Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:49 AM GMT

PDB ID	:	2BUH
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

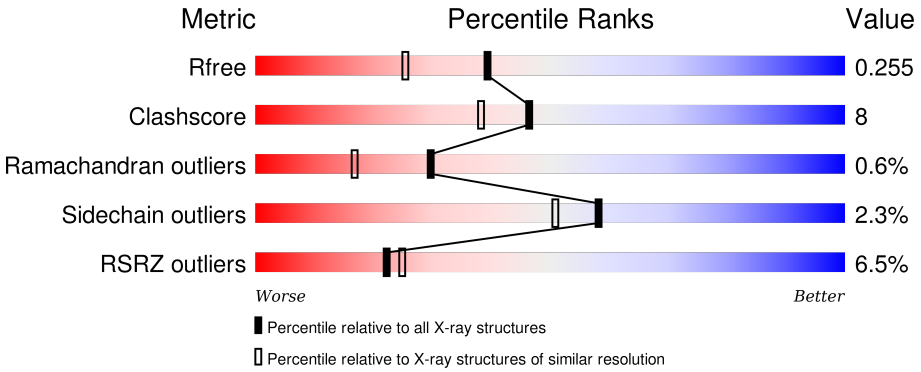
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	2% 85% 13%
1	B	406	10% 85% 14%
1	C	406	10% 82% 17%
1	D	406	4% 90% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NH4	A	901	-	-	-	X
2	NH4	B	901	-	-	-	X
2	NH4	C	901	-	-	-	X
2	NH4	D	901	-	-	-	X

2 Entry composition

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 (three-letter code: NH4) (formula: H_4N).

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.

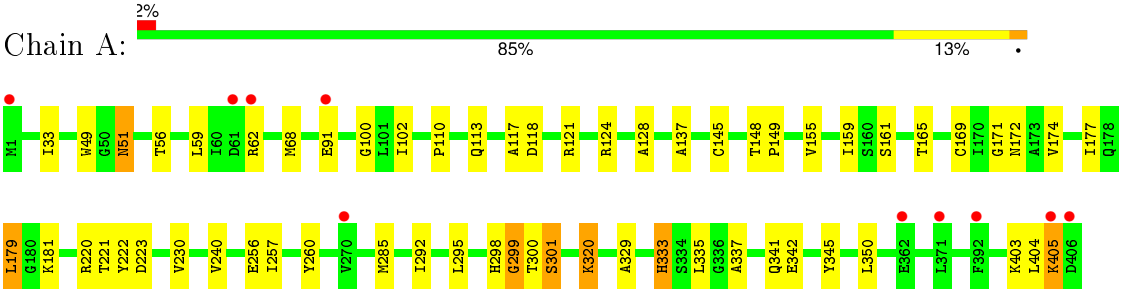
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	256	Total O 256 256	0	0
3	B	196	Total O 196 196	0	0
3	C	191	Total O 191 191	0	0
3	D	254	Total O 254 254	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

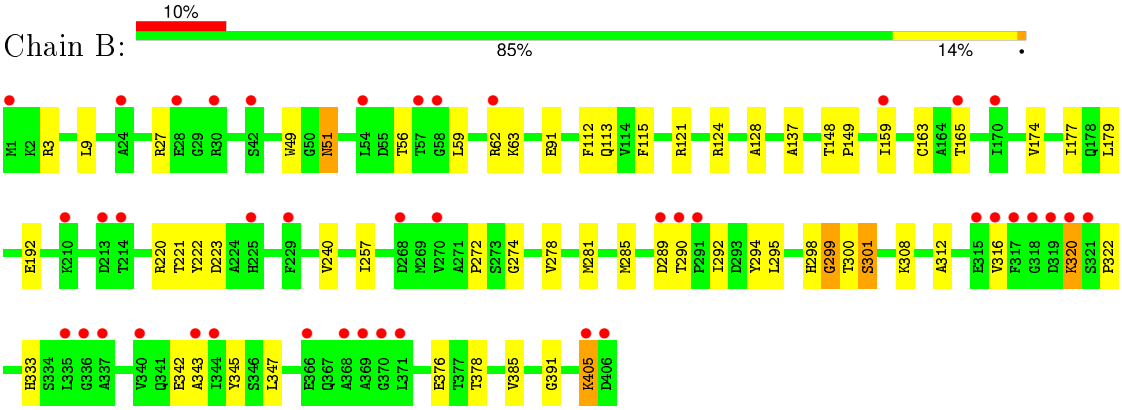
- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I

Chain A:



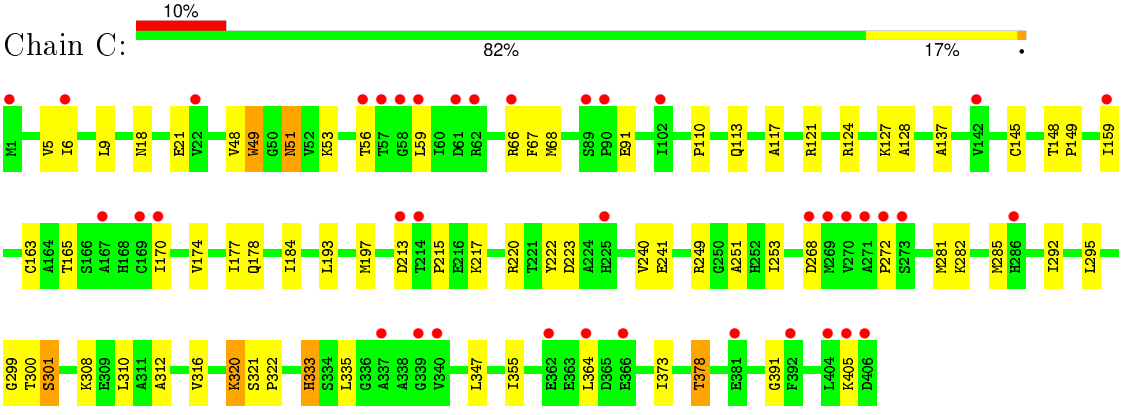
- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I

Chain B:



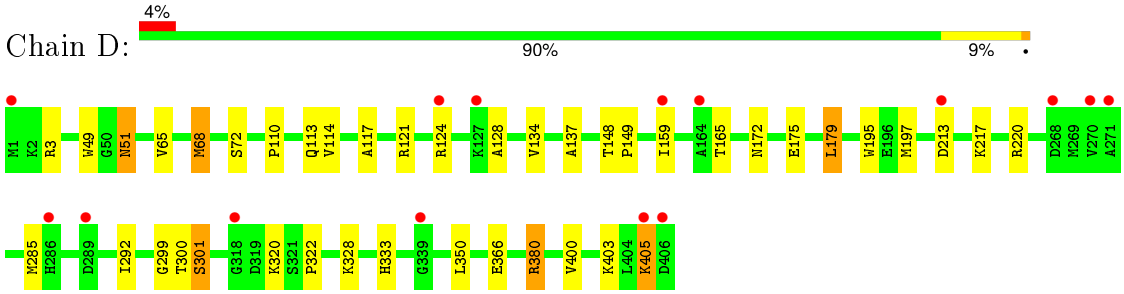
- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

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 30.10 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.5 (29.73-1.90) 89.6 (30.10-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.256 0.216 , 0.255	Depositor DCC
R_{free} test set	6276 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 124550 reflections (0.002%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.34	0/3029	0.61	0/4090
1	B	0.31	0/3029	0.55	0/4090
1	C	0.31	0/3029	0.56	0/4090
1	D	0.34	0/3029	0.60	0/4090
All	All	0.32	0/12116	0.58	0/16360

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

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	47	0
1	B	2981	0	2939	49	0
1	C	2981	0	2939	57	0
1	D	2981	0	2939	36	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	180	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 (180) 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:A:405:LYS:H	1:A:405:LYS:HD2	1.33	0.93
1:B:51:ASN:HD22	1:B:51:ASN:H	1.19	0.91
1:D:51:ASN:HD22	1:D:51:ASN:H	1.17	0.90
1:C:405:LYS:H	1:C:405:LYS:HD2	1.34	0.89
1:A:51:ASN:H	1:A:51:ASN:HD22	1.15	0.88
1:D:285:MET:HE3	1:D:292:ILE:HD11	1.60	0.82
1:B:3:ARG:HH22	1:B:405:LYS:HZ1	1.30	0.80
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: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:N	1:B:51:ASN:HD22	1.88	0.68
1:D:285:MET:HE2	1:D:285:MET:HA	1.74	0.68
1:A:405:LYS:N	1:A:405:LYS:HD2	2.08	0.67
1:A:51:ASN:N	1:A:51:ASN:HD22	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:ND2	1:B:51:ASN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:51:ASN:H	1:A:51:ASN:ND2	1.94	0.61
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:D:3:ARG:HH22	1:D:405:LYS:NZ	2.00	0.60
1:A:285:MET:SD	1:A:292:ILE:HD11	2.41	0.60
1:D:285:MET:CE	1:D:292:ILE:HD11	2.29	0.59
1:D:51:ASN:N	1:D:51:ASN:HD22	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
1:D:51:ASN:H	1:D:51:ASN:ND2	1.96	0.59
1:C:272:PRO:HG2	1:C:308:LYS:HG3	1.84	0.59
1:B:3:ARG:HH22	1:B:405:LYS:NZ	2.00	0.58
1:A:118:ASP:OD2	1:B:121:ARG:NH2	2.30	0.58
1:C:51:ASN:H	1:C:51:ASN:HD22	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:N	1:C:51:ASN:HD22	2.01	0.57
1:A:337:ALA:O	1:A:341:GLN:HG3	2.04	0.57
1:D:124:ARG:HB2	1:D:128:ALA:HB2	1.86	0.57
1:B:220:ARG:HD3	1:B:223:ASP:OD2	2.04	0.56
1:C:320:LYS:O	1:C:320:LYS:HD2	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: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:A:179:LEU:HD13	1:B:179:LEU:HD21	1.91	0.52
1:B:174:VAL:HG21	1:B:257:ILE:HG21	1.91	0.52
1:A:56:THR:HA	1:A:59:LEU:HD12	1.91	0.52
1:B:91:GLU:CD	1:B:91:GLU:H	2.12	0.52
1:B:285:MET:HE3	1:B:316:VAL:HG11	1.92	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:MET:HE3	1:A:145:CYS:HB3	1.92	0.51
1:A:220:ARG:HD3	1:A:223:ASP:OD2	2.09	0.51
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:B:177:ILE:CD1	1:B:240:VAL:HG12	2.41	0.50
1:B:320:LYS:HD2	1:B:320:LYS:O	2.12	0.50
1:A:350:LEU:HD11	1:A:403:LYS:HG3	1.94	0.50
1:B:292:ILE:O	1:B:322:PRO:HB3	2.13	0.49
1:B:281:MET:HB3	1:B:285:MET:CE	2.42	0.49
1:A:161:SER:OG	1:A:165:THR:HA	2.13	0.49
1:D:159:ILE:O	1:D:165:THR:HG23	2.13	0.49
1:D:3:ARG:HH22	1:D:405:LYS:HZ2	1.61	0.48
1:C:320:LYS:NZ	3:C:2157:HOH:O	2.46	0.48
1:A:91:GLU:H	1:A:91:GLU:CD	2.16	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:C:48:VAL:HG12	1:C:215:PRO:HB3	1.95	0.48
1:C:320:LYS:HG2	3:C:2064:HOH:O	2.14	0.48
1:C:282:LYS:HA	1:C:285:MET:HE2	1.95	0.48
1:C:113:GLN:HG3	1:C:137:ALA:HB1	1.94	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:C:113:GLN:OE1	1:D:113:GLN:HG3	2.13	0.47
1:A:342:GLU:HA	1:A:345:TYR:CD2	2.50	0.47
1:C:18:ASN:OD1	1:C:21:GLU:HG3	2.15	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:C:300:THR:O	1:C:301:SER:HB3	2.15	0.47
1:B:285:MET:CE	1:B:316:VAL:HG11	2.45	0.46
1:C:56:THR:HA	1:C:59:LEU:CD1	2.44	0.46
1:B:112:PHE:HA	1:B:115:PHE:HB3	1.97	0.46
1:A:117:ALA:O	1:A:121:ARG:CD	2.63	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:A:295:LEU:C	1:A:295:LEU:HD23	2.37	0.45
1:C:177:ILE:CD1	1:C:240:VAL:HG12	2.44	0.45
1:B:159:ILE:O	1:B:165:THR:HG23	2.16	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:B:292:ILE:H	1:B:320:LYS:NZ	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:MET:O	1:C:285:MET:HG3	2.16	0.45
1:D:285:MET:CE	1:D:285:MET:HA	2.45	0.44
1:C:6:ILE:CD1	1:C:347:LEU:HD11	2.48	0.44
1:B:342:GLU:HA	1:B:345:TYR:CD2	2.52	0.44
1:B:272:PRO:HG2	1:B:308:LYS:HG3	1.98	0.44
1:B:295:LEU:C	1:B:295:LEU:HD23	2.38	0.44
1:C:163:CYS:SG	1:C:391:GLY:HA2	2.58	0.44
1:D:300:THR:O	1:D:301:SER:CB	2.65	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:C:220:ARG:HD3	1:C:223:ASP:OD2	2.17	0.44
1:C:91:GLU:CD	1:C:91:GLU:H	2.20	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:C:285:MET:HE3	1:C:285:MET:HB2	1.80	0.43
1:C:121:ARG:HD2	1:D:195:TRP:HH2	1.83	0.43
1:A:145:CYS:O	1:A:149:PRO:HG2	2.18	0.43
1:C:124:ARG:CB	1:C:128:ALA:HB2	2.46	0.43
1:B:163:CYS:SG	1:B:391:GLY:HA2	2.58	0.43
1:A:100:GLY:HA3	1:A:155:VAL:HG22	1.99	0.43
1:C:145:CYS:O	1:C:149:PRO:HG2	2.18	0.43
1:A:256:GLU:HB2	1:A:404:LEU:HD11	2.01	0.43
1:A:174:VAL:HG21	1:A:257:ILE:HG21	2.00	0.43
1:A:113:GLN:CG	1:A:137:ALA:HB1	2.48	0.43
1:A:102:ILE:HD13	1:A:172:ASN:HD22	1.84	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:292:ILE:H	1:B:320:LYS:HZ3	1.65	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:282:LYS:HA	1:C:285:MET:CE	2.49	0.42
1:B:9:LEU:HD12	1:B:9:LEU:C	2.40	0.42
1:D:285:MET:CE	1:D:400:VAL:HG21	2.49	0.42
1:D:292:ILE:O	1:D:322:PRO:HB3	2.19	0.42
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:C:222:TYR:CD1	1:C:310:LEU:HD11	2.55	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: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:118:ASP:CG	1:B:121:ARG:HH22	2.19	0.42
1:B:312:ALA:O	1:B:316:VAL:HG23	2.19	0.42
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:C:333:HIS:CE1	1:C:335:LEU:HA	2.54	0.42
1:C:113:GLN:CG	1:C:137:ALA:HB1	2.50	0.41
1:A:350:LEU:O	1:A:403:LYS:HE2	2.19	0.41
1:C:249:ARG:CZ	1:C:251:ALA:HB2	2.51	0.41
1:B:298:HIS:O	1:B:299:GLY:C	2.59	0.41
1:A:179:LEU:HD12	1:A:179:LEU:HA	1.91	0.41
1:C:300:THR:O	1:C:301:SER:CB	2.68	0.41
1:A:300:THR:O	1:A:301:SER:CB	2.69	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:C:5:VAL:HB	1:C:253:ILE:HG23	2.03	0.41
1:B:192:GLU:HG2	3:B:2113:HOH:O	2.20	0.41
1:B:62:ARG:HH21	1:B:63:LYS:CE	2.33	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:C:295:LEU:C	1:C:295:LEU:HD23	2.41	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:298:HIS:O	1:A:299:GLY:C	2.60	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:366:GLU:HG3	3:D:2231:HOH:O	2.22	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	404/406 (100%)	385 (95%)	17 (4%)	2 (0%)	34	21
1	B	404/406 (100%)	383 (95%)	19 (5%)	2 (0%)	34	21
1	C	404/406 (100%)	385 (95%)	16 (4%)	3 (1%)	26	14
1	D	404/406 (100%)	390 (96%)	12 (3%)	2 (0%)	34	21
All	All	1616/1624 (100%)	1543 (96%)	64 (4%)	9 (1%)	30	17

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 (i)

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%)	303 (98%)	6 (2%)	65	59
1	B	309/309 (100%)	304 (98%)	5 (2%)	70	66
1	C	309/309 (100%)	302 (98%)	7 (2%)	58	51
1	D	309/309 (100%)	299 (97%)	10 (3%)	46	35
All	All	1236/1236 (100%)	1208 (98%)	28 (2%)	58	51

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	TRP
1	A	51	ASN

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Mol	Chain	Res	Type
1	A	179	LEU
1	A	320	LYS
1	A	333	HIS
1	A	405	LYS
1	B	49	TRP
1	B	51	ASN
1	B	320	LYS
1	B	333	HIS
1	B	405	LYS
1	C	49	TRP
1	C	51	ASN
1	C	68	MET
1	C	213	ASP
1	C	320	LYS
1	C	333	HIS
1	C	378	THR
1	D	49	TRP
1	D	51	ASN
1	D	68	MET
1	D	172	ASN
1	D	179	LEU
1	D	213	ASP
1	D	320	LYS
1	D	333	HIS
1	D	380	ARG
1	D	405	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	94	GLN
1	A	172	ASN
1	A	252	HIS
1	B	51	ASN
1	B	94	GLN
1	B	113	GLN
1	B	172	ASN
1	C	51	ASN
1	C	94	GLN
1	D	51	ASN
1	D	94	GLN

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Mol	Chain	Res	Type
1	D	95	ASN
1	D	252	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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, 95^{th} 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%)	0.39	10 (2%) 61 64	10, 20, 37, 58	0
1	B	406/406 (100%)	0.85	42 (10%) 9 9	14, 26, 46, 64	0
1	C	406/406 (100%)	0.81	39 (9%) 10 11	14, 25, 43, 67	0
1	D	406/406 (100%)	0.49	15 (3%) 45 49	11, 21, 39, 66	0
All	All	1624/1624 (100%)	0.64	106 (6%) 22 25	10, 23, 42, 67	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	406	ASP	12.0
1	C	270	VAL	9.8
1	B	406	ASP	7.7
1	C	1	MET	6.7
1	C	271	ALA	6.4
1	C	406	ASP	5.8
1	D	1	MET	5.8
1	A	406	ASP	5.6
1	B	319	ASP	5.5
1	B	371	LEU	5.0
1	C	405	LYS	4.8
1	B	270	VAL	4.6
1	D	286	HIS	4.5
1	C	272	PRO	4.5
1	B	1	MET	4.5
1	B	405	LYS	4.4
1	C	62	ARG	4.2
1	C	268	ASP	4.0
1	C	90	PRO	4.0
1	B	321	SER	3.9
1	B	213	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	366	GLU	3.8
1	B	320	LYS	3.6
1	B	214	THR	3.6
1	C	159	ILE	3.6
1	B	316	VAL	3.5
1	B	225	HIS	3.5
1	B	368	ALA	3.4
1	C	61	ASP	3.4
1	C	57	THR	3.4
1	B	317	PHE	3.3
1	D	405	LYS	3.3
1	D	289	ASP	3.3
1	D	271	ALA	3.3
1	B	315	GLU	3.3
1	B	57	THR	3.2
1	B	318	GLY	3.2
1	B	370	GLY	3.2
1	C	340	VAL	3.1
1	C	273	SER	3.0
1	C	213	ASP	3.0
1	C	362	GLU	3.0
1	B	369	ALA	3.0
1	B	62	ARG	3.0
1	A	62	ARG	3.0
1	B	28	GLU	2.9
1	B	366	GLU	2.8
1	B	268	ASP	2.8
1	C	286	HIS	2.8
1	A	405	LYS	2.8
1	A	270	VAL	2.8
1	B	58	GLY	2.7
1	A	362	GLU	2.7
1	C	170	ILE	2.7
1	C	56	THR	2.7
1	D	318	GLY	2.7
1	B	42	SER	2.7
1	B	337	ALA	2.6
1	B	30	ARG	2.6
1	D	213	ASP	2.6
1	B	289	ASP	2.5
1	D	268	ASP	2.5
1	C	89	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	339	GLY	2.5
1	C	102	ILE	2.4
1	B	335	LEU	2.4
1	C	167	ALA	2.4
1	C	66	ARG	2.4
1	C	364	LEU	2.4
1	A	1	MET	2.3
1	C	392	PHE	2.3
1	D	159	ILE	2.3
1	B	291	PRO	2.3
1	C	269	MET	2.3
1	C	337	ALA	2.3
1	B	340	VAL	2.3
1	D	270	VAL	2.2
1	C	404	LEU	2.2
1	B	343	ALA	2.2
1	C	381	GLU	2.2
1	C	58	GLY	2.2
1	B	54	LEU	2.2
1	D	124	ARG	2.2
1	B	344	ILE	2.2
1	A	392	PHE	2.1
1	C	169	CYS	2.1
1	C	59	LEU	2.1
1	C	6	ILE	2.1
1	A	61	ASP	2.1
1	A	371	LEU	2.1
1	D	339	GLY	2.1
1	B	210	LYS	2.1
1	C	225	HIS	2.1
1	B	170	ILE	2.1
1	B	24	ALA	2.1
1	D	164	ALA	2.1
1	C	22	VAL	2.1
1	B	336	GLY	2.1
1	B	159	ILE	2.0
1	C	142	VAL	2.0
1	A	91	GLU	2.0
1	B	229	PHE	2.0
1	B	165	THR	2.0
1	B	290	THR	2.0
1	C	214	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	127	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	NH4	C	901	1/1	0.98	0.48	22.95	19,19,19,19	0
2	NH4	A	901	1/1	0.97	0.30	14.98	16,16,16,16	0
2	NH4	D	901	1/1	0.97	0.39	9.29	15,15,15,15	0
2	NH4	B	901	1/1	0.96	0.37	8.29	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.