



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:40 AM UTC

PDB ID : 2BYZ / pdb_00002byz
Title : Structure of E.coli KAS I H298Q mutant in complex with C12 fatty acid
Authors : Olsen, J.G.; von Wettstein-Knowles, P.; Henriksen, A.
Deposited on : 2005-08-09
Resolution : 1.95 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

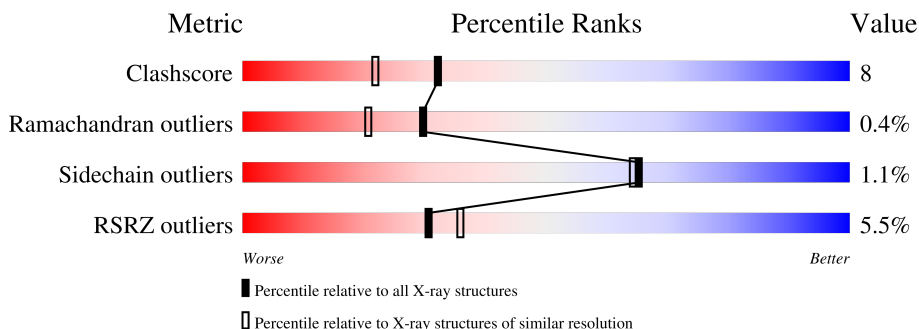
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	418	5% 81% 14% ..
1	B	418	8% 81% 15% ..
1	C	418	4% 82% 14% ..
1	D	418	4% 79% 17% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12957 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.

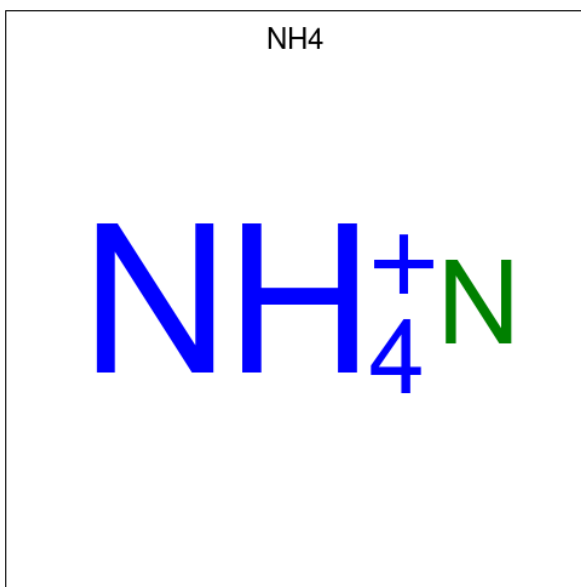
- Molecule 1 is a protein called 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	1
			2972	1848	518	583	23			
1	B	406	Total	C	N	O	S	0	0	1
			2972	1848	518	583	23			
1	C	406	Total	C	N	O	S	0	0	1
			2972	1848	518	583	23			
1	D	406	Total	C	N	O	S	0	0	1
			2972	1848	518	583	23			

There are 4 discrepancies between the modelled and reference sequences:

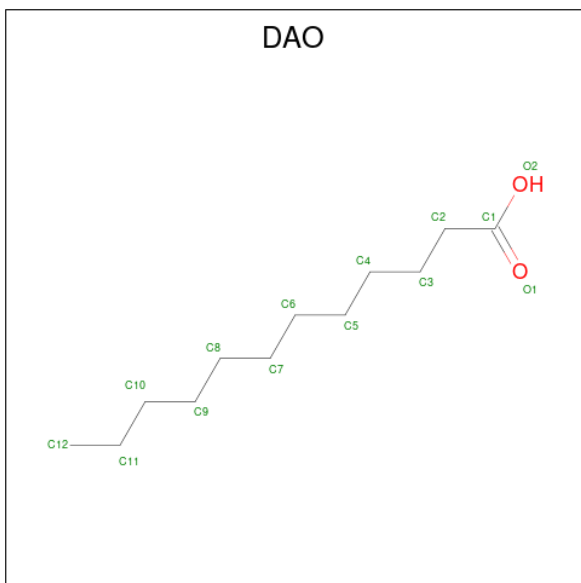
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLN	HIS	engineered mutation	UNP P14926
B	298	GLN	HIS	engineered mutation	UNP P14926
C	298	GLN	HIS	engineered mutation	UNP P14926
D	298	GLN	HIS	engineered mutation	UNP P14926

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



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

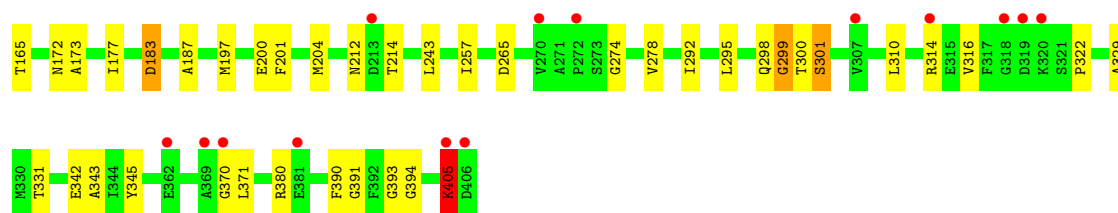
- Molecule 3 is LAURIC ACID (CCD ID: DAO) (formula: $C_{12}H_{24}O_2$).



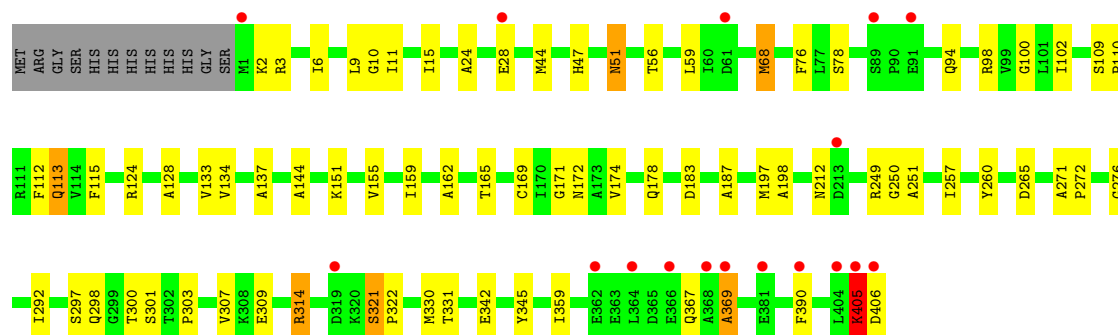
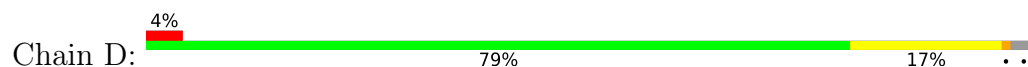
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	12	1		
3	B	1	Total	C	O	0	0
			13	12	1		
3	C	1	Total	C	O	0	0
			13	12	1		
3	D	1	Total	C	O	0	0
			13	12	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	253	Total	O	0	0
			253	253		
4	B	250	Total	O	0	0
			250	250		
4	C	272	Total	O	0	0
			272	272		
4	D	238	Total	O	0	0
			238	238		



● 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	59.10Å 139.25Å 212.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	116.40 – 1.95 116.40 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.6 (116.40-1.95) 94.7 (116.40-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.189 , 0.217 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12957	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DAO, 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	0.41	1/3019 (0.0%)	0.87	8/4078 (0.2%)
1	B	0.38	1/3019 (0.0%)	0.82	4/4078 (0.1%)
1	C	0.39	1/3019 (0.0%)	0.87	10/4078 (0.2%)
1	D	0.37	1/3019 (0.0%)	0.84	4/4078 (0.1%)
All	All	0.39	4/12076 (0.0%)	0.85	26/16312 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	405	LYS	C-N	-5.73	1.25	1.33
1	C	405	LYS	C-N	-5.69	1.25	1.33
1	D	405	LYS	C-N	-5.58	1.25	1.33
1	B	405	LYS	C-N	-5.49	1.25	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	MET	N-CA-C	6.97	121.39	110.17
1	B	68	MET	N-CA-C	6.81	121.14	110.17
1	A	298	GLN	N-CA-C	-6.77	103.98	111.36
1	C	68	MET	N-CA-C	6.60	120.79	110.17
1	D	68	MET	N-CA-C	6.53	120.33	109.95
1	C	69	SER	N-CA-C	-6.02	101.55	110.46
1	C	214	THR	CA-C-N	5.82	125.29	119.24
1	C	214	THR	C-N-CA	5.82	125.29	119.24
1	C	343	ALA	N-CA-C	-5.72	105.13	111.36
1	D	113	GLN	N-CA-C	-5.64	105.21	111.36
1	B	243	LEU	N-CA-C	5.58	117.82	111.02
1	A	162	ALA	CB-CA-C	-5.42	110.30	116.54
1	D	11	ILE	N-CA-C	5.37	114.93	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	ALA	N-CA-C	-5.36	105.52	111.36
1	C	183	ASP	N-CA-C	-5.35	106.88	113.41
1	A	133	VAL	N-CA-C	5.34	116.12	110.72
1	B	162	ALA	CB-CA-C	-5.30	110.48	116.63
1	D	162	ALA	CB-CA-C	-5.29	110.45	116.54
1	B	133	VAL	N-CA-C	5.28	116.05	110.72
1	C	243	LEU	N-CA-C	5.24	117.41	111.02
1	C	133	VAL	N-CA-C	5.21	115.98	110.72
1	A	113	GLN	N-CA-C	-5.21	105.68	111.36
1	A	11	ILE	N-CA-C	5.18	115.03	107.88
1	A	243	LEU	N-CA-C	5.12	117.25	111.11
1	C	316	VAL	N-CA-C	5.08	115.31	110.53
1	C	162	ALA	CB-CA-C	-5.03	110.76	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2972	0	2935	48	0
1	B	2972	0	2935	47	0
1	C	2972	0	2935	44	0
1	D	2972	0	2935	61	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	13	0	23	3	0
3	B	13	0	23	5	0
3	C	13	0	23	5	0
3	D	13	0	23	2	0
4	A	253	0	0	2	0
4	B	250	0	0	2	0
4	C	272	0	0	2	0
4	D	238	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12957	0	11832	189	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 (189) 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:D:314:ARG:HH11	1:D:314:ARG:HB2	1.36	0.90
1:B:51:ASN:H	1:B:51:ASN:HD22	1.20	0.90
1:C:51:ASN:HD22	1:C:51:ASN:H	1.20	0.89
1:A:51:ASN:H	1:A:51:ASN:HD22	1.24	0.86
1:C:298:GLN:NE2	1:C:390:PHE:H	1.80	0.80
1:D:124:ARG:HB2	1:D:128:ALA:HB2	1.63	0.80
1:D:51:ASN:H	1:D:51:ASN:HD22	1.34	0.75
1:D:197:MET:HE2	3:D:1407:DAO:H91	1.69	0.75
1:B:314:ARG:HB2	1:B:314:ARG:HH11	1.52	0.74
1:B:197:MET:HE2	3:B:1407:DAO:H82	1.69	0.74
1:D:307:VAL:HG13	1:D:367:GLN:HG3	1.69	0.74
1:C:172:ASN:HD21	1:D:172:ASN:HD21	1.35	0.73
1:A:62:ARG:HH12	1:A:63:LYS:HE2	1.55	0.72
1:A:197:MET:HE2	3:A:1407:DAO:H91	1.72	0.71
1:B:298:GLN:NE2	1:B:390:PHE:H	1.86	0.71
3:B:1407:DAO:H92	3:B:1407:DAO:H51	1.72	0.70
1:A:177:ILE:HD12	1:A:240:VAL:HG12	1.74	0.69
1:D:272:PRO:HG3	1:D:390:PHE:CE2	2.28	0.69
1:C:124:ARG:HB2	1:C:128:ALA:HB2	1.75	0.69
1:B:51:ASN:HD22	1:B:51:ASN:N	1.88	0.68
1:D:51:ASN:HD22	1:D:51:ASN:N	1.94	0.66
1:C:134:VAL:HG22	3:D:1407:DAO:H121	1.78	0.66
1:A:124:ARG:HB2	1:A:128:ALA:HB2	1.77	0.65
1:A:405:LYS:CD	1:A:405:LYS:H	2.09	0.65
1:A:298:GLN:NE2	1:A:390:PHE:H	1.95	0.65
1:B:159:ILE:O	1:B:165:THR:HG23	1.97	0.64
1:A:310:LEU:O	1:A:314:ARG:HG3	1.96	0.64
1:D:113:GLN:HG2	1:D:137:ALA:HB1	1.78	0.64
1:A:6:ILE:HD11	1:A:257:ILE:HD11	1.78	0.64
1:B:307:VAL:HG13	1:B:367:GLN:HG3	1.81	0.63
1:C:197:MET:HE2	3:C:1407:DAO:H92	1.80	0.62
1:C:6:ILE:HD11	1:C:257:ILE:HD11	1.81	0.62
1:B:51:ASN:H	1:B:51:ASN:ND2	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ASN:HB2	4:C:2146:HOH:O	2.00	0.62
1:B:124:ARG:HB2	1:B:128:ALA:HB2	1.82	0.61
1:C:3:ARG:HH22	1:C:405:LYS:HE2	1.67	0.60
1:D:292:ILE:O	1:D:322:PRO:HB3	2.02	0.59
1:C:100:GLY:HA3	1:C:155:VAL:HG12	1.85	0.59
1:D:100:GLY:HA3	1:D:155:VAL:HG12	1.85	0.58
1:D:314:ARG:NH2	1:D:369:ALA:HB3	2.19	0.58
1:D:174:VAL:O	1:D:178:GLN:HG3	2.05	0.56
1:D:298:GLN:HG3	1:D:300:THR:HG23	1.86	0.56
1:A:172:ASN:HD21	1:B:172:ASN:HD21	1.53	0.56
1:A:159:ILE:O	1:A:165:THR:HG23	2.05	0.55
1:A:295:LEU:C	1:A:295:LEU:HD23	2.31	0.55
1:D:98:ARG:HE	1:D:183:ASP:CG	2.13	0.55
1:B:285:MET:HG3	1:B:386:MET:HE1	1.86	0.55
1:D:6:ILE:HD11	1:D:257:ILE:HD11	1.90	0.54
1:B:329:ALA:HB3	4:B:2229:HOH:O	2.09	0.53
1:C:51:ASN:H	1:C:51:ASN:ND2	1.97	0.53
1:C:159:ILE:O	1:C:165:THR:HG23	2.09	0.53
1:C:295:LEU:HD23	1:C:295:LEU:C	2.34	0.52
1:A:155:VAL:HG22	1:A:157:TYR:CE1	2.45	0.52
1:C:200:GLU:HG2	1:D:133:VAL:CG1	2.39	0.51
1:D:47:HIS:H	1:D:212:ASN:HD21	1.58	0.51
1:B:24:ALA:O	1:B:28:GLU:HG2	2.10	0.51
1:B:3:ARG:HH22	1:B:405:LYS:HE2	1.75	0.51
1:B:310:LEU:HD13	1:B:368:ALA:HB2	1.93	0.51
1:D:314:ARG:HH21	1:D:369:ALA:HB3	1.75	0.51
3:C:1407:DAO:H122	1:D:134:VAL:HA	1.93	0.50
1:B:324:ILE:HB	1:B:373:ILE:HD13	1.93	0.50
1:D:51:ASN:H	1:D:51:ASN:ND2	2.07	0.50
1:A:324:ILE:HB	1:A:373:ILE:HD13	1.93	0.50
1:B:292:ILE:O	1:B:322:PRO:HB3	2.12	0.50
1:C:314:ARG:HH21	1:C:370:GLY:H	1.60	0.50
1:A:54:LEU:HD23	1:A:55:ASP:C	2.37	0.49
1:B:300:THR:O	1:B:301:SER:HB3	2.11	0.49
1:B:37:GLN:HG3	1:B:41:ASP:OD2	2.12	0.49
1:D:314:ARG:HH11	1:D:314:ARG:CB	2.19	0.49
1:A:68:MET:HE1	1:A:76:PHE:HB2	1.94	0.49
1:B:68:MET:HE1	1:B:76:PHE:HB2	1.95	0.49
1:A:54:LEU:HD23	1:A:54:LEU:C	2.38	0.49
1:A:113:GLN:HE21	1:B:110:PRO:HG3	1.78	0.49
1:B:33:ILE:HD12	1:B:230:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:GLU:OE2	3:C:1407:DAO:H121	2.13	0.49
1:D:159:ILE:O	1:D:165:THR:HG23	2.13	0.49
1:A:393:GLY:HA3	1:B:144:ALA:HB1	1.94	0.49
1:B:98:ARG:HE	1:B:183:ASP:CG	2.21	0.49
1:B:325:SER:HA	1:B:358:SER:OG	2.13	0.48
1:C:98:ARG:HE	1:C:183:ASP:CG	2.21	0.48
1:D:47:HIS:H	1:D:212:ASN:ND2	2.10	0.48
1:A:405:LYS:H	1:A:405:LYS:HD2	1.76	0.48
1:C:110:PRO:HG2	1:C:197:MET:HE3	1.95	0.48
1:C:173:ALA:O	1:C:177:ILE:HD13	2.14	0.48
1:C:329:ALA:HB3	4:C:2224:HOH:O	2.13	0.48
1:D:68:MET:HE1	1:D:76:PHE:HB2	1.96	0.48
1:B:53:LYS:N	1:B:53:LYS:HD3	2.29	0.48
1:A:51:ASN:HD22	1:A:51:ASN:N	2.01	0.47
1:A:110:PRO:HG2	1:A:197:MET:HE3	1.95	0.47
1:D:300:THR:O	1:D:301:SER:HB3	2.13	0.47
1:D:110:PRO:HG2	1:D:197:MET:HE3	1.95	0.47
1:B:51:ASN:N	1:B:51:ASN:ND2	2.60	0.47
1:C:314:ARG:HE	1:C:371:LEU:HG	1.79	0.47
1:B:15:ILE:HD13	1:B:331:THR:HG22	1.96	0.47
1:A:350:LEU:O	1:A:403:LYS:HE2	2.15	0.47
1:A:172:ASN:HB2	4:A:2136:HOH:O	2.14	0.47
1:D:24:ALA:O	1:D:28:GLU:HG2	2.15	0.46
1:A:174:VAL:O	1:A:178:GLN:HG3	2.14	0.46
1:A:329:ALA:HB3	4:A:2214:HOH:O	2.15	0.46
1:C:300:THR:O	1:C:301:SER:HB3	2.15	0.46
1:B:220:ARG:HB3	1:B:360:ASN:HB3	1.98	0.46
1:B:285:MET:CG	1:B:386:MET:HE1	2.44	0.46
1:C:47:HIS:H	1:C:212:ASN:ND2	2.14	0.46
1:A:264:SER:HB2	1:B:156:ASN:HB3	1.98	0.46
1:C:172:ASN:HD21	1:D:172:ASN:ND2	2.08	0.46
1:B:296:ASN:OD1	1:B:342:GLU:HG2	2.16	0.46
1:D:102:ILE:O	1:D:187:ALA:HA	2.16	0.46
1:D:159:ILE:HD12	1:D:169:CYS:HA	1.97	0.46
1:C:393:GLY:HA3	1:D:144:ALA:HB1	1.97	0.45
1:A:236:GLY:O	1:A:237:MET:HE2	2.16	0.45
1:A:300:THR:O	1:A:301:SER:HB3	2.17	0.45
1:C:274:GLY:O	1:C:278:VAL:HG23	2.17	0.45
1:D:405:LYS:HD2	1:D:406:ASP:N	2.31	0.45
1:A:310:LEU:HD22	1:A:371:LEU:HD13	1.97	0.45
1:C:15:ILE:HD13	1:C:331:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:LEU:HD22	1:C:371:LEU:CD1	2.47	0.45
1:A:47:HIS:H	1:A:212:ASN:HD21	1.64	0.45
1:C:200:GLU:HG2	1:D:133:VAL:HG11	1.99	0.45
1:A:56:THR:HA	1:A:59:LEU:HD12	1.99	0.45
1:B:192:GLU:HG2	4:B:2144:HOH:O	2.17	0.45
3:C:1407:DAO:H123	1:D:137:ALA:HB3	1.98	0.45
1:A:177:ILE:CD1	1:A:240:VAL:HG12	2.44	0.45
1:B:361:ILE:HD12	1:B:375:THR:HG22	1.98	0.45
1:D:56:THR:HA	1:D:59:LEU:HD12	1.99	0.45
1:C:300:THR:O	1:C:301:SER:CB	2.64	0.44
1:A:200:GLU:OE1	3:A:1407:DAO:H121	2.17	0.44
1:D:109:SER:O	1:D:113:GLN:HG3	2.18	0.44
1:A:47:HIS:H	1:A:212:ASN:ND2	2.15	0.44
1:C:342:GLU:HA	1:C:345:TYR:CD2	2.52	0.44
1:D:2:LYS:HE2	4:D:2097:HOH:O	2.17	0.44
1:D:15:ILE:HD13	1:D:331:THR:HG22	2.00	0.44
1:B:307:VAL:CG1	1:B:367:GLN:HG3	2.48	0.44
1:D:51:ASN:N	1:D:51:ASN:ND2	2.65	0.44
1:C:172:ASN:ND2	1:D:172:ASN:HD21	2.11	0.43
1:A:201:PHE:HZ	3:A:1407:DAO:H42	1.82	0.43
1:A:102:ILE:O	1:A:187:ALA:HA	2.19	0.43
1:C:155:VAL:CG2	1:C:157:TYR:CE1	3.02	0.43
1:A:144:ALA:HB1	1:B:393:GLY:HA3	2.00	0.43
1:B:310:LEU:HD22	1:B:371:LEU:HD13	2.01	0.43
1:D:297:SER:HB2	1:D:309:GLU:CD	2.44	0.43
1:A:124:ARG:NH2	1:A:127:LYS:HE2	2.34	0.42
1:A:174:VAL:HG21	1:A:257:ILE:HG21	2.01	0.42
3:B:1407:DAO:H51	3:B:1407:DAO:C9	2.46	0.42
1:C:110:PRO:O	1:C:114:VAL:HG23	2.19	0.42
1:C:292:ILE:O	1:C:322:PRO:HB3	2.19	0.42
1:A:138:MET:HA	3:B:1407:DAO:H102	2.01	0.42
1:D:321:SER:HB3	4:D:2226:HOH:O	2.20	0.42
1:D:265:ASP:OD1	1:D:276:GLY:HA3	2.20	0.42
1:B:285:MET:HG3	1:B:386:MET:CE	2.49	0.42
1:B:197:MET:HG3	3:B:1407:DAO:H112	2.02	0.42
1:A:271:ALA:HA	1:A:272:PRO:HD3	1.90	0.42
1:D:94:GLN:HB3	1:D:151:LYS:HB2	2.02	0.42
1:C:68:MET:HB3	1:C:72:SER:HB2	2.00	0.41
1:C:113:GLN:CD	1:D:110:PRO:HB3	2.45	0.41
1:D:249:ARG:CZ	1:D:251:ALA:HB2	2.50	0.41
1:A:98:ARG:HE	1:A:183:ASP:CG	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:GLY:HA3	1:D:78:SER:O	2.20	0.41
1:B:265:ASP:OD1	1:B:276:GLY:HA3	2.20	0.41
1:A:259:GLY:HA3	1:A:284:ALA:O	2.21	0.41
1:A:264:SER:HB2	1:B:156:ASN:CB	2.50	0.41
1:C:110:PRO:CD	1:C:197:MET:HE3	2.51	0.41
1:B:223:ASP:OD2	1:B:225:HIS:HB2	2.20	0.41
1:C:298:GLN:O	1:C:299:GLY:C	2.63	0.41
1:D:44:MET:HE1	1:D:198:ALA:HB1	2.03	0.41
1:D:56:THR:HA	1:D:59:LEU:CD1	2.50	0.41
1:D:171:GLY:HA3	1:D:260:TYR:CE1	2.56	0.41
1:D:271:ALA:HA	1:D:272:PRO:HD3	1.84	0.41
1:B:94:GLN:HG2	1:B:150:PHE:O	2.21	0.41
1:D:330:MET:HB3	1:D:359:ILE:CD1	2.51	0.41
1:B:113:GLN:HE21	1:B:113:GLN:HB2	1.49	0.41
1:B:113:GLN:CD	1:B:137:ALA:HB1	2.46	0.41
1:D:171:GLY:HA3	1:D:260:TYR:CZ	2.55	0.41
1:A:298:GLN:O	1:A:299:GLY:C	2.64	0.41
1:A:323:ALA:HA	1:A:372:ASN:ND2	2.35	0.41
1:D:314:ARG:HB2	1:D:314:ARG:NH1	2.19	0.41
1:A:54:LEU:HD23	1:A:55:ASP:N	2.35	0.40
1:B:297:SER:HB2	1:B:309:GLU:CD	2.46	0.40
1:C:102:ILE:O	1:C:187:ALA:HA	2.21	0.40
1:C:201:PHE:O	1:C:204:MET:HB2	2.21	0.40
1:D:3:ARG:HH22	1:D:405:LYS:HE3	1.85	0.40
1:D:112:PHE:HA	1:D:115:PHE:HB3	2.03	0.40
1:D:250:GLY:HA2	4:D:2167:HOH:O	2.20	0.40
1:D:300:THR:O	1:D:301:SER:CB	2.69	0.40
1:B:271:ALA:HA	1:B:272:PRO:HD3	1.92	0.40
1:C:265:ASP:HB2	1:C:394:GLY:HA3	2.03	0.40
1:C:391:GLY:HA2	3:C:1407:DAO:O1	2.22	0.40
1:D:9:LEU:HD12	1:D:9:LEU:O	2.22	0.40
1:C:148:THR:HB	1:C:149:PRO:CD	2.52	0.40
1:D:342:GLU:HA	1:D:345:TYR:CD2	2.57	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	404/418 (97%)	383 (95%)	19 (5%)	2 (0%)	24	16
1	B	404/418 (97%)	384 (95%)	19 (5%)	1 (0%)	43	36
1	C	404/418 (97%)	388 (96%)	14 (4%)	2 (0%)	24	16
1	D	404/418 (97%)	385 (95%)	17 (4%)	2 (0%)	24	16
All	All	1616/1672 (97%)	1540 (95%)	69 (4%)	7 (0%)	30	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	369	ALA
1	C	299	GLY
1	A	299	GLY
1	A	369	ALA
1	B	299	GLY
1	C	301	SER
1	D	303	PRO

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	308/319 (97%)	305 (99%)	3 (1%)	68	67
1	B	308/319 (97%)	304 (99%)	4 (1%)	61	58
1	C	308/319 (97%)	305 (99%)	3 (1%)	68	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	308/319 (97%)	304 (99%)	4 (1%)	61	58
All	All	1232/1276 (97%)	1218 (99%)	14 (1%)	65	64

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	155	VAL
1	A	405	LYS
1	B	51	ASN
1	B	113	GLN
1	B	314	ARG
1	B	405	LYS
1	C	51	ASN
1	C	380	ARG
1	C	405	LYS
1	D	51	ASN
1	D	314	ARG
1	D	321	SER
1	D	405	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	51	ASN
1	A	95	ASN
1	A	176	GLN
1	A	178	GLN
1	A	212	ASN
1	A	225	HIS
1	A	360	ASN
1	A	367	GLN
1	B	51	ASN
1	B	95	ASN
1	B	113	GLN
1	B	172	ASN
1	B	176	GLN
1	B	212	ASN
1	B	360	ASN
1	B	372	ASN

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Mol	Chain	Res	Type
1	C	37	GLN
1	C	51	ASN
1	C	172	ASN
1	C	176	GLN
1	C	178	GLN
1	C	212	ASN
1	C	396	ASN
1	D	37	GLN
1	D	51	ASN
1	D	176	GLN
1	D	178	GLN
1	D	212	ASN
1	D	252	HIS
1	D	360	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 8 ligands modelled in this entry, 4 are modelled with single atom - leaving 4 for Mogul analysis.

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
3	DAO	A	1407	1	11,12,13	0.31	0	10,11,13	0.69	0
3	DAO	C	1407	1	11,12,13	0.39	0	10,11,13	0.56	0
3	DAO	D	1407	1	11,12,13	0.33	0	10,11,13	0.65	0
3	DAO	B	1407	1	11,12,13	0.31	0	10,11,13	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DAO	A	1407	1	-	2/10/10/11	-
3	DAO	C	1407	1	-	1/10/10/11	-
3	DAO	D	1407	1	-	2/10/10/11	-
3	DAO	B	1407	1	-	2/10/10/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1407	DAO	O1-C1-C2-C3
3	B	1407	DAO	O1-C1-C2-C3
3	C	1407	DAO	O1-C1-C2-C3
3	D	1407	DAO	O1-C1-C2-C3
3	B	1407	DAO	C5-C6-C7-C8
3	A	1407	DAO	C4-C5-C6-C7
3	D	1407	DAO	C4-C5-C6-C7

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1407	DAO	3	0
3	C	1407	DAO	5	0
3	D	1407	DAO	2	0
3	B	1407	DAO	5	0

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	406/418 (97%)	-0.03	22 (5%) 31 37	5, 12, 26, 44	0
1	B	406/418 (97%)	0.37	34 (8%) 17 19	6, 16, 37, 52	0
1	C	406/418 (97%)	0.02	17 (4%) 40 47	6, 13, 27, 41	0
1	D	406/418 (97%)	0.25	17 (4%) 40 47	7, 17, 29, 44	0
All	All	1624/1672 (97%)	0.15	90 (5%) 30 36	5, 14, 30, 52	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	370	GLY	11.2
1	A	370	GLY	9.8
1	C	406	ASP	6.4
1	A	289	ASP	5.9
1	B	370	GLY	5.6
1	A	319	ASP	5.4
1	A	320	LYS	5.1
1	A	369	ALA	4.7
1	B	406	ASP	4.7
1	D	405	LYS	4.3
1	B	319	ASP	4.3
1	C	381	GLU	4.3
1	D	369	ALA	4.2
1	B	213	ASP	4.2
1	A	405	LYS	3.9
1	B	371	LEU	3.8
1	A	285	MET	3.8
1	B	318	GLY	3.8
1	B	368	ALA	3.7
1	C	1	MET	3.6
1	A	1	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	381	GLU	3.5
1	A	404	LEU	3.4
1	D	362	GLU	3.3
1	B	321	SER	3.3
1	A	381	GLU	3.2
1	C	307	VAL	3.1
1	C	405	LYS	3.1
1	B	405	LYS	3.1
1	B	364	LEU	3.0
1	B	1	MET	3.0
1	D	1	MET	3.0
1	C	159	ILE	3.0
1	B	314	ARG	2.9
1	D	61	ASP	2.9
1	B	366	GLU	2.9
1	B	390	PHE	2.9
1	B	369	ALA	2.9
1	B	361	ILE	2.9
1	B	372	ASN	2.8
1	A	376	GLU	2.8
1	D	319	ASP	2.8
1	D	91	GLU	2.8
1	C	319	ASP	2.8
1	D	368	ALA	2.7
1	B	28	GLU	2.7
1	B	376	GLU	2.7
1	C	314	ARG	2.7
1	D	28	GLU	2.6
1	B	225	HIS	2.6
1	A	366	GLU	2.6
1	B	381	GLU	2.6
1	B	367	GLN	2.6
1	D	406	ASP	2.6
1	C	61	ASP	2.5
1	B	317	PHE	2.5
1	D	404	LEU	2.5
1	B	298	GLN	2.5
1	B	362	GLU	2.5
1	C	270	VAL	2.5
1	A	268	ASP	2.5
1	A	62	ARG	2.4
1	A	91	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	366	GLU	2.4
1	B	217	LYS	2.4
1	B	113	GLN	2.4
1	D	89	SER	2.4
1	D	390	PHE	2.3
1	A	368	ALA	2.3
1	C	272	PRO	2.3
1	B	30	ARG	2.3
1	B	289	ASP	2.3
1	C	213	ASP	2.3
1	B	374	VAL	2.3
1	C	320	LYS	2.3
1	A	108	GLY	2.2
1	A	61	ASP	2.2
1	B	379	ASP	2.2
1	A	54	LEU	2.2
1	D	213	ASP	2.1
1	B	404	LEU	2.1
1	D	364	LEU	2.1
1	C	362	GLU	2.1
1	A	390	PHE	2.1
1	A	321	SER	2.1
1	B	91	GLU	2.1
1	C	318	GLY	2.1
1	A	307	VAL	2.1
1	C	369	ALA	2.1
1	B	320	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 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($\text{\AA}^2$)	Q<0.9
3	DAO	D	1407	13/14	0.80	0.19	24,29,41,42	0
3	DAO	C	1407	13/14	0.84	0.15	19,25,32,33	0
3	DAO	A	1407	13/14	0.86	0.13	21,26,34,34	0
3	DAO	B	1407	13/14	0.90	0.15	22,30,35,37	0
2	NH4	C	1406	1/1	0.95	0.04	13,13,13,13	0
2	NH4	B	1406	1/1	0.96	0.19	27,27,27,27	0
2	NH4	A	1406	1/1	0.98	0.07	8,8,8,8	0
2	NH4	D	1406	1/1	0.98	0.09	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.