1:D:179:LEU:HB2	2.20	0.41
1:B:62:ARG:HH21	1:B:63:LYS:CE	2.33	0.41
1:C:204:MET:HE1	1:C:392:PHE:CE1	2.56	0.41
1:B:124:ARG:CB	1:B:128:ALA:HB2	2.43	0.41
1:B:113:GLN:HG2	1:B:137:ALA:HB1	2.01	0.40
1:B:343:ALA:O	1:B:347:LEU:HG	2.21	0.40
1:A:159:ILE:O	1:A:165:THR:HG23	2.21	0.40
1:C:9:LEU:HD12	1:C:9:LEU:O	2.21	0.40
1:A:179:LEU:HB3	1:A:181:LYS:HG3	2.04	0.40
1:A:333:HIS:CE1	1:A:335:LEU:HA	2.56	0.40
1:D:9:LEU:C	1:D:9:LEU:HD12	2.46	0.40
1:D:146:LEU:C	1:D:149:PRO:HD2	2.46	0.40
1:D:366:GLU:HG3	3:D:2231:HOH:O	2.22	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	404/406 (100%)	385 (95%)	17 (4%)	2 (0%)	24	16
1	B	404/406 (100%)	383 (95%)	19 (5%)	2 (0%)	24	16
1	C	404/406 (100%)	385 (95%)	16 (4%)	3 (1%)	18	10
1	D	404/406 (100%)	390 (96%)	12 (3%)	2 (0%)	24	16
All	All	1616/1624 (100%)	1543 (96%)	64 (4%)	9 (1%)	21	13

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	GLY
1	B	299	GLY
1	C	299	GLY
1	D	299	GLY
1	C	268	ASP
1	A	301	SER
1	B	301	SER
1	C	301	SER
1	D	301	SER

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	309/309 (100%)	305 (99%)	4 (1%)	61	61
1	B	309/309 (100%)	305 (99%)	4 (1%)	61	61
1	C	309/309 (100%)	303 (98%)	6 (2%)	50	47
1	D	309/309 (100%)	300 (97%)	9 (3%)	37	31
All	All	1236/1236 (100%)	1213 (98%)	23 (2%)	50	47

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	91	GLU

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Mol	Chain	Res	Type
1	A	179	LEU
1	A	405	LYS
1	B	51	ASN
1	B	91	GLU
1	B	121	ARG
1	B	405	LYS
1	C	51	ASN
1	C	91	GLU
1	C	121	ARG
1	C	179	LEU
1	C	213	ASP
1	C	378	THR
1	D	51	ASN
1	D	68	MET
1	D	121	ARG
1	D	179	LEU
1	D	213	ASP
1	D	315	GLU
1	D	320	LYS
1	D	380	ARG
1	D	405	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	51	ASN
1	A	94	GLN
1	A	95	ASN
1	A	176	GLN
1	A	178	GLN
1	A	252	HIS
1	A	396	ASN
1	B	37	GLN
1	B	51	ASN
1	B	94	GLN
1	B	95	ASN
1	B	113	GLN
1	B	176	GLN
1	B	225	HIS
1	C	51	ASN
1	C	94	GLN

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Mol	Chain	Res	Type
1	D	51	ASN
1	D	94	GLN
1	D	95	ASN
1	D	252	HIS
1	D	396	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](#)

Of 4 ligands modelled in this entry, 4 are modelled with single atom - leaving 0 for Mogul analysis.

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	406/406 (100%)	0.16	13 (3%)	50	54	10, 20, 37, 58	0
1	B	406/406 (100%)	0.68	35 (8%)	16	17	14, 26, 46, 64	0
1	C	406/406 (100%)	0.58	29 (7%)	22	23	14, 25, 43, 67	0
1	D	406/406 (100%)	0.19	15 (3%)	45	48	11, 21, 39, 66	0
All	All	1624/1624 (100%)	0.40	92 (5%)	29	31	10, 23, 42, 67	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	270	VAL	6.8
1	C	268	ASP	5.5
1	A	405	LYS	5.3
1	D	406	ASP	5.0
1	C	405	LYS	4.3
1	C	271	ALA	4.2
1	B	270	VAL	4.1
1	D	270	VAL	4.1
1	C	406	ASP	4.0
1	B	406	ASP	3.8
1	A	406	ASP	3.6
1	B	368	ALA	3.4
1	A	1	MET	3.4
1	A	392	PHE	3.3
1	B	321	SER	3.3
1	C	392	PHE	3.3
1	A	270	VAL	3.2
1	B	371	LEU	3.2
1	C	267	ALA	3.1
1	B	319	ASP	3.1
1	C	269	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	273	SER	3.1
1	B	213	ASP	3.0
1	C	213	ASP	3.0
1	C	272	PRO	2.9
1	D	213	ASP	2.9
1	B	271	ALA	2.9
1	C	364	LEU	2.8
1	C	61	ASP	2.7
1	B	291	PRO	2.7
1	B	369	ALA	2.7
1	B	268	ASP	2.7
1	C	362	GLU	2.7
1	B	225	HIS	2.7
1	B	211	TYR	2.6
1	D	267	ALA	2.6
1	D	392	PHE	2.6
1	D	404	LEU	2.6
1	A	319	ASP	2.5
1	A	320	LYS	2.5
1	B	405	LYS	2.5
1	C	307	VAL	2.5
1	B	320	LYS	2.5
1	C	320	LYS	2.5
1	D	320	LYS	2.5
1	B	366	GLU	2.5
1	C	92	ALA	2.5
1	D	271	ALA	2.5
1	A	404	LEU	2.4
1	C	404	LEU	2.4
1	D	268	ASP	2.4
1	C	368	ALA	2.4
1	A	30	ARG	2.4
1	A	268	ASP	2.4
1	B	322	PRO	2.4
1	A	127	LYS	2.4
1	A	271	ALA	2.3
1	D	205	GLY	2.3
1	B	307	VAL	2.3
1	C	193	LEU	2.3
1	C	1	MET	2.3
1	B	323	ALA	2.3
1	C	59	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	61	ASP	2.2
1	B	316	VAL	2.2
1	B	362	GLU	2.2
1	B	215	PRO	2.2
1	B	287	GLY	2.2
1	D	286	HIS	2.2
1	C	248	ALA	2.2
1	C	217	LYS	2.2
1	D	62	ARG	2.2
1	B	28	GLU	2.2
1	C	367	GLN	2.2
1	B	378	THR	2.2
1	B	314	ARG	2.2
1	C	225	HIS	2.1
1	B	392	PHE	2.1
1	B	290	THR	2.1
1	B	131	PRO	2.1
1	C	62	ARG	2.1
1	B	24	ALA	2.1
1	B	224	ALA	2.1
1	C	361	ILE	2.1
1	D	289	ASP	2.1
1	B	89	SER	2.1
1	D	61	ASP	2.1
1	B	325	SER	2.0
1	D	405	LYS	2.0
1	A	286	HIS	2.0
1	B	229	PHE	2.0
1	C	352	HIS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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	NH4	B	901	1/1	0.95	0.09	25,25,25,25	0
2	NH4	A	901	1/1	0.96	0.05	16,16,16,16	0
2	NH4	D	901	1/1	0.97	0.06	15,15,15,15	0
2	NH4	C	901	1/1	0.99	0.09	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.