



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:51 AM GMT

PDB ID : 2BZ4  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

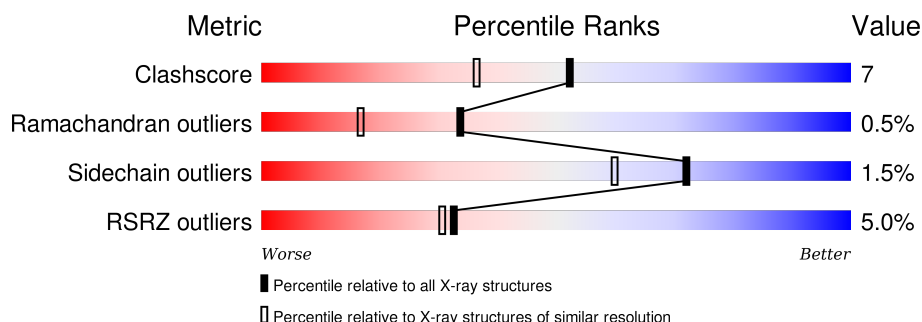
# 1 Overall quality at a glance

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	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	
1	B	418	
1	C	418	
1	D	418	

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	B	1406	-	-	-	X
2	NH4	C	1406	-	-	-	X
2	NH4	D	1406	-	-	-	X

## 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.

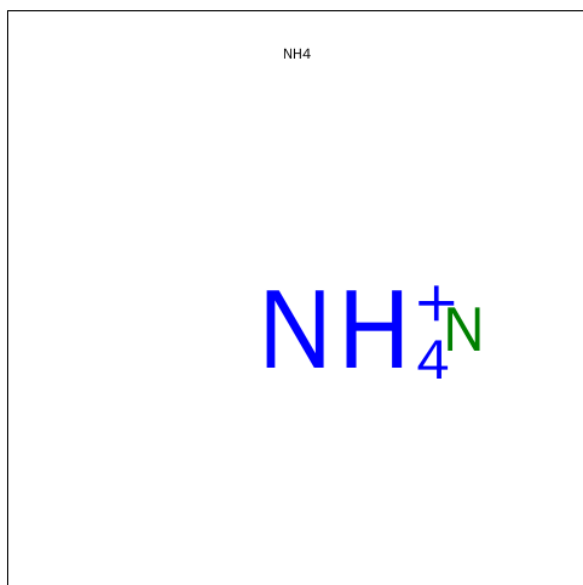
- Molecule 1 is a protein called 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I.

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 (three-letter code: NH4) (formula: H<sub>4</sub>N).



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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

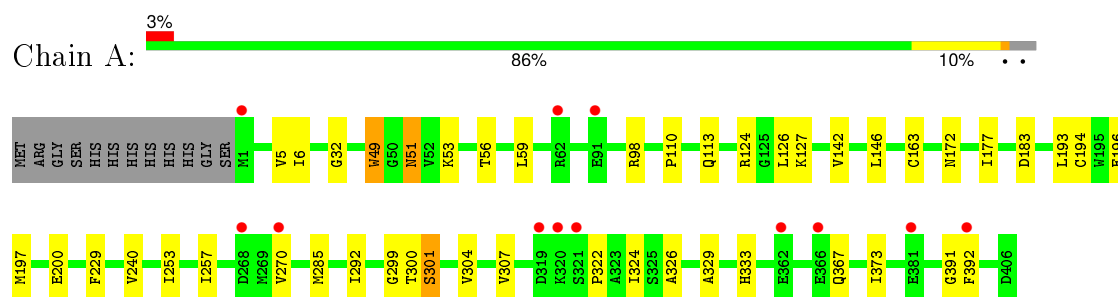
- Molecule 4 is water.

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		

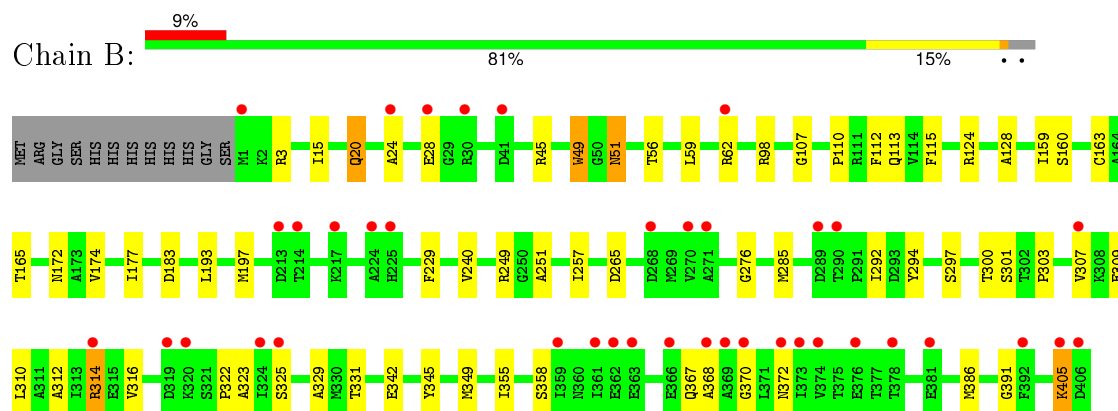
### 3 Residue-property plots

These plots are drawn for all protein, RNA 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.

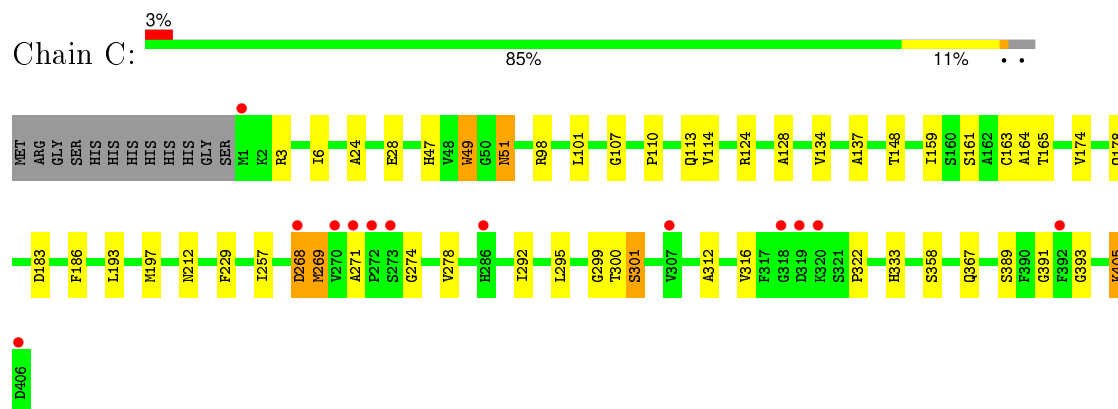
#### • Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I



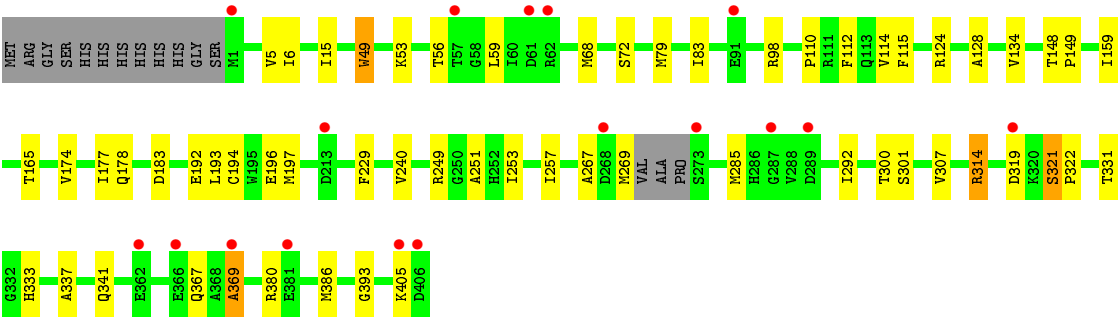
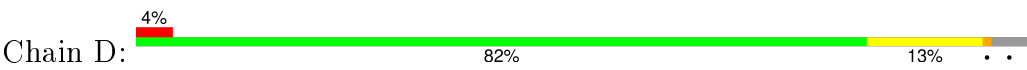
#### • Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I



#### • 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, $\alpha$ , $\beta$ , $\gamma$	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) 98.4 (26.07-1.86)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.41 (at 1.87Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.204 , 0.234 0.205 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	15.6	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 57.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 144860 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13012	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.33	0/3019	0.59	0/4078
1	B	0.30	0/3019	0.52	0/4078
1	C	0.32	0/3019	0.59	0/4078
1	D	0.31	0/2998	0.54	0/4046
All	All	0.32	0/12055	0.56	0/16280

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 [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	2936	34	0
1	B	2972	0	2936	56	0
1	C	2972	0	2936	35	0
1	D	2953	0	2914	43	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
4	D	264	0	0	7	0
All	All	13012	0	11722	158	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 (158) 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:H	1:C:51:ASN:HD22	1.17	0.93
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:B:349:MET:HE3	1:B:355:ILE:HA	1.67	0.77
1:A:124:ARG:HH21	1:A:127:LYS:HE2	1.50	0.77
1:B:51:ASN:HD22	1:B:51:ASN:H	1.36	0.73
1:C:51:ASN:N	1:C:51:ASN:HD22	1.90	0.70
1:B:20:GLN:H	1:B:20:GLN:HE21	1.40	0.69
1:B:51:ASN:N	1:B:51:ASN:HD22	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:NH1	1:D:314:ARG:HB2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:314:ARG:NH2	1:D:369:ALA:HB3	2.20	0.56
1:B:329:ALA:HB3	4:B:2219:HOH:O	2.05	0.55
1:B:300:THR:O	1:B:301:SER:HB3	2.07	0.55
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:HD12	1:B:257:ILE:H	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:B:62:ARG:HG3	4:B:2073:HOH:O	2.08	0.53
1:B:56:THR:HA	1:B:59:LEU:HD12	1.91	0.53
1:C:51:ASN:ND2	1:C:51:ASN:H	1.95	0.52
1:A:51:ASN:N	1:A:51:ASN:HD22	1.95	0.52
1:C:101:LEU:HD23	1:C:186:PHE:HB2	1.92	0.52
1:B:294:TYR:CE1	1:B:325:SER:HB3	2.45	0.51
1:D:285:MET:HG3	1:D:386:MET:HE1	1.91	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:D:124:ARG:HD3	4:D:2111:HOH:O	2.12	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:D:98:ARG:HE	1:D:183:ASP:CG	2.15	0.50
1:B:285:MET:HG3	1:B:386:MET:CE	2.42	0.49
1:C:124:ARG:HB2	1:C:128:ALA:HB2	1.94	0.49
1:B:257:ILE:N	1:B:257:ILE:HD12	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:ND2	1:B:51:ASN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:98:ARG:HE	1:C:183:ASP:CG	2.16	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:D:314:ARG:HH21	1:D:369:ALA:HB3	1.79	0.48
1:A:163:CYS:SG	1:A:391:GLY:HA2	2.54	0.48
1:B:24:ALA:O	1:B:28:GLU:HG2	2.14	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:C:300:THR:O	1:C:301:SER:HB3	2.15	0.47
1:C:292:ILE:O	1:C:322:PRO:HB3	2.14	0.47
1:A:285:MET:SD	1:A:292:ILE:HD11	2.55	0.47
1:C:300:THR:O	1:C:301:SER:CB	2.62	0.47
1:D:269:MET:HE1	1:D:393:GLY:HA2	1.96	0.47
1:D:110:PRO:O	1:D:114:VAL:HG23	2.15	0.47
1:D:134:VAL:HB	4:D:2119:HOH:O	2.15	0.46
1:B:49:TRP:CE3	1:B:193:LEU:HG	2.50	0.46
1:A:5:VAL:HB	1:A:253:ILE:HG23	1.98	0.46
1:B:349:MET:CE	1:B:355:ILE:HA	2.43	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:98:ARG:HE	1:B:183:ASP:CG	2.18	0.46
1:D:285:MET:CG	1:D:386:MET:HE1	2.46	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:D:300:THR:O	1:D:301:SER:HB3	2.15	0.46
1:C:269:MET:CE	1:C:393:GLY:HA2	2.45	0.46
1:D:269:MET:CE	1:D:393:GLY:HA2	2.46	0.45
1:C:113:GLN:OE1	1:D:110:PRO:HB3	2.16	0.45
1:B:107:GLY:HA3	1:B:197:MET:HE1	1.98	0.45
1:B:112:PHE:HA	1:B:115:PHE:HB3	1.99	0.45
1:A:270:VAL:HG12	1:A:392:PHE:HD2	1.82	0.45
1:C:159:ILE:O	1:C:165:THR:HG23	2.16	0.45
1:B:297:SER:HB2	1:B:309:GLU:CD	2.37	0.45
1:D:229:PHE:HB3	1:D:300:THR:HG22	1.98	0.45
1:C:51:ASN:N	1:C:51:ASN:ND2	2.61	0.45
1:B:314:ARG:NH2	1:B:370:GLY:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ILE:O	1:B:322:PRO:HB3	2.17	0.45
1:D:249:ARG:CZ	1:D:251:ALA:HB2	2.47	0.44
1:B:285:MET:HG3	1:B:386:MET:HE1	1.98	0.44
1:B:249:ARG:CZ	1:B:251:ALA:HB2	2.47	0.44
1:B:303:PRO:O	1:B:307:VAL:HG23	2.18	0.44
1:A:300:THR:O	1:A:301:SER:HB3	2.17	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:B:107:GLY:HA3	1:B:197:MET:CE	2.48	0.44
1:A:32:GLY:O	1:A:53:LYS:NZ	2.50	0.44
1:C:269:MET:HE1	1:C:393:GLY:HA2	2.01	0.43
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:D:380:ARG:HG2	1:D:380:ARG:HH11	1.83	0.43
1:C:107:GLY:HA3	1:C:197:MET:CE	2.48	0.42
1:C:268:ASP:OD1	1:C:271:ALA:HB3	2.18	0.42
1:A:367:GLN:NE2	1:C:367:GLN:HG2	2.34	0.42
1:A:329:ALA:HB3	4:A:2286:HOH:O	2.19	0.42
1:A:49:TRP:CE3	1:A:193:LEU:HG	2.54	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:A:113:GLN:CD	1:B:110:PRO:HB3	2.40	0.42
1:C:134:VAL:HG23	4:D:2143:HOH:O	2.19	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:D:177:ILE:CD1	1:D:240:VAL:HG12	2.48	0.41
1:B:300:THR:O	1:B:301:SER:CB	2.67	0.41
1:D:300:THR:O	1:D:301:SER:CB	2.67	0.41
1:D:159:ILE:O	1:D:165:THR:HG23	2.21	0.41
1:D:148:THR:N	1:D:149:PRO:HD2	2.35	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:295:LEU:C	1:C:295:LEU:HD23	2.40	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:174:VAL:HG21	1:B:257:ILE:HG21	2.02	0.41
1:B:159:ILE:O	1:B:165:THR:HG23	2.20	0.41
1:D:194:CYS:HB2	1:D:196:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:98:ARG:HE	1:A:183:ASP:CG	2.24	0.40
1:C:107:GLY:HA3	1:C:197:MET:HE1	2.04	0.40
1:B:312:ALA:O	1:B:316:VAL:HG23	2.21	0.40
1:B:177:ILE:CD1	1:B:240:VAL:HG12	2.46	0.40
1:A:194:CYS:HB2	1:A:196:GLU:OE2	2.21	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%)	386 (96%)	16 (4%)	2 (0%)	34	17
1	B	404/418 (97%)	375 (93%)	29 (7%)	0	100	100
1	C	404/418 (97%)	387 (96%)	12 (3%)	5 (1%)	16	4
1	D	399/418 (96%)	380 (95%)	18 (4%)	1 (0%)	46	29
All	All	1611/1672 (96%)	1528 (95%)	75 (5%)	8 (0%)	34	17

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%)	305 (99%)	3 (1%)	82	76
1	B	308/319 (97%)	303 (98%)	5 (2%)	70	57
1	C	308/319 (97%)	303 (98%)	5 (2%)	70	57
1	D	306/319 (96%)	300 (98%)	6 (2%)	63	47
All	All	1230/1276 (96%)	1211 (98%)	19 (2%)	72	60

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	TRP
1	A	51	ASN
1	A	333	HIS
1	B	20	GLN
1	B	49	TRP
1	B	51	ASN
1	B	314	ARG
1	B	405	LYS
1	C	49	TRP
1	C	51	ASN
1	C	333	HIS
1	C	358	SER
1	C	405	LYS
1	D	49	TRP
1	D	53	LYS
1	D	314	ARG
1	D	321	SER
1	D	333	HIS
1	D	405	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	51	ASN
1	A	172	ASN
1	A	367	GLN
1	B	20	GLN
1	B	51	ASN
1	B	372	ASN
1	C	51	ASN
1	C	95	ASN
1	C	113	GLN
1	C	212	ASN
1	C	252	HIS
1	C	372	ASN
1	D	225	HIS
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 carbohydrates 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	0.25	0	6,6,6	0.08	0
3	SO4	D	1407	-	4,4,4	0.35	0	6,6,6	0.11	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	SO4	C	1407	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1407	-	-	0/0/0/0	0/0/0/0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	406/418 (97%)	-0.16	12 (2%) 54 51	4, 14, 32, 46	0
1	B	406/418 (97%)	0.59	39 (9%) 10 10	7, 22, 44, 55	0
1	C	406/418 (97%)	-0.04	13 (3%) 51 48	6, 15, 32, 50	0
1	D	403/418 (96%)	0.28	17 (4%) 40 37	8, 19, 34, 49	0
All	All	1621/1672 (96%)	0.17	81 (4%) 32 31	4, 17, 37, 55	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	406	ASP	8.7
1	B	319	ASP	5.6
1	B	406	ASP	5.6
1	C	273	SER	5.3
1	C	1	MET	4.8
1	B	213	ASP	4.5
1	C	406	ASP	4.5
1	C	270	VAL	4.3
1	C	271	ALA	4.1
1	B	370	GLY	4.0
1	D	1	MET	4.0
1	D	273	SER	3.9
1	D	405	LYS	3.9
1	B	270	VAL	3.8
1	A	270	VAL	3.8
1	D	62	ARG	3.8
1	D	268	ASP	3.8
1	C	268	ASP	3.7
1	B	28	GLU	3.7
1	C	319	ASP	3.6
1	B	1	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	361	ILE	3.5
1	B	362	GLU	3.5
1	A	319	ASP	3.4
1	C	318	GLY	3.4
1	A	268	ASP	3.3
1	C	320	LYS	3.3
1	A	321	SER	3.2
1	B	372	ASN	3.2
1	D	91	GLU	3.1
1	B	405	LYS	3.1
1	B	24	ALA	3.0
1	B	271	ALA	3.0
1	B	366	GLU	3.0
1	D	381	GLU	3.0
1	A	1	MET	3.0
1	C	272	PRO	3.0
1	A	62	ARG	2.9
1	B	30	ARG	2.9
1	D	369	ALA	2.9
1	B	374	VAL	2.8
1	C	286	HIS	2.8
1	A	366	GLU	2.8
1	D	366	GLU	2.8
1	D	61	ASP	2.7
1	B	359	ILE	2.7
1	B	307	VAL	2.7
1	D	57	THR	2.7
1	D	213	ASP	2.7
1	B	325	SER	2.6
1	D	287	GLY	2.6
1	A	392	PHE	2.6
1	C	392	PHE	2.6
1	B	363	GLU	2.6
1	A	320	LYS	2.5
1	D	362	GLU	2.5
1	A	362	GLU	2.5
1	B	320	LYS	2.5
1	A	381	GLU	2.5
1	B	373	ILE	2.5
1	A	91	GLU	2.4
1	B	369	ALA	2.3
1	D	319	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	314	ARG	2.3
1	C	307	VAL	2.3
1	B	225	HIS	2.3
1	B	289	ASP	2.3
1	B	224	ALA	2.2
1	B	268	ASP	2.2
1	B	290	THR	2.2
1	B	368	ALA	2.2
1	B	214	THR	2.2
1	B	378	THR	2.2
1	B	381	GLU	2.1
1	B	392	PHE	2.1
1	B	324	ILE	2.1
1	B	62	ARG	2.1
1	B	376	GLU	2.1
1	D	289	ASP	2.0
1	B	217	LYS	2.0
1	B	41	ASP	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NH4	D	1406	1/1	0.98	0.21	11.02	14,14,14,14	0
2	NH4	C	1406	1/1	0.97	0.15	3.19	14,14,14,14	0
2	NH4	B	1406	1/1	0.91	0.24	2.53	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NH4	A	1406	1/1	0.99	0.12	2.00	9,9,9,9	0
3	SO4	D	1407	5/5	0.73	0.33	-	46,46,48,49	0
3	SO4	C	1407	5/5	0.96	0.23	-	42,43,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.