Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:51 AM GMT

PDB ID	:	2BYY
Title	:	E.coli KAS I H298E Mutation
Authors	:	Olsen, J.G.; von Wettstein-Knowles, P.; Henriksen, A.
Deposited on	:	2005-08-09
Resolution	:	2.20 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:

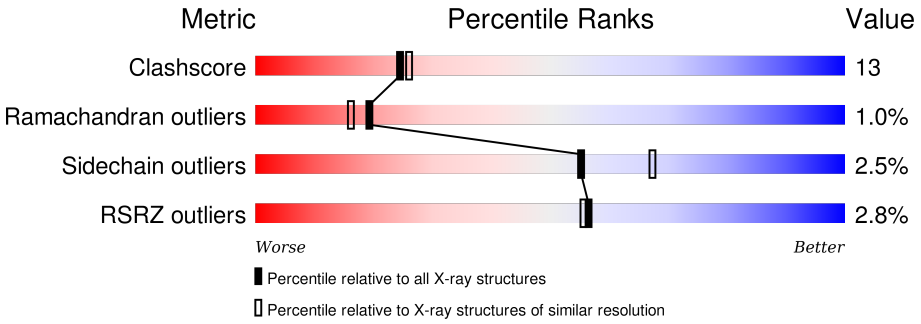
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	418	3% 72% 24%
1	B	418	4% 70% 26%
1	C	418	% 72% 23%
1	D	418	3% 73% 22%

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

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12464 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	517	584	23			
1	B	406	Total	C	N	O	S	0	0	1
			2972	1848	517	584	23			
1	C	406	Total	C	N	O	S	0	0	1
			2972	1848	517	584	23			
1	D	406	Total	C	N	O	S	0	0	1
			2972	1848	517	584	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	HIS	ENGINEERED MUTATION	UNP P14926
B	298	GLU	HIS	ENGINEERED MUTATION	UNP P14926
C	298	GLU	HIS	ENGINEERED MUTATION	UNP P14926
D	298	GLU	HIS	ENGINEERED MUTATION	UNP P14926

- Molecule 2 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).

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 water.

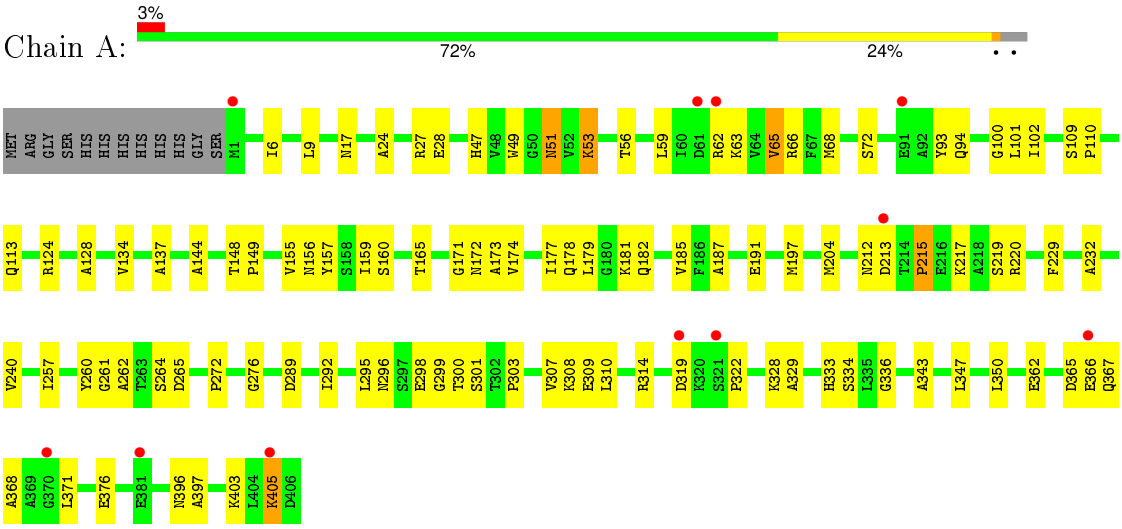
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	171	Total O 171 171	0	0
3	B	125	Total O 125 125	0	0
3	C	151	Total O 151 151	0	0
3	D	125	Total O 125 125	0	0

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.

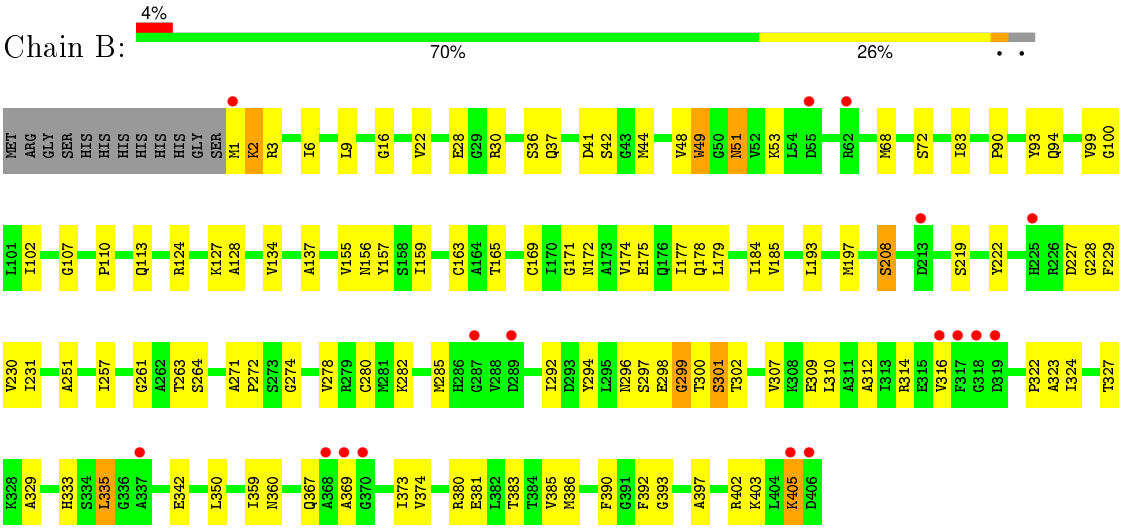
- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I

Chain A:



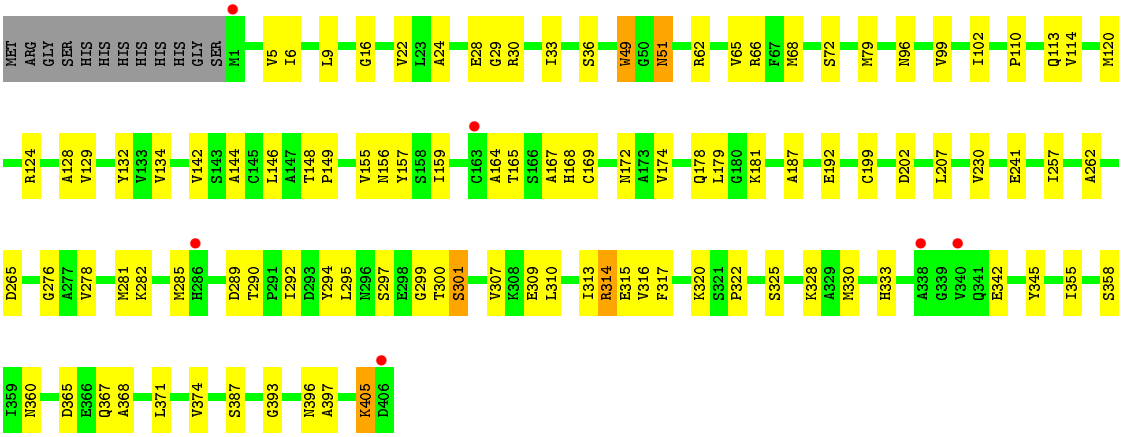
- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I

Chain B:



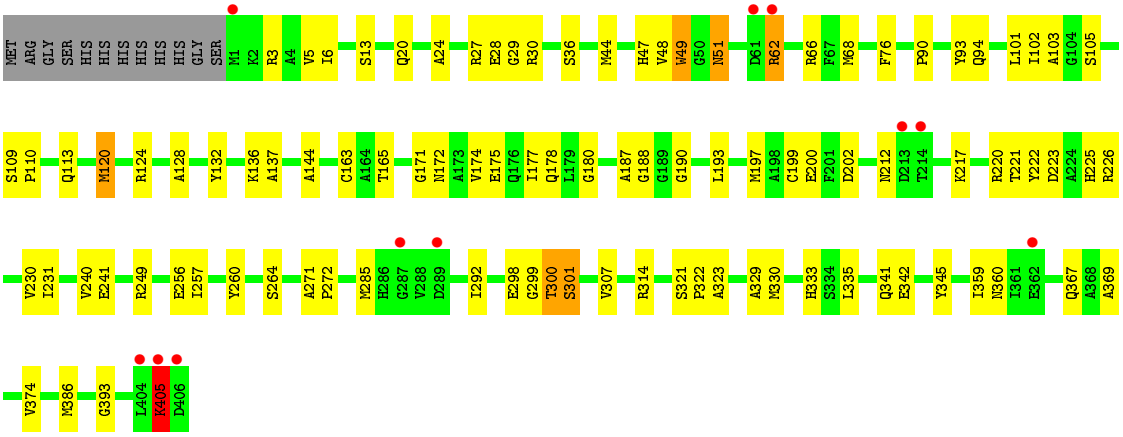
- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I

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	59.13Å 139.39Å 213.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.49 – 2.20 32.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.9 (32.49-2.20) 88.0 (32.49-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.88 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.272 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	15.2	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 49.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 79506 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12464	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 3.01% 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	0.60	0/3019	0.74	0/4078
1	B	0.55	0/3019	0.70	0/4078
1	C	0.57	0/3019	0.72	0/4078
1	D	0.56	0/3019	0.69	0/4078
All	All	0.57	0/12076	0.71	0/16312

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	2972	0	2934	76	0
1	B	2972	0	2934	80	0
1	C	2972	0	2934	85	0
1	D	2972	0	2934	84	0
2	A	1	0	0	1	0
2	B	1	0	0	1	0
2	C	1	0	0	1	0
2	D	1	0	0	0	0
3	A	171	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	125	0	0	2	0
3	C	151	0	0	6	0
3	D	125	0	0	4	0
All	All	12464	0	11736	305	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 13.

All (305) 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:405:LYS:H	1:A:405:LYS:HD2	1.09	1.17
1:D:307:VAL:HG13	1:D:367:GLN:HG3	1.37	1.07
1:C:172:ASN:HD21	1:D:172:ASN:HD21	1.16	0.91
1:A:6:ILE:HD11	1:A:257:ILE:HD11	1.62	0.82
1:B:51:ASN:H	1:B:51:ASN:HD22	1.24	0.82
1:A:405:LYS:N	1:A:405:LYS:HD2	1.93	0.80
1:A:24:ALA:O	1:A:28:GLU:HG2	1.81	0.80
1:A:51:ASN:HD22	1:A:51:ASN:H	1.30	0.79
1:C:51:ASN:H	1:C:51:ASN:HD22	1.29	0.78
1:D:3:ARG:HH22	1:D:405:LYS:HE3	1.49	0.77
1:C:124:ARG:HB2	1:C:128:ALA:HB2	1.65	0.77
1:C:6:ILE:HD11	1:C:257:ILE:HD11	1.67	0.74
1:D:124:ARG:HB2	1:D:128:ALA:HB2	1.69	0.73
1:A:405:LYS:H	1:A:405:LYS:CD	1.90	0.72
1:D:298:GLU:OE2	1:D:300:THR:HG23	1.89	0.72
1:A:124:ARG:HB2	1:A:128:ALA:HB2	1.72	0.72
1:B:307:VAL:HG13	1:B:367:GLN:HG3	1.72	0.71
1:D:51:ASN:HD22	1:D:51:ASN:N	1.88	0.71
1:A:229:PHE:HB3	1:A:300:THR:HG22	1.72	0.70
1:D:51:ASN:ND2	1:D:51:ASN:H	1.90	0.69
1:D:51:ASN:HD22	1:D:51:ASN:H	1.40	0.69
1:A:308:LYS:HE2	3:C:2140:HOH:O	1.90	0.69
1:C:314:ARG:HH11	1:C:314:ARG:HB2	1.56	0.69
1:B:324:ILE:HB	1:B:373:ILE:HD13	1.73	0.68
1:C:181:LYS:NZ	1:D:175:GLU:OE1	2.25	0.68
1:A:68:MET:HE2	1:A:72:SER:HB3	1.75	0.67
1:D:62:ARG:HG2	3:D:2017:HOH:O	1.94	0.66
1:B:134:VAL:HB	3:B:2060:HOH:O	1.94	0.66
1:C:172:ASN:HD21	1:D:172:ASN:ND2	1.90	0.66
1:D:177:ILE:HD12	1:D:240:VAL:HG12	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ASP:OD2	1:D:225:HIS:HB2	1.96	0.66
1:C:300:THR:O	1:C:301:SER:HB3	1.93	0.66
1:A:110:PRO:HG2	1:A:197:MET:HB2	1.77	0.65
1:B:292:ILE:O	1:B:322:PRO:HB3	1.97	0.65
1:A:51:ASN:N	1:A:51:ASN:HD22	1.95	0.65
1:B:42:SER:OG	1:B:44:MET:HG3	1.96	0.64
1:B:294:TYR:HB3	1:B:385:VAL:HG12	1.79	0.64
1:B:51:ASN:N	1:B:51:ASN:HD22	1.93	0.64
1:C:120:MET:HG3	1:D:199:CYS:SG	2.39	0.63
1:B:36:SER:HB2	1:B:49:TRP:CE2	2.33	0.63
1:A:300:THR:HG23	1:A:333:HIS:HD2	1.64	0.62
1:B:107:GLY:O	1:B:110:PRO:HD3	2.00	0.62
1:C:310:LEU:HD22	1:C:371:LEU:CD1	2.30	0.62
1:C:120:MET:HG2	1:C:129:VAL:HG21	1.80	0.61
1:C:310:LEU:HD22	1:C:371:LEU:HD13	1.82	0.61
1:B:51:ASN:ND2	1:B:51:ASN:H	1.98	0.61
1:C:393:GLY:HA3	1:D:144:ALA:HB1	1.83	0.61
1:B:229:PHE:HB3	1:B:300:THR:HG22	1.83	0.60
1:C:292:ILE:O	1:C:322:PRO:HB3	2.02	0.60
1:C:144:ALA:HB1	1:D:393:GLY:HA3	1.83	0.60
1:B:36:SER:HB2	1:B:49:TRP:NE1	2.17	0.60
1:C:172:ASN:ND2	1:D:172:ASN:HD21	1.94	0.59
1:C:328:LYS:NZ	1:C:342:GLU:OE2	2.33	0.59
1:B:68:MET:HB3	1:B:72:SER:HB2	1.85	0.59
1:A:134:VAL:HG11	1:B:392:PHE:HE2	1.68	0.59
1:C:297:SER:HB2	1:C:309:GLU:OE1	2.02	0.58
1:D:163:CYS:HG	1:D:333:HIS:HE2	1.51	0.58
1:B:300:THR:HG23	1:B:333:HIS:HD2	1.68	0.58
1:A:295:LEU:HD23	1:A:295:LEU:C	2.24	0.58
1:D:27:ARG:HD3	3:D:2005:HOH:O	2.02	0.58
1:C:278:VAL:O	1:C:282:LYS:HG3	2.03	0.58
1:B:285:MET:HG3	1:B:386:MET:HE1	1.85	0.57
1:B:285:MET:HG3	1:B:386:MET:CE	2.34	0.57
1:A:232:ALA:O	1:A:334:SER:HA	2.05	0.57
1:B:314:ARG:NH2	1:B:367:GLN:O	2.38	0.57
1:A:310:LEU:CD1	1:A:368:ALA:HB2	2.34	0.57
1:C:134:VAL:HB	3:C:2063:HOH:O	2.04	0.57
1:C:66:ARG:HD2	1:C:132:TYR:CZ	2.39	0.56
1:A:171:GLY:HA3	1:A:260:TYR:CZ	2.40	0.56
1:B:124:ARG:HB2	1:B:128:ALA:HB2	1.87	0.56
1:A:124:ARG:CB	1:A:128:ALA:HB2	2.34	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:ASN:ND2	1:D:51:ASN:N	2.51	0.56
1:C:355:ILE:HG21	1:C:374:VAL:HG21	1.87	0.56
1:C:68:MET:HB3	1:C:72:SER:HB2	1.87	0.56
1:A:159:ILE:O	1:A:165:THR:HG23	2.05	0.56
1:C:360:ASN:ND2	3:C:2137:HOH:O	2.39	0.56
1:C:309:GLU:O	1:C:313:ILE:HG13	2.06	0.56
1:D:24:ALA:O	1:D:28:GLU:HG2	2.06	0.56
1:C:281:MET:O	1:C:285:MET:HG3	2.06	0.55
1:A:303:PRO:O	1:A:307:VAL:HG23	2.07	0.55
1:A:9:LEU:HD12	1:A:9:LEU:C	2.27	0.55
1:B:300:THR:O	1:B:301:SER:HB3	2.07	0.55
1:A:134:VAL:HG11	1:B:392:PHE:CE2	2.41	0.55
1:D:285:MET:CG	1:D:386:MET:HE1	2.36	0.55
1:C:62:ARG:HA	1:C:65:VAL:HG12	1.88	0.55
1:D:28:GLU:HG3	1:D:30:ARG:HB2	1.87	0.55
1:C:192:GLU:HB3	3:C:2077:HOH:O	2.07	0.55
1:B:110:PRO:HG2	1:B:197:MET:HB2	1.89	0.54
1:A:27:ARG:NE	3:A:2017:HOH:O	2.40	0.54
1:D:342:GLU:HA	1:D:345:TYR:CD2	2.42	0.54
1:A:217:LYS:HE2	3:A:2153:HOH:O	2.06	0.54
1:B:383:THR:O	1:B:402:ARG:HG3	2.08	0.54
1:A:213:ASP:C	1:A:215:PRO:HD3	2.27	0.54
1:C:120:MET:HG2	1:C:129:VAL:CG2	2.38	0.54
1:C:310:LEU:CD1	1:C:368:ALA:HB2	2.37	0.54
1:A:51:ASN:ND2	1:A:51:ASN:H	2.01	0.54
1:A:171:GLY:HA3	1:A:260:TYR:CE1	2.43	0.54
1:C:159:ILE:O	1:C:165:THR:HG23	2.07	0.54
1:D:3:ARG:HH22	1:D:405:LYS:CE	2.19	0.53
1:B:37:GLN:HG3	1:B:41:ASP:OD2	2.08	0.53
1:C:310:LEU:HD13	1:C:368:ALA:HB2	1.89	0.53
1:D:226:ARG:NH2	1:D:307:VAL:HG23	2.24	0.53
1:B:296:ASN:OD1	2:B:1406:NH4:N	2.40	0.53
1:B:3:ARG:HH22	1:B:405:LYS:HZ2	1.56	0.53
1:D:66:ARG:HD2	1:D:132:TYR:CZ	2.44	0.53
1:D:93:TYR:CE1	1:D:94:GLN:HG2	2.44	0.53
1:C:278:VAL:HG13	1:C:316:VAL:HG22	1.90	0.53
1:A:155:VAL:CG2	1:A:157:TYR:CE1	2.92	0.52
1:B:171:GLY:O	1:B:175:GLU:HG3	2.09	0.52
1:C:295:LEU:HD23	1:C:295:LEU:C	2.29	0.52
1:C:36:SER:HB2	1:C:49:TRP:CE2	2.44	0.52
1:D:36:SER:HB2	1:D:49:TRP:CE2	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:CYS:HG	1:D:333:HIS:CE1	2.27	0.52
1:B:228:GLY:HA2	1:B:302:THR:HG22	1.92	0.52
1:D:333:HIS:CE1	1:D:335:LEU:HA	2.45	0.51
1:A:109:SER:HB3	1:A:137:ALA:HA	1.93	0.51
1:A:177:ILE:HD12	1:A:240:VAL:HG12	1.92	0.51
1:A:367:GLN:HE22	1:C:367:GLN:HE22	1.59	0.51
1:D:47:HIS:H	1:D:212:ASN:ND2	2.09	0.51
1:B:208:SER:HB2	1:B:227:ASP:OD1	2.11	0.51
1:A:179:LEU:HD21	1:B:179:LEU:HG	1.92	0.51
1:D:5:VAL:HG12	1:D:256:GLU:HB2	1.93	0.51
1:C:265:ASP:OD1	1:C:276:GLY:HA3	2.10	0.51
1:B:49:TRP:CE3	1:B:193:LEU:HG	2.45	0.51
1:A:217:LYS:HE3	3:A:2104:HOH:O	2.09	0.51
1:D:330:MET:HB3	1:D:359:ILE:HD11	1.93	0.51
1:B:278:VAL:O	1:B:282:LYS:HG3	2.11	0.51
1:C:110:PRO:O	1:C:114:VAL:HG23	2.11	0.51
1:C:142:VAL:O	1:C:146:LEU:HD13	2.11	0.51
1:C:307:VAL:HG22	1:C:367:GLN:HG3	1.92	0.50
1:D:292:ILE:O	1:D:322:PRO:HB3	2.10	0.50
1:B:359:ILE:O	1:B:360:ASN:HB2	2.10	0.50
1:A:292:ILE:O	1:A:322:PRO:HB3	2.10	0.50
1:C:102:ILE:O	1:C:187:ALA:HA	2.12	0.50
1:C:68:MET:HE2	1:C:72:SER:HB3	1.93	0.50
1:A:376:GLU:HG3	1:A:376:GLU:O	2.10	0.50
1:A:101:LEU:C	1:A:101:LEU:HD23	2.31	0.50
1:C:113:GLN:NE2	1:D:200:GLU:OE2	2.44	0.50
1:C:192:GLU:HG2	3:C:2076:HOH:O	2.12	0.50
1:D:29:GLY:HA2	1:D:330:MET:SD	2.51	0.49
1:B:307:VAL:HG22	1:B:367:GLN:HG3	1.93	0.49
1:C:156:ASN:HB2	1:D:264:SER:HB2	1.93	0.49
1:D:231:ILE:HD11	1:D:335:LEU:HD11	1.94	0.49
1:C:79:MET:SD	1:C:146:LEU:HD23	2.52	0.49
1:D:174:VAL:CG2	1:D:257:ILE:HD13	2.42	0.49
1:A:100:GLY:HA3	1:A:155:VAL:HG12	1.93	0.49
1:B:297:SER:HB2	1:B:309:GLU:CD	2.33	0.49
1:A:329:ALA:HB3	3:A:2150:HOH:O	2.12	0.49
1:A:310:LEU:HD22	1:A:371:LEU:HD13	1.95	0.49
1:A:63:LYS:O	1:A:66:ARG:HG2	2.13	0.49
1:D:323:ALA:HB1	1:D:374:VAL:HG21	1.94	0.49
1:D:44:MET:HB3	1:D:202:ASP:OD2	2.12	0.49
1:C:314:ARG:HH11	1:C:314:ARG:CB	2.22	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:THR:HG23	1:A:333:HIS:CD2	2.47	0.48
1:B:155:VAL:CG2	1:B:157:TYR:CE1	2.96	0.48
1:C:148:THR:HB	1:C:149:PRO:CD	2.43	0.48
1:B:48:VAL:HG23	1:B:230:VAL:HG13	1.95	0.48
1:B:159:ILE:HD11	1:B:172:ASN:ND2	2.28	0.48
1:D:180:GLY:HA2	3:D:2057:HOH:O	2.12	0.48
1:C:124:ARG:CB	1:C:128:ALA:HB2	2.41	0.48
1:D:300:THR:HG22	1:D:333:HIS:CD2	2.49	0.48
1:B:49:TRP:HD1	1:B:49:TRP:O	1.95	0.48
1:D:241:GLU:OE1	1:D:249:ARG:NE	2.46	0.48
1:A:173:ALA:HB1	1:A:185:VAL:HB	1.95	0.48
1:A:156:ASN:HB2	1:B:264:SER:HB2	1.95	0.47
1:A:296:ASN:OD1	2:A:1406:NH4:N	2.47	0.47
1:D:103:ALA:HA	1:D:188:GLY:O	2.14	0.47
1:C:28:GLU:HG3	1:C:30:ARG:HB2	1.96	0.47
1:D:300:THR:HG22	1:D:333:HIS:HD2	1.79	0.47
1:D:101:LEU:HD23	1:D:101:LEU:C	2.35	0.47
1:B:261:GLY:O	1:B:397:ALA:HA	2.13	0.47
1:A:298:GLU:HB3	1:A:309:GLU:OE1	2.14	0.47
1:A:113:GLN:HG3	1:A:137:ALA:HB1	1.97	0.47
1:B:100:GLY:HA3	1:B:155:VAL:HG12	1.97	0.47
1:D:13:SER:HB3	1:D:341:GLN:NE2	2.30	0.47
1:A:174:VAL:O	1:A:178:GLN:HG3	2.15	0.47
1:C:278:VAL:HG13	1:C:316:VAL:CG2	2.45	0.47
1:C:365:ASP:OD2	1:C:367:GLN:HG2	2.15	0.47
1:C:51:ASN:H	1:C:51:ASN:ND2	2.06	0.46
1:A:181:LYS:C	1:A:182:GLN:HG2	2.34	0.46
1:D:68:MET:HE1	1:D:76:PHE:HB2	1.96	0.46
1:A:365:ASP:OD2	1:A:366:GLU:N	2.49	0.46
1:A:265:ASP:OD1	1:A:276:GLY:HA3	2.15	0.46
1:D:6:ILE:HD11	1:D:257:ILE:HD11	1.96	0.46
1:A:262:ALA:HA	1:A:396:ASN:O	2.15	0.46
1:C:300:THR:O	1:C:301:SER:CB	2.60	0.46
1:C:307:VAL:HG13	1:C:367:GLN:HG3	1.97	0.46
1:B:312:ALA:O	1:B:316:VAL:HG23	2.15	0.46
1:A:264:SER:HB2	1:B:156:ASN:HB2	1.97	0.46
1:D:217:LYS:HB3	1:D:217:LYS:HE3	1.74	0.46
1:D:314:ARG:NH1	1:D:367:GLN:O	2.49	0.46
1:B:219:SER:OG	1:B:329:ALA:HA	2.17	0.45
1:C:317:PHE:HB3	1:C:320:LYS:O	2.16	0.45
1:B:251:ALA:HB1	3:B:2041:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:ALA:O	1:C:167:ALA:HB3	2.16	0.45
1:D:174:VAL:O	1:D:178:GLN:HG3	2.16	0.45
1:B:174:VAL:O	1:B:178:GLN:HG3	2.16	0.45
1:B:99:VAL:HG22	1:B:184:ILE:HB	1.98	0.45
1:C:199:CYS:SG	1:D:120:MET:HG2	2.57	0.45
1:D:285:MET:HG3	1:D:386:MET:HE1	1.98	0.45
1:B:163:CYS:HB2	1:B:390:PHE:O	2.16	0.45
1:D:49:TRP:CE3	1:D:193:LEU:HG	2.50	0.45
1:B:99:VAL:HA	1:B:184:ILE:O	2.17	0.45
1:D:300:THR:O	1:D:301:SER:HB3	2.17	0.44
1:D:109:SER:HB3	1:D:137:ALA:HA	1.98	0.44
1:A:6:ILE:CD1	1:A:257:ILE:HD11	2.40	0.44
1:B:307:VAL:CG1	1:B:367:GLN:HG3	2.44	0.44
1:B:263:THR:OG1	1:B:280:CYS:HB2	2.16	0.44
1:A:160:SER:HB3	3:A:2065:HOH:O	2.17	0.44
1:A:51:ASN:ND2	1:A:53:LYS:HE3	2.33	0.44
1:C:16:GLY:HA3	1:C:22:VAL:HG23	1.99	0.44
1:B:124:ARG:NH2	1:B:127:LYS:HD2	2.32	0.44
1:B:274:GLY:O	1:B:278:VAL:HG23	2.18	0.44
1:C:294:TYR:HE1	1:C:325:SER:HB3	1.82	0.44
1:B:49:TRP:O	1:B:49:TRP:CD1	2.71	0.44
1:A:298:GLU:O	1:A:328:LYS:HD2	2.18	0.44
1:D:113:GLN:HG3	1:D:137:ALA:HB1	1.98	0.44
1:A:102:ILE:O	1:A:187:ALA:HA	2.18	0.44
1:B:222:TYR:CE1	1:B:310:LEU:HD21	2.53	0.44
1:D:405:LYS:N	1:D:405:LYS:HD2	2.33	0.44
1:B:231:ILE:HD11	1:B:335:LEU:HD11	1.99	0.44
1:B:300:THR:HG23	1:B:333:HIS:CD2	2.51	0.44
1:D:48:VAL:HG23	1:D:230:VAL:HG13	2.00	0.44
1:B:90:PRO:HA	1:B:94:GLN:HG3	2.00	0.44
1:C:294:TYR:CE1	1:C:325:SER:HB3	2.52	0.43
1:A:62:ARG:HA	1:A:65:VAL:HG12	2.00	0.43
1:D:330:MET:HB3	1:D:359:ILE:CD1	2.47	0.43
1:C:168:HIS:CE1	1:C:397:ALA:HB2	2.53	0.43
1:A:56:THR:O	1:A:59:LEU:HG	2.18	0.43
1:C:300:THR:HG23	1:C:333:HIS:CD2	2.54	0.43
1:D:314:ARG:NH1	1:D:314:ARG:HB2	2.33	0.43
1:B:51:ASN:ND2	1:B:51:ASN:N	2.62	0.43
1:C:155:VAL:CG2	1:C:157:TYR:CE1	3.01	0.43
1:D:329:ALA:HB3	3:D:2110:HOH:O	2.17	0.43
1:D:110:PRO:HG2	1:D:197:MET:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:GLN:HE22	1:C:367:GLN:NE2	2.16	0.43
1:A:261:GLY:O	1:A:397:ALA:HA	2.19	0.43
1:A:17:ASN:HB3	3:A:2005:HOH:O	2.18	0.43
1:C:342:GLU:HA	1:C:345:TYR:CD2	2.54	0.43
1:B:298:GLU:O	1:B:299:GLY:C	2.57	0.43
1:B:350:LEU:HD11	1:B:403:LYS:HG3	2.01	0.43
1:A:93:TYR:CE1	1:A:94:GLN:HG3	2.54	0.43
1:C:202:ASP:HB2	1:C:207:LEU:HD12	2.00	0.43
1:A:174:VAL:HG21	1:A:257:ILE:HG21	2.00	0.42
1:A:272:PRO:HG3	3:A:2120:HOH:O	2.19	0.42
1:C:387:SER:OG	2:C:1406:NH4:N	2.51	0.42
1:B:51:ASN:HD21	1:B:53:LYS:HE3	1.84	0.42
1:D:66:ARG:HD2	1:D:132:TYR:OH	2.20	0.42
1:C:33:ILE:HD12	1:C:230:VAL:HG11	2.01	0.42
1:C:289:ASP:OD1	1:C:290:THR:HG23	2.18	0.42
1:B:300:THR:O	1:B:301:SER:CB	2.67	0.42
1:B:28:GLU:OE2	1:B:30:ARG:HD2	2.19	0.42
1:A:51:ASN:ND2	1:A:51:ASN:N	2.65	0.42
1:C:144:ALA:CB	1:D:393:GLY:HA3	2.48	0.42
1:B:271:ALA:HA	1:B:272:PRO:HD3	1.90	0.42
1:D:405:LYS:H	1:D:405:LYS:HD2	1.85	0.42
1:D:174:VAL:HG21	1:D:257:ILE:HG21	2.01	0.42
1:D:241:GLU:CD	1:D:249:ARG:HE	2.23	0.42
1:C:30:ARG:O	1:C:330:MET:HB2	2.19	0.42
1:B:102:ILE:O	1:B:169:CYS:HB3	2.19	0.42
1:C:96:ASN:HB3	1:C:99:VAL:CG2	2.50	0.42
1:C:28:GLU:O	1:C:29:GLY:C	2.59	0.42
1:D:171:GLY:HA3	1:D:260:TYR:CZ	2.55	0.42
1:B:323:ALA:HB1	1:B:374:VAL:CG2	2.50	0.42
1:B:51:ASN:ND2	1:B:53:LYS:HE3	2.35	0.42
1:B:159:ILE:O	1:B:165:THR:HG23	2.20	0.42
1:D:47:HIS:H	1:D:212:ASN:HD21	1.67	0.41
1:A:219:SER:OG	1:A:329:ALA:HA	2.20	0.41
1:A:148:THR:HB	1:A:149:PRO:CD	2.50	0.41
1:A:343:ALA:O	1:A:347:LEU:HG	2.20	0.41
1:D:314:ARG:HB2	1:D:314:ARG:HH11	1.84	0.41
1:A:144:ALA:HB1	1:B:393:GLY:HA3	2.02	0.41
1:B:184:ILE:HG22	1:B:185:VAL:N	2.35	0.41
1:D:217:LYS:O	1:D:220:ARG:HD2	2.19	0.41
1:D:220:ARG:HB3	1:D:360:ASN:HB3	2.02	0.41
1:C:314:ARG:HH11	1:C:314:ARG:CG	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:ARG:HD2	3:C:2039:HOH:O	2.20	0.41
1:C:9:LEU:HD12	1:C:9:LEU:C	2.40	0.41
1:C:262:ALA:HA	1:C:396:ASN:O	2.20	0.41
1:B:83:ILE:HD13	1:B:93:TYR:CZ	2.55	0.41
1:C:24:ALA:O	1:C:28:GLU:HG2	2.20	0.41
1:A:191:GLU:OE1	1:A:336:GLY:N	2.46	0.41
1:D:105:SER:HB3	1:D:190:GLY:O	2.21	0.41
1:D:221:THR:HG22	1:D:222:TYR:CG	2.56	0.41
1:A:47:HIS:H	1:A:212:ASN:ND2	2.18	0.41
1:C:5:VAL:HG22	1:C:241:GLU:O	2.20	0.41
1:D:285:MET:SD	1:D:386:MET:HE1	2.61	0.41
1:D:90:PRO:O	1:D:94:GLN:HG3	2.20	0.41
1:B:16:GLY:HA3	1:B:22:VAL:HG23	2.03	0.41
1:C:174:VAL:O	1:C:178:GLN:HG3	2.20	0.41
1:A:220:ARG:HH22	1:A:362:GLU:CD	2.23	0.41
1:B:296:ASN:OD1	1:B:342:GLU:HG2	2.21	0.40
1:B:6:ILE:HD11	1:B:257:ILE:HD11	2.02	0.40
1:B:1:MET:O	1:B:2:LYS:HB2	2.22	0.40
1:C:393:GLY:HA3	1:D:144:ALA:CB	2.51	0.40
1:C:179:LEU:HD23	1:C:179:LEU:HA	1.87	0.40
1:C:285:MET:HE1	1:C:317:PHE:HE2	1.86	0.40
1:D:132:TYR:O	1:D:136:LYS:HG3	2.21	0.40
1:B:380:ARG:HG3	1:B:381:GLU:N	2.36	0.40
1:D:271:ALA:HA	1:D:272:PRO:HD3	1.93	0.40
1:D:102:ILE:O	1:D:187:ALA:HA	2.20	0.40
1:A:350:LEU:HD11	1:A:403:LYS:HG3	2.04	0.40
1:A:307:VAL:HG13	1:A:367:GLN:HG3	2.04	0.40
1:C:159:ILE:HB	1:C:169:CYS:SG	2.61	0.40
1:B:113:GLN:HG2	1:B:137:ALA:HB1	2.04	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%)	382 (95%)	20 (5%)	2 (0%)	34 35
1	B	404/418 (97%)	377 (93%)	21 (5%)	6 (2%)	13 9
1	C	404/418 (97%)	378 (94%)	23 (6%)	3 (1%)	26 25
1	D	404/418 (97%)	371 (92%)	28 (7%)	5 (1%)	16 12
All	All	1616/1672 (97%)	1508 (93%)	92 (6%)	16 (1%)	19 16

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	369	ALA
1	C	405	LYS
1	D	405	LYS
1	D	369	ALA
1	C	299	GLY
1	A	301	SER
1	B	299	GLY
1	B	405	LYS
1	D	301	SER
1	B	2	LYS
1	C	301	SER
1	D	165	THR
1	D	299	GLY
1	B	301	SER
1	B	335	LEU
1	A	299	GLY

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%)	297 (96%)	11 (4%)	42 52
1	B	308/319 (97%)	302 (98%)	6 (2%)	65 77
1	C	308/319 (97%)	302 (98%)	6 (2%)	65 77
1	D	308/319 (97%)	300 (97%)	8 (3%)	54 66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1232/1276 (97%)	1201 (98%)	31 (2%)	55 67

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	TRP
1	A	51	ASN
1	A	53	LYS
1	A	65	VAL
1	A	172	ASN
1	A	204	MET
1	A	215	PRO
1	A	289	ASP
1	A	314	ARG
1	A	319	ASP
1	A	405	LYS
1	B	9	LEU
1	B	49	TRP
1	B	51	ASN
1	B	177	ILE
1	B	208	SER
1	B	327	THR
1	C	49	TRP
1	C	51	ASN
1	C	314	ARG
1	C	315	GLU
1	C	358	SER
1	C	405	LYS
1	D	20	GLN
1	D	49	TRP
1	D	51	ASN
1	D	62	ARG
1	D	120	MET
1	D	300	THR
1	D	321	SER
1	D	405	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	212	ASN
1	A	360	ASN
1	A	367	GLN
1	B	51	ASN
1	B	113	GLN
1	B	212	ASN
1	B	225	HIS
1	B	252	HIS
1	B	360	ASN
1	C	51	ASN
1	C	172	ASN
1	C	212	ASN
1	C	360	ASN
1	C	367	GLN
1	D	20	GLN
1	D	51	ASN
1	D	212	ASN
1	D	360	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 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	406/418 (97%)	-0.09	11 (2%) 58 57	3, 13, 27, 45	0
1	B	406/418 (97%)	0.28	17 (4%) 40 39	4, 18, 38, 53	0
1	C	406/418 (97%)	0.06	6 (1%) 76 75	4, 15, 32, 45	0
1	D	406/418 (97%)	0.21	11 (2%) 58 57	11, 20, 27, 37	0
All	All	1624/1672 (97%)	0.11	45 (2%) 56 55	3, 17, 32, 53	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	406	ASP	8.8
1	C	406	ASP	7.4
1	D	406	ASP	6.1
1	B	369	ALA	5.7
1	B	1	MET	4.4
1	B	318	GLY	4.3
1	B	370	GLY	4.2
1	B	319	ASP	4.0
1	C	1	MET	4.0
1	A	62	ARG	3.7
1	A	319	ASP	3.7
1	D	404	LEU	3.5
1	D	61	ASP	3.5
1	A	370	GLY	3.5
1	C	286	HIS	3.0
1	B	62	ARG	3.0
1	D	289	ASP	2.9
1	A	1	MET	2.9
1	D	1	MET	2.9
1	A	213	ASP	2.9
1	B	213	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	405	LYS	2.8
1	D	214	THR	2.7
1	B	405	LYS	2.5
1	B	289	ASP	2.5
1	A	91	GLU	2.5
1	D	287	GLY	2.4
1	B	337	ALA	2.4
1	B	368	ALA	2.3
1	A	321	SER	2.3
1	D	62	ARG	2.3
1	B	317	PHE	2.2
1	B	287	GLY	2.2
1	C	340	VAL	2.2
1	D	213	ASP	2.2
1	A	366	GLU	2.2
1	B	225	HIS	2.2
1	C	338	ALA	2.2
1	C	163	CYS	2.1
1	A	405	LYS	2.1
1	B	55	ASP	2.1
1	A	381	GLU	2.0
1	B	316	VAL	2.1
1	A	61	ASP	2.0
1	D	362	GLU	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	1406	1/1	0.98	0.38	10.34	14,14,14,14	0
2	NH4	A	1406	1/1	0.99	0.30	8.05	4,4,4,4	0
2	NH4	D	1406	1/1	0.98	0.29	7.90	4,4,4,4	0
2	NH4	B	1406	1/1	0.96	0.24	2.39	4,4,4,4	0

6.5 Other polymers (i)

There are no such residues in this entry.