



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:48 AM UTC

PDB ID : 2BZ4 / pdb_00002bz4
Title : structure of E.coli KAS I H298Q mutant
Authors : Olsen, J.G.; von Wettstein-Knowles, P.; Henriksen, A.
Deposited on : 2005-08-10
Resolution : 1.86 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

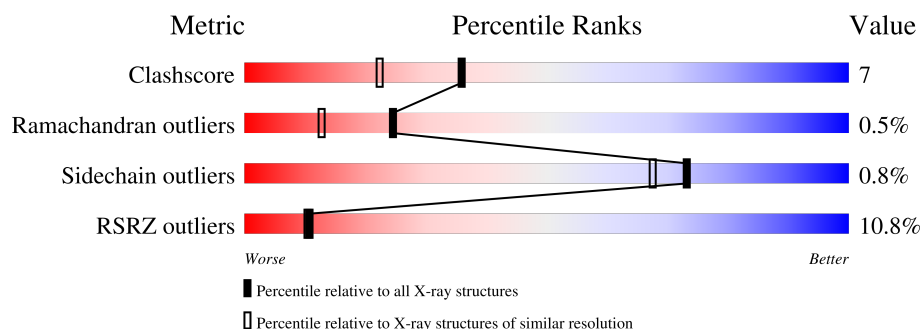
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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% 83% 13% ..
1	B	418	25% 80% 16% ..
1	C	418	5% 82% 14% ..
1	D	418	7% 79% 16% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13012 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.

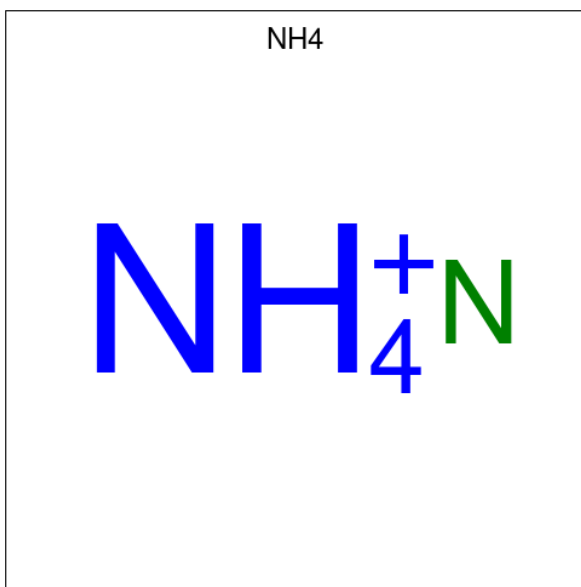
- Molecule 1 is a protein called 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I.

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	403	Total	C	N	O	S	0	0	1
			2953	1835	515	580	23			

There are 4 discrepancies between the modelled and reference sequences:

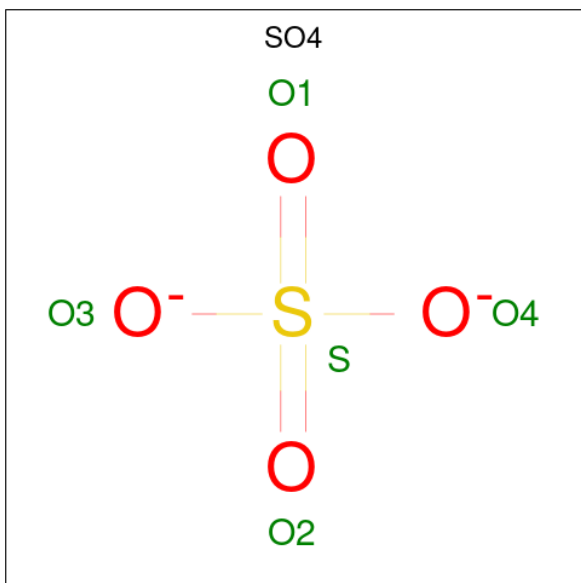
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLN	HIS	engineered mutation	UNP P14926
B	298	GLN	HIS	engineered mutation	UNP P14926
C	298	GLN	HIS	engineered mutation	UNP P14926
D	298	GLN	HIS	engineered mutation	UNP P14926

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



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

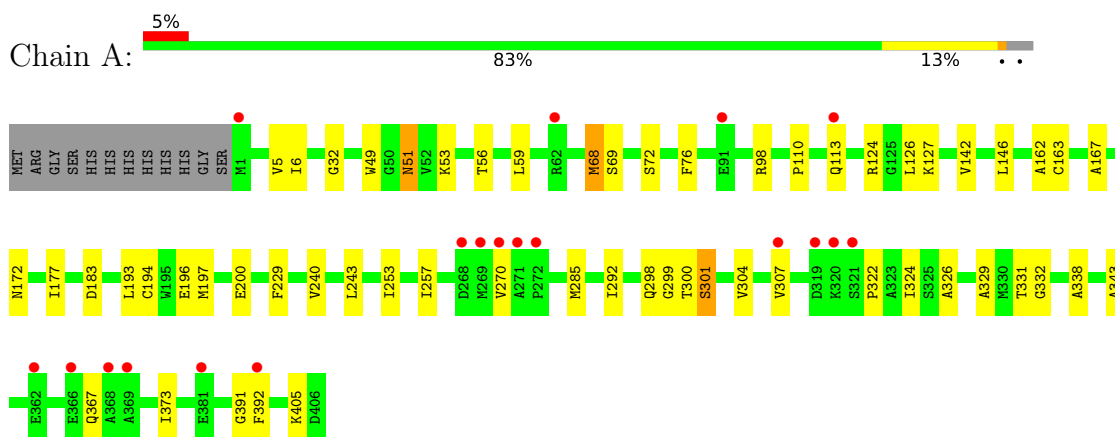
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	318	Total	O	0	0
			318	318		
4	B	230	Total	O	0	0
			230	230		
4	C	317	Total	O	0	0
			317	317		
4	D	264	Total	O	0	0
			264	264		

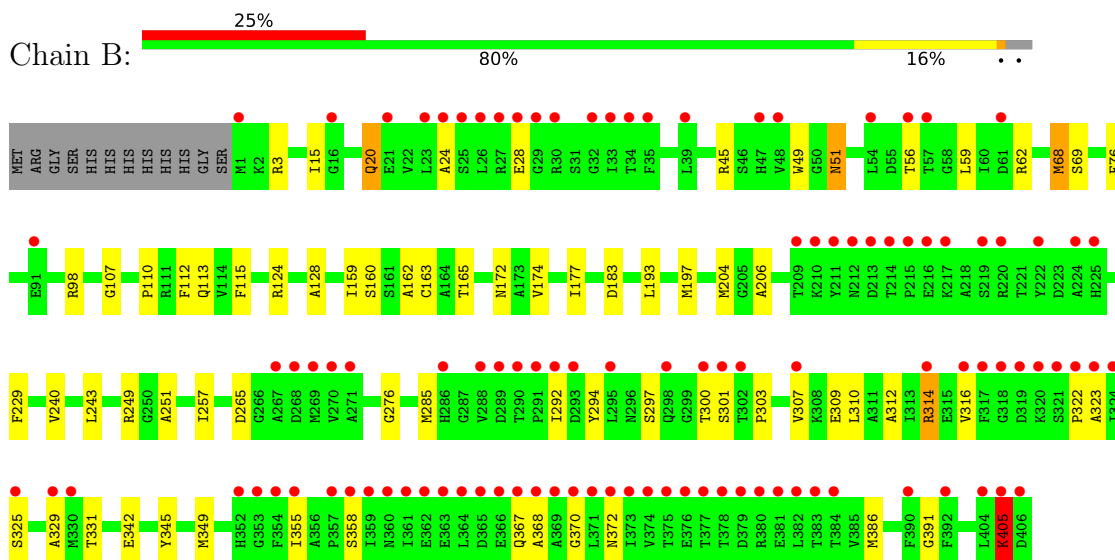
3 Residue-property plots

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.

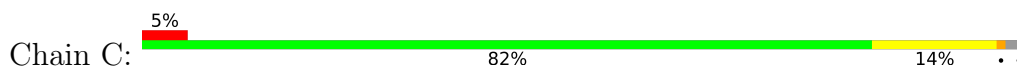
• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I

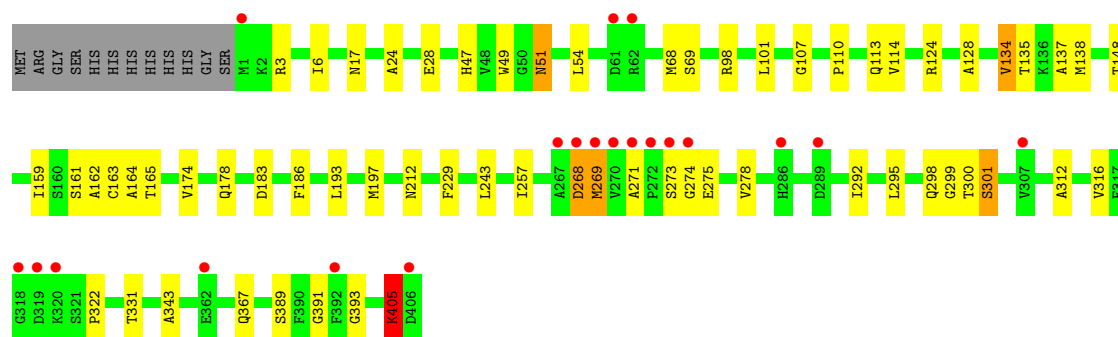


• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I



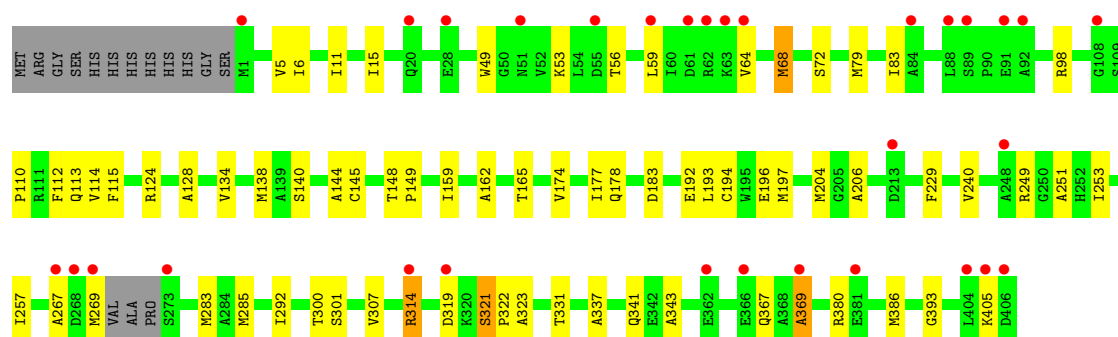
• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I





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

Chain D: 7% 79% 16%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.15Å 138.67Å 212.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.07 – 1.86 26.07 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.2 (26.07-1.86) 98.3 (26.07-1.86)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 1.87Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.234 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13012	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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, 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	1/3019 (0.0%)	0.88	10/4078 (0.2%)
1	B	0.36	1/3019 (0.0%)	0.80	4/4078 (0.1%)
1	C	0.39	1/3019 (0.0%)	0.87	8/4078 (0.2%)
1	D	0.38	1/2998 (0.0%)	0.80	6/4046 (0.1%)
All	All	0.38	4/12055 (0.0%)	0.84	28/16280 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	405	LYS	C-N	-5.67	1.25	1.33
1	A	405	LYS	C-N	-5.66	1.25	1.33
1	C	405	LYS	C-N	-5.64	1.25	1.33
1	B	405	LYS	C-N	-5.63	1.25	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	MET	N-CA-C	7.26	121.85	110.17
1	A	298	GLN	N-CA-C	-7.22	103.35	111.07
1	B	68	MET	N-CA-C	6.73	121.00	110.17
1	C	68	MET	N-CA-C	6.65	120.87	110.17
1	A	331	THR	N-CA-C	6.60	121.41	113.23
1	C	343	ALA	N-CA-C	-6.54	104.23	111.36
1	C	331	THR	N-CA-C	6.44	121.21	113.23
1	D	11	ILE	N-CA-C	6.10	115.87	108.06
1	D	68	MET	N-CA-C	5.92	119.71	110.17
1	C	69	SER	N-CA-C	-5.88	101.28	110.17
1	B	69	SER	N-CA-C	-5.72	101.99	110.46
1	B	162	ALA	CB-CA-C	-5.59	110.15	116.63
1	D	113	GLN	N-CA-C	-5.54	105.15	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	ALA	N-CA-C	-5.53	105.33	111.36
1	A	243	LEU	N-CA-C	5.49	117.71	111.02
1	C	162	ALA	CB-CA-C	-5.43	110.29	116.54
1	C	298	GLN	N-CA-C	-5.43	105.26	111.07
1	D	323	ALA	N-CA-C	-5.33	102.38	110.28
1	A	167	ALA	N-CA-C	-5.32	105.14	111.69
1	D	162	ALA	CB-CA-C	-5.30	110.44	116.54
1	A	69	SER	N-CA-C	-5.28	102.64	110.46
1	B	243	LEU	N-CA-C	5.23	117.39	111.02
1	A	162	ALA	CB-CA-C	-5.15	110.61	116.54
1	C	134	VAL	N-CA-C	5.07	115.69	110.36
1	C	243	LEU	N-CA-C	5.05	117.19	111.02
1	A	332	GLY	N-CA-C	-5.05	104.24	112.83
1	D	343	ALA	N-CA-C	-5.02	105.89	111.36
1	A	338	ALA	N-CA-C	5.02	117.14	111.11

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	2972	0	2936	36	0
1	B	2972	0	2936	61	0
1	C	2972	0	2936	38	0
1	D	2953	0	2914	49	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	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	318	0	0	4	0
4	B	230	0	0	3	0
4	C	317	0	0	1	0
4	D	264	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13012	0	11722	173	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (173) 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:C:51:ASN:HD22	1:C:51:ASN:H	1.17	0.93
1:B:349:MET:HE3	1:B:355:ILE:HA	1.53	0.88
1:A:172:ASN:HD21	1:B:172:ASN:HD21	1.16	0.88
1:A:51:ASN:H	1:A:51:ASN:HD22	1.20	0.85
1:D:314:ARG:HH11	1:D:314:ARG:HB2	1.41	0.83
1:B:307:VAL:HG13	1:B:367:GLN:HG3	1.59	0.83
1:D:307:VAL:HG13	1:D:367:GLN:HG3	1.61	0.82
1:B:314:ARG:HB2	1:B:314:ARG:HH11	1.46	0.78
1:A:124:ARG:HH21	1:A:127:LYS:HE2	1.50	0.77
1:B:51:ASN:H	1:B:51:ASN:HD22	1.36	0.73
1:D:204:MET:HE2	1:D:206:ALA:HB2	1.69	0.73
1:C:51:ASN:HD22	1:C:51:ASN:N	1.90	0.70
1:B:20:GLN:HE21	1:B:20:GLN:H	1.40	0.69
1:B:51:ASN:HD22	1:B:51:ASN:N	1.92	0.68
4:A:2176:HOH:O	1:B:160:SER:HB2	1.94	0.67
1:B:177:ILE:HD12	1:B:240:VAL:HG12	1.76	0.67
1:C:229:PHE:HB3	1:C:300:THR:HG22	1.77	0.66
1:C:6:ILE:HD11	1:C:257:ILE:HD11	1.77	0.66
1:D:177:ILE:HD12	1:D:240:VAL:HG12	1.80	0.64
1:B:124:ARG:HB2	1:B:128:ALA:HB2	1.80	0.64
1:D:68:MET:HB2	1:D:72:SER:HB2	1.79	0.64
1:D:319:ASP:HB3	4:D:2217:HOH:O	1.97	0.64
1:D:56:THR:HA	1:D:59:LEU:HD12	1.80	0.63
1:A:229:PHE:HB3	1:A:300:THR:HG22	1.80	0.63
1:A:172:ASN:HB2	4:A:2178:HOH:O	1.98	0.63
1:A:177:ILE:HD12	1:A:240:VAL:HG12	1.79	0.63
1:C:113:GLN:HG2	1:C:137:ALA:HB1	1.80	0.63
1:A:6:ILE:HD11	1:A:257:ILE:HD11	1.80	0.62
1:D:314:ARG:HB2	1:D:314:ARG:NH1	2.15	0.61
1:B:285:MET:HG3	1:B:386:MET:HE1	1.83	0.60
1:A:110:PRO:HG2	1:A:197:MET:HB2	1.84	0.60
1:B:110:PRO:HG2	1:B:197:MET:HB2	1.82	0.60
1:D:292:ILE:O	1:D:322:PRO:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ARG:HB2	1:D:128:ALA:HB2	1.85	0.59
1:A:172:ASN:HD21	1:B:172:ASN:ND2	1.94	0.59
1:A:304:VAL:O	1:A:307:VAL:HG22	2.02	0.58
1:A:51:ASN:H	1:A:51:ASN:ND2	1.98	0.58
1:C:3:ARG:HH22	1:C:405:LYS:HE2	1.69	0.57
1:D:251:ALA:HB1	4:D:2002:HOH:O	2.03	0.57
1:C:107:GLY:HA3	1:C:197:MET:HE2	1.87	0.57
1:D:314:ARG:NH2	1:D:369:ALA:HB3	2.20	0.56
1:A:68:MET:HE1	1:A:76:PHE:HB2	1.86	0.56
1:D:138:MET:HE3	1:D:140:SER:OG	2.05	0.56
1:B:329:ALA:HB3	4:B:2219:HOH:O	2.05	0.55
4:C:2139:HOH:O	1:D:283:MET:HE1	2.06	0.55
1:B:300:THR:O	1:B:301:SER:HB3	2.07	0.55
1:D:98:ARG:HE	1:D:183:ASP:CG	2.15	0.54
1:C:269:MET:HE3	1:C:393:GLY:HA2	1.88	0.54
1:B:323:ALA:HA	1:B:372:ASN:HD22	1.72	0.54
1:D:6:ILE:HD11	1:D:257:ILE:HD11	1.89	0.54
1:B:3:ARG:HH22	1:B:405:LYS:HE2	1.73	0.54
1:B:257:ILE:H	1:B:257:ILE:HD12	1.73	0.54
1:D:174:VAL:O	1:D:178:GLN:HG3	2.07	0.54
1:B:20:GLN:H	1:B:20:GLN:NE2	2.05	0.53
1:B:294:TYR:HE1	1:B:325:SER:HB3	1.74	0.53
1:C:98:ARG:HE	1:C:183:ASP:CG	2.16	0.53
1:D:269:MET:HE1	1:D:393:GLY:HA2	1.90	0.53
1:B:62:ARG:HG3	4:B:2073:HOH:O	2.08	0.53
1:A:68:MET:HE2	1:A:72:SER:HB3	1.91	0.53
1:B:110:PRO:HG2	1:B:197:MET:HE3	1.90	0.53
1:B:56:THR:HA	1:B:59:LEU:HD12	1.91	0.53
1:A:51:ASN:HD22	1:A:51:ASN:N	1.95	0.52
1:C:101:LEU:HD23	1:C:186:PHE:HB2	1.92	0.52
1:D:285:MET:CG	1:D:386:MET:HE1	2.39	0.52
1:B:294:TYR:CE1	1:B:325:SER:HB3	2.45	0.51
1:D:56:THR:HA	1:D:59:LEU:CD1	2.39	0.51
1:B:265:ASP:OD1	1:B:276:GLY:HA3	2.10	0.51
1:C:163:CYS:SG	1:C:391:GLY:HA2	2.51	0.51
1:B:98:ARG:HE	1:B:183:ASP:CG	2.18	0.50
1:D:124:ARG:HD3	4:D:2111:HOH:O	2.12	0.50
1:D:285:MET:HG3	1:D:386:MET:HE1	1.94	0.50
1:C:24:ALA:O	1:C:28:GLU:HG3	2.11	0.50
1:A:126:LEU:HD12	1:B:45:ARG:HD3	1.93	0.50
1:B:285:MET:HG3	1:B:386:MET:CE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ARG:HB2	1:C:128:ALA:HB2	1.94	0.49
1:B:297:SER:HB2	1:B:309:GLU:CD	2.37	0.49
1:B:257:ILE:HD12	1:B:257:ILE:N	2.28	0.49
1:C:47:HIS:H	1:C:212:ASN:ND2	2.11	0.49
1:C:148:THR:HG23	1:D:267:ALA:O	2.12	0.49
1:B:51:ASN:H	1:B:51:ASN:ND2	2.05	0.49
1:B:163:CYS:SG	1:B:391:GLY:HA2	2.53	0.49
1:D:15:ILE:HD13	1:D:331:THR:HG22	1.95	0.49
1:C:51:ASN:H	1:C:51:ASN:ND2	1.95	0.49
1:D:49:TRP:CE3	1:D:193:LEU:HG	2.48	0.49
1:A:56:THR:HA	1:A:59:LEU:HD12	1.95	0.49
1:B:204:MET:HE2	1:B:206:ALA:HB2	1.94	0.48
1:C:174:VAL:O	1:C:178:GLN:HG3	2.12	0.48
1:B:229:PHE:HB3	1:B:300:THR:HG22	1.95	0.48
1:A:163:CYS:SG	1:A:391:GLY:HA2	2.54	0.48
1:D:314:ARG:HH21	1:D:369:ALA:HB3	1.79	0.48
1:B:24:ALA:O	1:B:28:GLU:HG2	2.14	0.47
1:D:64:VAL:HG12	1:D:68:MET:HE3	1.96	0.47
1:D:110:PRO:HG2	1:D:197:MET:HB2	1.96	0.47
1:D:321:SER:HB3	4:D:2243:HOH:O	2.14	0.47
1:A:285:MET:SD	1:A:292:ILE:HD11	2.55	0.47
1:C:292:ILE:O	1:C:322:PRO:HB3	2.14	0.47
1:C:300:THR:O	1:C:301:SER:HB3	2.15	0.47
1:A:113:GLN:CD	1:B:110:PRO:HB3	2.40	0.47
1:C:135:THR:HA	1:C:138:MET:HE2	1.96	0.47
1:C:300:THR:O	1:C:301:SER:CB	2.62	0.47
1:D:110:PRO:O	1:D:114:VAL:HG23	2.15	0.47
1:B:49:TRP:CE3	1:B:193:LEU:HG	2.50	0.46
1:D:134:VAL:HB	4:D:2119:HOH:O	2.15	0.46
1:A:5:VAL:HB	1:A:253:ILE:HG23	1.98	0.46
1:C:49:TRP:CE3	1:C:193:LEU:HG	2.51	0.46
1:A:326:ALA:HB1	4:A:2265:HOH:O	2.16	0.46
1:B:15:ILE:HD13	1:B:331:THR:HG22	1.98	0.46
1:A:300:THR:O	1:A:301:SER:CB	2.63	0.46
1:B:310:LEU:HD13	1:B:368:ALA:HB2	1.98	0.46
1:B:110:PRO:CG	1:B:197:MET:HE3	2.45	0.46
1:A:126:LEU:CD1	1:B:45:ARG:HD3	2.46	0.46
1:A:292:ILE:O	1:A:322:PRO:HB3	2.15	0.46
1:C:295:LEU:HD23	1:C:295:LEU:C	2.40	0.46
1:D:300:THR:O	1:D:301:SER:HB3	2.15	0.46
1:D:269:MET:CE	1:D:393:GLY:HA2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:GLN:OE1	1:D:110:PRO:HB3	2.16	0.45
1:A:270:VAL:HG12	1:A:392:PHE:HD2	1.82	0.45
1:B:112:PHE:HA	1:B:115:PHE:HB3	1.99	0.45
1:B:285:MET:CG	1:B:386:MET:HE1	2.47	0.45
1:C:269:MET:CE	1:C:393:GLY:HA2	2.45	0.45
1:C:159:ILE:O	1:C:165:THR:HG23	2.16	0.45
1:A:98:ARG:HE	1:A:183:ASP:CG	2.24	0.45
1:D:229:PHE:HB3	1:D:300:THR:HG22	1.98	0.45
1:B:292:ILE:O	1:B:322:PRO:HB3	2.17	0.45
1:B:314:ARG:NH2	1:B:370:GLY:H	2.14	0.45
1:B:68:MET:HE1	1:B:76:PHE:HB2	1.98	0.44
1:D:249:ARG:CZ	1:D:251:ALA:HB2	2.47	0.44
1:B:249:ARG:CZ	1:B:251:ALA:HB2	2.47	0.44
1:A:300:THR:O	1:A:301:SER:HB3	2.17	0.44
1:B:303:PRO:O	1:B:307:VAL:HG23	2.18	0.44
1:C:113:GLN:HE21	1:C:137:ALA:HB1	1.83	0.44
1:A:200:GLU:OE1	1:B:113:GLN:NE2	2.50	0.44
1:A:324:ILE:HB	1:A:373:ILE:HD13	1.99	0.44
1:A:32:GLY:O	1:A:53:LYS:NZ	2.50	0.44
1:B:107:GLY:HA3	1:B:197:MET:CE	2.48	0.44
1:C:269:MET:HE1	1:D:144:ALA:HB1	1.99	0.44
1:D:68:MET:HE2	1:D:145:CYS:HB3	1.98	0.44
1:D:5:VAL:HB	1:D:253:ILE:HG23	1.99	0.43
1:B:342:GLU:HA	1:B:345:TYR:CD2	2.53	0.43
1:B:107:GLY:HA3	1:B:197:MET:HE2	2.01	0.43
1:D:380:ARG:HG2	1:D:380:ARG:HH11	1.83	0.43
1:A:367:GLN:NE2	1:C:367:GLN:HG2	2.34	0.42
1:C:268:ASP:OD1	1:C:271:ALA:HB3	2.18	0.42
1:A:49:TRP:CE3	1:A:193:LEU:HG	2.54	0.42
1:A:329:ALA:HB3	4:A:2286:HOH:O	2.19	0.42
1:D:79:MET:O	1:D:83:ILE:HG13	2.20	0.42
1:D:337:ALA:O	1:D:341:GLN:HG3	2.20	0.42
1:C:134:VAL:HG23	4:D:2143:HOH:O	2.19	0.42
1:C:273:SER:C	1:C:275:GLU:H	2.27	0.42
1:C:274:GLY:O	1:C:278:VAL:HG23	2.20	0.42
1:B:358:SER:HB3	4:B:2163:HOH:O	2.20	0.42
1:C:312:ALA:O	1:C:316:VAL:HG23	2.20	0.41
1:B:300:THR:O	1:B:301:SER:CB	2.67	0.41
1:D:159:ILE:O	1:D:165:THR:HG23	2.21	0.41
1:D:177:ILE:CD1	1:D:240:VAL:HG12	2.48	0.41
1:D:300:THR:O	1:D:301:SER:CB	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:THR:N	1:D:149:PRO:HD2	2.35	0.41
1:B:49:TRP:C	1:B:49:TRP:CD1	2.98	0.41
1:C:110:PRO:O	1:C:114:VAL:HG23	2.19	0.41
1:B:314:ARG:HB2	1:B:314:ARG:NH1	2.26	0.41
1:C:107:GLY:HA3	1:C:197:MET:CE	2.48	0.41
1:D:112:PHE:HA	1:D:115:PHE:HB3	2.02	0.41
1:A:110:PRO:HB3	1:B:113:GLN:NE2	2.36	0.41
1:D:192:GLU:HG2	4:D:2135:HOH:O	2.20	0.41
1:B:159:ILE:O	1:B:165:THR:HG23	2.20	0.41
1:B:174:VAL:HG21	1:B:257:ILE:HG21	2.02	0.41
1:D:194:CYS:HB2	1:D:196:GLU:OE2	2.21	0.41
1:A:142:VAL:O	1:A:146:LEU:HD13	2.21	0.40
1:C:164:ALA:HA	1:C:389:SER:HB3	2.03	0.40
1:C:17:ASN:CG	1:C:54:LEU:HB2	2.46	0.40
1:B:312:ALA:O	1:B:316:VAL:HG23	2.21	0.40
1:A:194:CYS:HB2	1:A:196:GLU:OE2	2.21	0.40
1:B:177:ILE:CD1	1:B:240:VAL:HG12	2.46	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	404/418 (97%)	386 (96%)	16 (4%)	2 (0%)	24	13
1	B	404/418 (97%)	375 (93%)	29 (7%)	0	100	100
1	C	404/418 (97%)	387 (96%)	12 (3%)	5 (1%)	10	2
1	D	399/418 (96%)	380 (95%)	18 (4%)	1 (0%)	36	25
All	All	1611/1672 (96%)	1528 (95%)	75 (5%)	8 (0%)	24	13

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	369	ALA
1	C	269	MET
1	C	301	SER
1	A	301	SER
1	C	268	ASP
1	C	161	SER
1	C	299	GLY
1	A	299	GLY

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	308/319 (97%)	307 (100%)	1 (0%)	86	85
1	B	308/319 (97%)	304 (99%)	4 (1%)	61	51
1	C	308/319 (97%)	306 (99%)	2 (1%)	78	73
1	D	306/319 (96%)	303 (99%)	3 (1%)	68	60
All	All	1230/1276 (96%)	1220 (99%)	10 (1%)	73	67

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	B	20	GLN
1	B	51	ASN
1	B	314	ARG
1	B	405	LYS
1	C	51	ASN
1	C	405	LYS
1	D	53	LYS
1	D	314	ARG
1	D	321	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	95	ASN
1	A	172	ASN
1	A	176	GLN
1	A	178	GLN
1	A	367	GLN
1	A	396	ASN
1	B	20	GLN
1	B	51	ASN
1	B	95	ASN
1	B	176	GLN
1	B	178	GLN
1	B	372	ASN
1	B	396	ASN
1	C	51	ASN
1	C	95	ASN
1	C	113	GLN
1	C	176	GLN
1	C	178	GLN
1	C	212	ASN
1	C	252	HIS
1	C	372	ASN
1	C	396	ASN
1	D	20	GLN
1	D	176	GLN
1	D	225	HIS
1	D	360	ASN
1	D	396	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are modelled with single atom - leaving 2 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	SO4	C	1407	-	4,4,4	0.37	0	6,6,6	0.07	0
3	SO4	D	1407	-	4,4,4	0.44	0	6,6,6	0.09	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	406/418 (97%)	0.01	19 (4%) 36 39	4, 14, 32, 46	0
1	B	406/418 (97%)	1.07	105 (25%) 1 1	7, 22, 44, 55	0
1	C	406/418 (97%)	0.07	20 (4%) 35 38	6, 14, 32, 50	0
1	D	403/418 (96%)	0.52	31 (7%) 19 20	8, 19, 34, 49	0
All	All	1621/1672 (96%)	0.42	175 (10%) 11 10	4, 17, 37, 55	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	406	ASP	6.2
1	B	372	ASN	6.1
1	B	370	GLY	5.9
1	A	270	VAL	5.8
1	B	361	ILE	5.7
1	B	406	ASP	5.7
1	D	405	LYS	5.4
1	A	321	SER	5.3
1	D	273	SER	5.2
1	C	270	VAL	5.1
1	C	271	ALA	5.0
1	C	273	SER	4.9
1	A	268	ASP	4.8
1	C	272	PRO	4.8
1	B	28	GLU	4.7
1	A	271	ALA	4.5
1	B	374	VAL	4.5
1	B	325	SER	4.4
1	B	373	ILE	4.4
1	B	371	LEU	4.3
1	D	268	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	406	ASP	4.2
1	A	319	ASP	4.2
1	B	368	ALA	4.1
1	B	290	THR	4.1
1	C	268	ASP	4.1
1	B	224	ALA	4.0
1	B	378	THR	4.0
1	B	366	GLU	3.9
1	A	320	LYS	3.8
1	B	359	ILE	3.8
1	C	392	PHE	3.8
1	D	362	GLU	3.8
1	B	213	ASP	3.8
1	A	369	ALA	3.8
1	D	61	ASP	3.8
1	B	369	ALA	3.8
1	B	211	TYR	3.7
1	B	362	GLU	3.7
1	C	319	ASP	3.7
1	B	381	GLU	3.7
1	D	369	ALA	3.7
1	D	319	ASP	3.6
1	B	364	LEU	3.6
1	C	267	ALA	3.6
1	B	322	PRO	3.6
1	D	91	GLU	3.6
1	C	318	GLY	3.6
1	C	307	VAL	3.6
1	B	319	ASP	3.6
1	B	270	VAL	3.5
1	B	24	ALA	3.5
1	A	381	GLU	3.5
1	D	381	GLU	3.5
1	A	392	PHE	3.5
1	B	271	ALA	3.4
1	B	289	ASP	3.4
1	D	366	GLU	3.3
1	B	321	SER	3.3
1	C	1	MET	3.3
1	B	360	ASN	3.3
1	B	392	PHE	3.3
1	B	363	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	320	LYS	3.2
1	B	379	ASP	3.2
1	B	355	ILE	3.1
1	B	324	ILE	3.1
1	B	358	SER	3.1
1	B	35	PHE	3.1
1	B	380	ARG	3.1
1	B	317	PHE	3.0
1	B	29	GLY	3.0
1	B	376	GLU	3.0
1	B	214	THR	3.0
1	B	383	THR	3.0
1	B	212	ASN	3.0
1	B	307	VAL	2.9
1	B	354	PHE	2.9
1	B	1	MET	2.9
1	D	92	ALA	2.9
1	D	20	GLN	2.9
1	A	366	GLU	2.9
1	B	48	VAL	2.9
1	A	113	GLN	2.9
1	B	314	ARG	2.9
1	B	353	GLY	2.9
1	A	272	PRO	2.8
1	D	267	ALA	2.8
1	B	32	GLY	2.8
1	B	57	THR	2.8
1	B	375	THR	2.8
1	B	30	ARG	2.8
1	D	62	ARG	2.8
1	B	222	TYR	2.8
1	B	323	ALA	2.8
1	B	217	LYS	2.8
1	B	27	ARG	2.7
1	C	286	HIS	2.7
1	B	267	ALA	2.7
1	D	64	VAL	2.7
1	C	289	ASP	2.6
1	B	405	LYS	2.6
1	A	307	VAL	2.6
1	B	318	GLY	2.6
1	B	268	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	390	PHE	2.6
1	B	316	VAL	2.6
1	B	301	SER	2.6
1	B	302	THR	2.6
1	B	367	GLN	2.5
1	B	54	LEU	2.5
1	B	286	HIS	2.5
1	B	209	THR	2.5
1	A	62	ARG	2.5
1	C	269	MET	2.5
1	B	295	LEU	2.5
1	B	365	ASP	2.5
1	B	320	LYS	2.5
1	B	292	ILE	2.5
1	D	28	GLU	2.5
1	B	26	LEU	2.4
1	A	91	GLU	2.4
1	B	298	GLN	2.4
1	A	1	MET	2.4
1	C	274	GLY	2.4
1	B	225	HIS	2.4
1	B	34	THR	2.4
1	B	329	ALA	2.4
1	B	291	PRO	2.4
1	D	108	GLY	2.4
1	D	269	MET	2.3
1	B	219	SER	2.3
1	D	213	ASP	2.3
1	B	23	LEU	2.3
1	B	382	LEU	2.3
1	B	404	LEU	2.3
1	B	377	THR	2.3
1	D	1	MET	2.3
1	B	216	GLU	2.3
1	B	47	HIS	2.3
1	D	248	ALA	2.3
1	B	21	GLU	2.3
1	B	91	GLU	2.3
1	B	293	ASP	2.2
1	B	288	VAL	2.2
1	B	300	THR	2.2
1	D	314	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	59	LEU	2.2
1	B	352	HIS	2.2
1	B	39	LEU	2.2
1	B	220	ARG	2.2
1	C	62	ARG	2.2
1	D	51	ASN	2.1
1	C	362	GLU	2.1
1	B	16	GLY	2.1
1	B	330	MET	2.1
1	A	368	ALA	2.1
1	B	61	ASP	2.1
1	C	61	ASP	2.1
1	D	55	ASP	2.1
1	D	89	SER	2.1
1	B	210	LYS	2.1
1	B	357	PRO	2.1
1	A	362	GLU	2.1
1	A	269	MET	2.1
1	D	88	LEU	2.1
1	B	25	SER	2.0
1	B	33	ILE	2.0
1	B	56	THR	2.0
1	B	215	PRO	2.0
1	D	404	LEU	2.0
1	D	84	ALA	2.0
1	D	63	LYS	2.0
1	B	269	MET	2.0
1	B	384	THR	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	SO4	D	1407	5/5	0.71	0.20	46,46,48,49	0
2	NH4	B	1406	1/1	0.86	0.14	23,23,23,23	0
3	SO4	C	1407	5/5	0.92	0.13	42,43,44,44	0
2	NH4	C	1406	1/1	0.96	0.05	14,14,14,14	0
2	NH4	D	1406	1/1	0.98	0.08	14,14,14,14	0
2	NH4	A	1406	1/1	0.99	0.03	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.