Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:33 AM GMT

PDB ID	:	3ITA
Title	:	Crystal structure of Penicillin-Binding Protein 6 (PBP6) from E. coli in acyl-enzyme complex with ampicillin
Authors	:	Chen, Y.; Zhang, W.; Shi, Q.; Hesek, D.; Lee, M.; Mobashery, S.; Shoichet, B.K.
Deposited on	:	2009-08-27
Resolution	:	1.80 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:

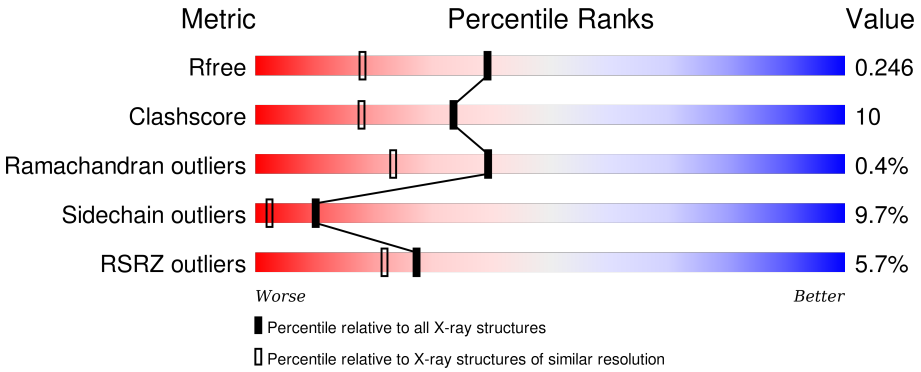
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	352	4% 81% 16%
1	B	352	2% 86% 11%
1	C	352	8% 64% 24% 6% 6%
1	D	352	8% 71% 19% 5%

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
3	SO4	C	355	-	-	X	X
4	AIC	D	501	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11223 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.

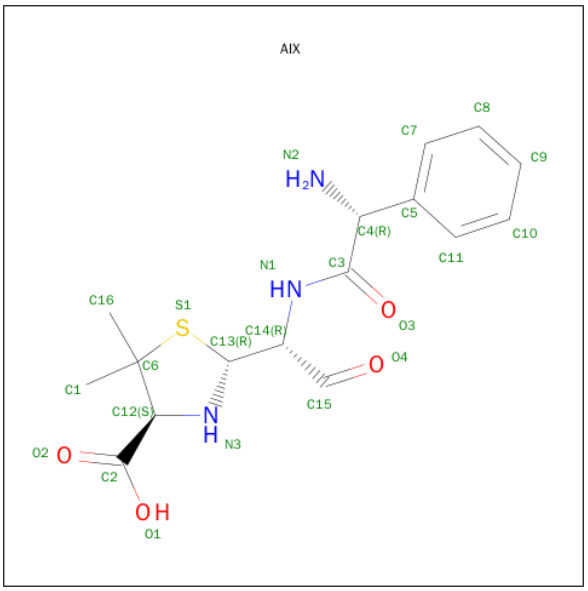
- Molecule 1 is a protein called D-alanyl-D-alanine carboxypeptidase dacC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2644	1670	454	510	10			
1	B	347	Total	C	N	O	S	0	0	0
			2637	1666	453	508	10			
1	C	330	Total	C	N	O	S	0	1	0
			2532	1604	431	487	10			
1	D	333	Total	C	N	O	S	0	3	0
			2558	1610	441	498	9			

There are 4 discrepancies between the modelled and reference sequences:

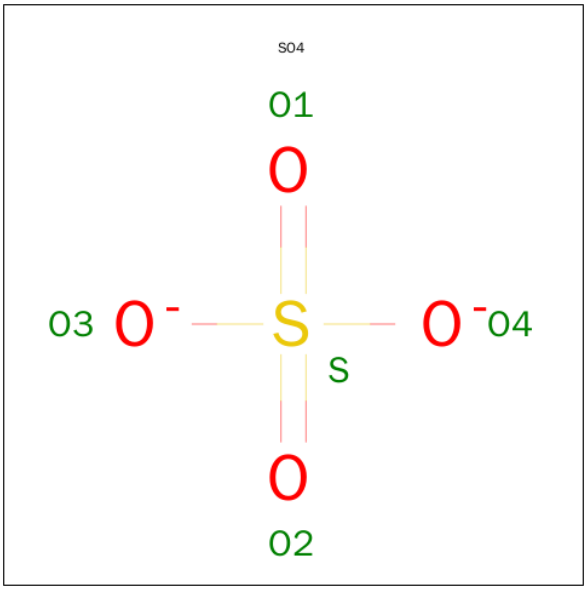
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP P08506
B	1	MET	-	INITIATING METHIONINE	UNP P08506
C	1	MET	-	INITIATING METHIONINE	UNP P08506
D	1	MET	-	INITIATING METHIONINE	UNP P08506

- Molecule 2 is (2R,4S)-2-[(1R)-1-{[(2R)-2-AMINO-2-PHENYLACETYL]AMINO}-2-OXOETHYL]-5,5-DIMETHYL-1,3-THIAZOLIDINE-4-CARBOXYLIC ACID (three-letter code: AIX) (formula: $C_{16}H_{21}N_3O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			24	16	3	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	O	S		0	0
			5	4	1			
3	B	1	Total	O	S		0	0
			5	4	1			
3	B	1	Total	O	S		0	0
			5	4	1			

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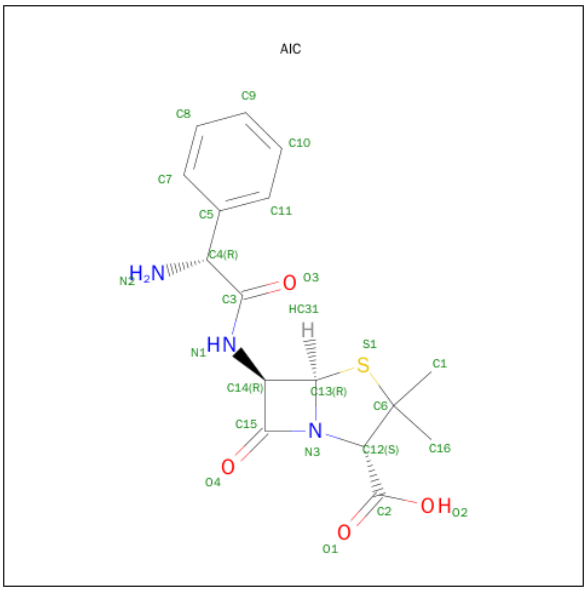
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is (2S,5R,6R)-6-{[(2R)-2-AMINO-2-PHENYLETHANOYL]AMINO}-3,3-DIMETHYL-7-OXO-4-THIA-1-AZABICYCLO[3.2.0]HEPTANE-2-CARBOXYLIC ACID (three-letter code: AIC) (formula: $C_{16}H_{19}N_3O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C N O S 24 16 3 4 1	0	0

- Molecule 5 is water.

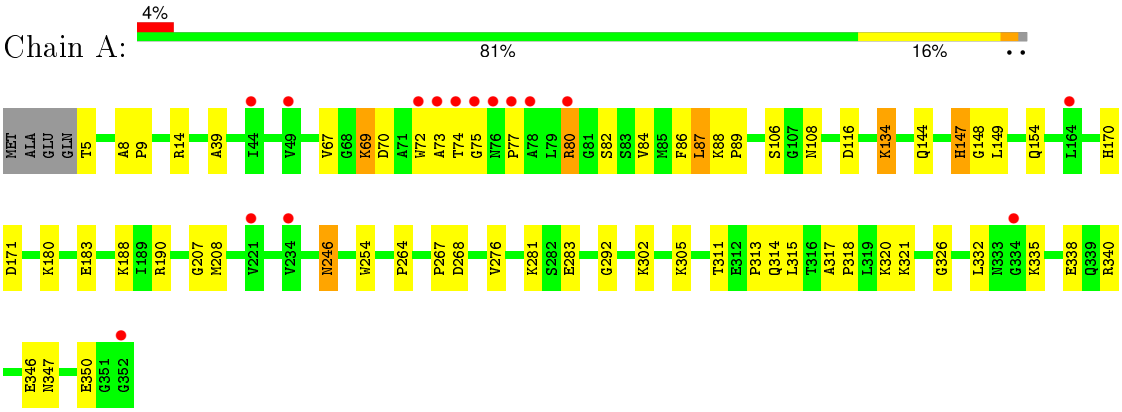
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	286	Total O 286 286	0	0
5	B	234	Total O 234 234	0	0
5	C	99	Total O 99 99	0	0
5	D	155	Total O 155 155	0	0

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.

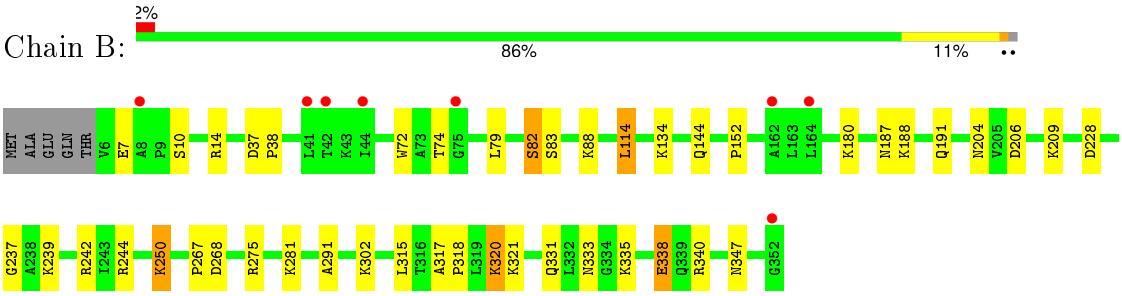
- Molecule 1: D-alanyl-D-alanine carboxypeptidase dacC

Chain A:



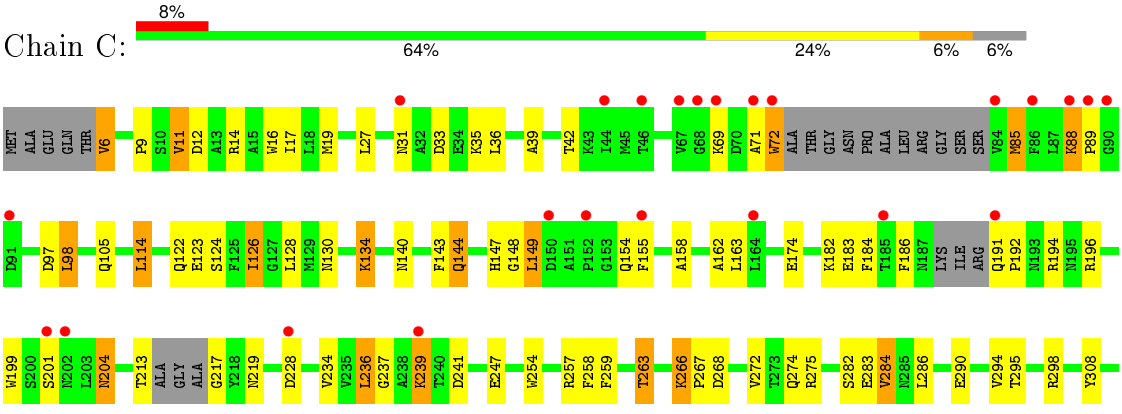
- Molecule 1: D-alanyl-D-alanine carboxypeptidase dacC

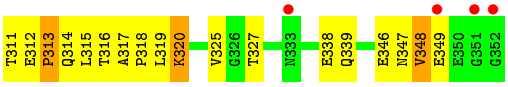
Chain B:



- Molecule 1: D-alanyl-D-alanine carboxypeptidase dacC

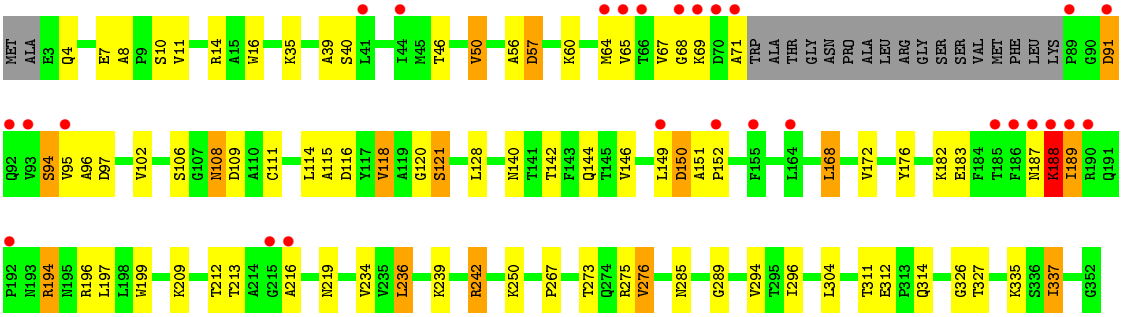
Chain C:





• Molecule 1: D-alanyl-D-alanine carboxypeptidase dacC

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.94Å 185.98Å 83.04Å 90.00° 101.37° 90.00°	Depositor
Resolution (Å)	35.81 – 1.80 34.35 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.8 (35.81-1.80) 94.8 (34.35-1.80)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.203 , 0.250 0.201 , 0.246	Depositor DCC
R_{free} test set	7301 reflections (5.18%)	DCC
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 148303 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11223	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: AIX, AIC, 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	0.59	0/2689	0.67	0/3639
1	B	0.56	0/2682	0.65	1/3629 (0.0%)
1	C	0.42	0/2576	0.57	0/3481
1	D	0.46	0/2601	0.58	0/3516
All	All	0.51	0/10548	0.62	1/14265 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	114	LEU	CB-CG-CD1	5.54	120.41	111.00

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	2644	0	2668	42	0
1	B	2637	0	2662	20	0
1	C	2532	0	2552	82	0
1	D	2558	0	2575	67	0
2	A	24	0	19	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	0	0
3	C	15	0	0	2	0
4	D	24	0	18	3	0
5	A	286	0	0	5	0
5	B	234	0	0	2	0
5	C	99	0	0	0	0
5	D	155	0	0	3	0
All	All	11223	0	10494	214	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 10.

All (214) 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:183:GLU:OE2	1:A:190:ARG:HD2	1.48	1.13
1:C:88:LYS:HG2	1:C:89:PRO:HD2	1.16	1.09
1:C:267:PRO:O	1:C:268:ASP:HB2	1.54	1.07
1:C:327:THR:HG21	1:C:339:GLN:HE21	1.24	1.02
1:A:338:GLU:HG3	1:A:340:ARG:NH2	1.75	1.01
1:C:130:ASN:HD21	1:C:143:PHE:H	1.07	0.99
4:D:501:AIC:O2	4:D:501:AIC:HC2	1.65	0.96
1:D:39:ALA:CB	1:D:213:THR:HG22	1.97	0.93
1:D:108:ASN:HD22	1:D:108:ASN:N	1.62	0.93
1:B:267:PRO:O	1:B:268:ASP:HB2	1.66	0.92
1:A:338:GLU:HG3	1:A:340:ARG:HH22	1.32	0.92
1:C:88:LYS:HG2	1:C:89:PRO:CD	1.99	0.91
1:C:213:THR:HG23	1:C:219:ASN:HD21	1.36	0.91
1:B:338:GLU:HG2	1:B:340:ARG:NH2	1.87	0.89
1:D:8:ALA:HB2	5:D:733:HOH:O	1.71	0.88
1:D:213:THR:HG23	1:D:219:ASN:HD21	1.39	0.87
1:D:94:SER:HB3	1:D:97:ASP:H	1.42	0.85
1:D:39:ALA:HB2	1:D:213:THR:HG22	1.57	0.84
1:C:126:ILE:HD12	1:C:126:ILE:C	1.98	0.83
1:D:144:GLN:HE21	1:D:144:GLN:HA	1.43	0.83
1:A:14:ARG:HD3	5:A:457:HOH:O	1.79	0.83
1:D:94:SER:HB3	1:D:97:ASP:HB2	1.62	0.82
1:D:94:SER:CB	1:D:97:ASP:HB2	2.09	0.82
1:D:91:ASP:OD1	1:D:91:ASP:N	2.13	0.82
1:A:144:GLN:H	1:A:154:GLN:HE21	1.26	0.82
1:D:242[B]:ARG:HG3	1:D:242[B]:ARG:HH11	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:GLN:NE2	1:D:144:GLN:HA	1.95	0.80
1:C:217:GLY:HA3	1:C:237:GLY:HA2	1.63	0.80
1:C:122:GLN:O	1:C:126:ILE:HG23	1.83	0.79
1:C:85:MET:O	1:C:85:MET:HG2	1.82	0.78
1:B:79:LEU:O	1:B:82:SER:HB2	1.85	0.77
1:A:84:VAL:HG13	1:A:86:PHE:H	1.49	0.77
1:C:294:VAL:HG13	1:C:338:GLU:CD	2.07	0.75
1:D:39:ALA:HB3	1:D:213:THR:HG22	1.67	0.75
1:C:315:LEU:HD11	1:C:325:VAL:HG11	1.68	0.74
4:D:501:AIC:O2	4:D:501:AIC:C1	2.36	0.74
1:D:108:ASN:ND2	1:D:108:ASN:N	2.36	0.73
1:A:311:THR:HG23	1:A:326:GLY:HA2	1.71	0.73
3:C:355:SO4:O2	1:D:242[A]:ARG:HD3	1.89	0.72
1:C:213:THR:CG2	1:C:219:ASN:HD21	2.03	0.71
1:D:213:THR:HG23	1:D:219:ASN:ND2	2.04	0.71
1:D:213:THR:CG2	1:D:219:ASN:HD21	2.03	0.71
1:C:126:ILE:HD12	1:C:126:ILE:O	1.90	0.71
1:B:180:LYS:HG3	1:B:206:ASP:HB2	1.73	0.70
1:A:170:HIS:HD2	1:A:171:ASP:OD1	1.75	0.69
1:C:6:VAL:HG11	1:C:258:PHE:HB3	1.73	0.69
1:C:325:VAL:O	1:C:325:VAL:HG12	1.91	0.69
1:A:82:SER:HB2	1:A:108:ASN:ND2	2.06	0.69
1:D:8:ALA:CB	5:D:733:HOH:O	2.37	0.69
1:A:134:LYS:HE3	1:A:134:LYS:CA	2.21	0.68
1:A:338:GLU:CG	1:A:340:ARG:HH22	2.04	0.67
1:C:85:MET:HB2	1:C:105:GLN:OE1	1.95	0.67
1:D:294:VAL:HG12	1:D:296:ILE:HG23	1.78	0.66
1:D:4:GLN:HB2	1:D:335:LYS:NZ	2.11	0.65
1:C:71:ALA:O	1:C:72:TRP:HB3	1.97	0.65
1:C:184:PHE:O	1:C:191:GLN:HB2	1.96	0.65
1:C:199:TRP:NE1	3:C:355:SO4:O2	2.29	0.65
1:C:257:ARG:HG2	1:C:258:PHE:CE2	2.32	0.65
1:C:213:THR:HG23	1:C:219:ASN:ND2	2.09	0.64
1:C:327:THR:CG2	1:C:339:GLN:HE21	2.07	0.64
1:D:168:LEU:HD23	1:D:172:VAL:CG2	2.28	0.64
1:A:338:GLU:CG	1:A:340:ARG:NH2	2.56	0.64
1:A:8:ALA:HB2	5:A:479:HOH:O	1.98	0.63
1:B:320:LYS:HA	1:B:347:ASN:HD22	1.63	0.63
1:D:242[B]:ARG:HG3	1:D:242[B]:ARG:NH1	2.11	0.63
4:D:501:AIC:H162	5:D:680:HOH:O	1.99	0.62
1:C:183:GLU:HA	1:C:191:GLN:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:GLN:HG3	1:D:152:PRO:O	2.00	0.61
1:A:82:SER:CB	1:A:108:ASN:HD22	2.13	0.61
1:A:267:PRO:O	1:A:268:ASP:HB2	2.01	0.61
1:C:98:LEU:HB3	1:C:114:LEU:HD22	1.83	0.61
1:D:108:ASN:H	1:D:108:ASN:HD22	1.46	0.60
1:C:325:VAL:O	1:C:325:VAL:CG1	2.50	0.60
1:C:39:ALA:HA	1:C:148:GLY:O	2.00	0.60
1:D:115:ALA:HB2	1:D:146:VAL:HG11	1.84	0.60
1:D:168:LEU:CD2	1:D:172:VAL:HG23	2.31	0.60
1:D:11:VAL:HG22	1:D:16:TRP:CE3	2.37	0.60
1:C:284:VAL:HG13	1:C:348:VAL:HG11	1.84	0.59
1:B:10:SER:O	1:B:250:LYS:HE2	2.03	0.59
1:A:82:SER:HB2	1:A:108:ASN:HD22	1.65	0.59
1:D:196:ARG:HG2	1:D:196:ARG:HH11	1.68	0.58
1:D:213:THR:OG1	1:D:216:ALA:HB3	2.03	0.58
1:D:168:LEU:HD23	1:D:172:VAL:HG23	1.85	0.58
1:D:182:LYS:HG2	1:D:199:TRP:CZ2	2.38	0.58
1:A:321:LYS:H	1:A:347:ASN:ND2	2.02	0.58
1:D:94:SER:HB2	1:D:97:ASP:HB2	1.84	0.58
1:B:317:ALA:HB1	1:B:318:PRO:HA	1.85	0.58
1:C:263:THR:HB	1:C:266:LYS:HE2	1.86	0.57
1:C:11:VAL:HA	1:C:247:GLU:OE2	2.04	0.57
1:D:151:ALA:HB1	1:D:152:PRO:HD2	1.87	0.56
1:D:144:GLN:HE21	1:D:144:GLN:CA	2.10	0.56
1:B:37:ASP:OD1	1:B:38:PRO:HD2	2.05	0.56
1:C:12:ASP:N	1:C:247:GLU:OE2	2.36	0.56
1:D:46:THR:O	1:D:50:VAL:HG13	2.06	0.56
1:D:234:VAL:HG12	1:D:236:LEU:HD13	1.87	0.56
1:A:183:GLU:OE2	1:A:190:ARG:CD	2.40	0.55
1:C:105:GLN:HE21	1:C:191:GLN:HB3	1.69	0.55
1:B:321:LYS:H	1:B:347:ASN:ND2	2.05	0.55
1:C:266:LYS:N	1:C:266:LYS:HD2	2.20	0.55
1:C:183:GLU:HG3	1:C:192:PRO:HA	1.88	0.55
1:D:120:GLY:O	1:D:121:SER:HB3	2.06	0.55
1:C:311:THR:O	1:C:313:PRO:HD3	2.07	0.54
1:C:105:GLN:NE2	1:C:191:GLN:HB3	2.22	0.54
1:A:147:HIS:CE1	1:A:149:LEU:HD12	2.42	0.54
1:D:67:VAL:CG1	1:D:71:ALA:CB	2.87	0.53
1:D:311:THR:HG23	1:D:326:GLY:HA2	1.89	0.53
1:C:182:LYS:HE3	1:C:199:TRP:NE1	2.23	0.53
1:D:56:ALA:O	1:D:57:ASP:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:GLU:HG2	1:B:340:ARG:CZ	2.40	0.52
1:B:180:LYS:CG	1:B:206:ASP:HB2	2.38	0.52
1:D:65:VAL:O	1:D:65:VAL:CG2	2.58	0.52
1:A:320:LYS:HA	1:A:347:ASN:HD22	1.75	0.52
1:D:109:ASP:N	1:D:109:ASP:OD1	2.42	0.51
1:C:19:MET:HE2	1:C:162:ALA:HB1	1.92	0.51
1:D:67:VAL:HG23	1:D:91:ASP:O	2.10	0.51
1:D:168:LEU:HD13	1:D:176:TYR:HD1	1.76	0.51
1:A:9:PRO:HD3	1:A:254:TRP:CE2	2.46	0.51
1:C:239:LYS:HD2	1:C:239:LYS:N	2.26	0.51
1:D:187:ASN:O	1:D:188:LYS:C	2.50	0.50
1:D:149:LEU:O	1:D:150:ASP:C	2.49	0.50
1:A:134:LYS:HE3	1:A:134:LYS:N	2.26	0.50
1:B:267:PRO:O	1:B:268:ASP:CB	2.44	0.49
1:A:317:ALA:HB1	1:A:318:PRO:HA	1.94	0.49
1:B:291:ALA:O	1:B:340:ARG:HD2	2.12	0.49
1:C:184:PHE:N	1:C:191:GLN:O	2.38	0.49
1:C:42:THR:HB	1:C:148:GLY:HA3	1.95	0.49
1:A:70:ASP:OD1	1:A:116:ASP:OD2	2.31	0.49
1:D:187:ASN:O	1:D:189:ILE:N	2.45	0.49
1:A:72:TRP:CE3	1:A:89:PRO:HG2	2.47	0.49
1:C:204:ASN:HD22	1:C:204:ASN:C	2.15	0.49
1:C:35:LYS:NZ	1:C:140:ASN:OD1	2.40	0.49
1:A:77:PRO:O	1:A:80:ARG:HB2	2.13	0.48
1:A:72:TRP:CG	1:A:89:PRO:HD3	2.49	0.48
1:C:105:GLN:HE22	1:C:191:GLN:CG	2.26	0.48
1:C:315:LEU:HD11	1:C:325:VAL:CG1	2.39	0.48
1:D:187:ASN:O	1:D:189:ILE:HG13	2.13	0.48
1:D:94:SER:HB3	1:D:97:ASP:N	2.21	0.48
1:C:144:GLN:HB2	1:C:154:GLN:HB2	1.95	0.48
1:A:69:LYS:NZ	1:A:69:LYS:HB2	2.28	0.47
1:A:134:LYS:HE3	1:A:134:LYS:HA	1.95	0.47
1:D:146:VAL:O	1:D:146:VAL:HG12	2.14	0.47
1:C:9:PRO:HD3	1:C:254:TRP:CZ2	2.50	0.47
1:A:281:LYS:NZ	1:A:346:GLU:OE2	2.44	0.47
1:D:116:ASP:OD1	1:D:121:SER:HA	2.14	0.47
1:B:242:ARG:NH1	5:B:444:HOH:O	2.48	0.47
1:A:69:LYS:HG2	1:A:75:GLY:HA3	1.97	0.47
1:C:290:GLU:HA	1:C:290:GLU:OE1	2.14	0.47
1:C:311:THR:O	1:C:313:PRO:CD	2.63	0.46
1:B:14:ARG:HG3	1:B:237:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:CYS:HB3	1:D:146:VAL:HG12	1.98	0.46
1:D:108:ASN:H	1:D:108:ASN:ND2	2.08	0.46
1:C:140:ASN:O	1:C:155:PHE:HD1	1.98	0.46
1:C:149:LEU:HD22	1:C:149:LEU:HA	1.85	0.46
1:D:146:VAL:CG1	1:D:146:VAL:O	2.63	0.45
1:A:264:PRO:HD2	1:A:292:GLY:O	2.16	0.45
1:D:275:ARG:HG3	1:D:276:VAL:N	2.31	0.45
1:C:267:PRO:O	1:C:268:ASP:CB	2.38	0.45
1:C:134:LYS:O	1:C:134:LYS:HD2	2.16	0.45
1:B:333:ASN:O	5:B:586:HOH:O	2.21	0.45
1:B:275:ARG:HG2	1:B:275:ARG:HH11	1.81	0.45
1:C:294:VAL:HG13	1:C:338:GLU:OE1	2.17	0.45
1:C:312:GLU:HA	1:C:313:PRO:HD2	1.67	0.45
1:C:9:PRO:HG3	1:C:254:TRP:CG	2.51	0.45
1:D:194:ARG:H	1:D:194:ARG:HG2	1.54	0.45
1:C:17:ILE:HG22	1:C:234:VAL:HB	1.99	0.45
1:B:187:ASN:O	1:B:188:LYS:HB2	2.17	0.45
1:D:267:PRO:HA	1:D:289:GLY:O	2.17	0.44
1:C:9:PRO:HG3	1:C:254:TRP:CD2	2.52	0.44
1:D:60:LYS:HB3	1:D:60:LYS:HE2	1.81	0.44
1:C:16:TRP:HA	1:C:234:VAL:O	2.18	0.44
1:C:35:LYS:C	1:C:36:LEU:HD23	2.38	0.44
1:B:72:TRP:CE2	1:B:74:THR:HB	2.52	0.44
1:A:313:PRO:O	1:A:314:GLN:HG3	2.18	0.43
1:A:67:VAL:HG11	1:A:87:LEU:HB3	1.98	0.43
1:C:317:ALA:HB1	1:C:318:PRO:HA	2.00	0.43
1:D:188:LYS:HD3	1:D:188:LYS:HA	1.22	0.43
1:A:39:ALA:HA	1:A:148:GLY:O	2.17	0.43
1:A:246:ASN:HB3	5:A:715:HOH:O	2.18	0.43
1:A:332:LEU:HA	1:A:332:LEU:HD12	1.81	0.43
1:C:294:VAL:HA	1:C:338:GLU:OE2	2.19	0.43
1:D:197:LEU:HA	1:D:197:LEU:HD23	1.85	0.43
1:C:272:VAL:HG23	1:C:286:LEU:HB2	2.01	0.43
1:C:213:THR:O	1:C:213:THR:OG1	2.30	0.43
1:C:284:VAL:HG21	1:C:315:LEU:HD23	2.01	0.43
1:C:134:LYS:HD2	1:C:134:LYS:C	2.38	0.43
1:D:35:LYS:NZ	1:D:140:ASN:OD1	2.52	0.43
1:C:31:ASN:C	1:C:33:ASP:H	2.21	0.43
1:C:105:GLN:HE22	1:C:191:GLN:HG2	1.84	0.42
1:D:95:VAL:O	1:D:96:ALA:C	2.58	0.42
1:C:105:GLN:NE2	1:C:191:GLN:CG	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:ALA:O	1:D:57:ASP:CB	2.66	0.42
1:D:273:THR:HG22	1:D:285:ASN:HD22	1.84	0.42
1:C:257:ARG:HG2	1:C:258:PHE:CD2	2.54	0.42
1:D:65:VAL:O	1:D:65:VAL:HG22	2.19	0.42
1:C:36:LEU:HD12	1:C:236:LEU:HB3	2.02	0.42
1:A:207:GLY:HA2	1:A:208:MET:HA	1.87	0.42
1:C:158:ALA:HB2	1:C:236:LEU:HD22	2.01	0.42
1:C:191:GLN:HA	1:C:192:PRO:HD3	1.94	0.42
1:C:272:VAL:HG11	1:C:308:TYR:CZ	2.54	0.42
1:A:77:PRO:HA	1:A:80:ARG:HH11	1.84	0.41
1:C:259:PHE:O	1:C:298:ARG:NH1	2.53	0.41
1:A:350:GLU:HB3	5:A:498:HOH:O	2.20	0.41
1:C:320:LYS:HA	1:C:347:ASN:HD22	1.85	0.41
1:C:196[A]:ARG:NH1	1:C:241:ASP:OD2	2.53	0.41
1:C:284:VAL:HG13	1:C:348:VAL:CG1	2.50	0.41
1:C:274:GLN:O	1:C:283:GLU:HA	2.20	0.41
1:D:304:LEU:CD1	1:D:337:ILE:HD11	2.50	0.41
1:A:180:LYS:NZ	5:A:425:HOH:O	2.52	0.41
1:C:97:ASP:OD2	1:C:186:PHE:HE1	2.04	0.41
1:C:140:ASN:O	1:C:155:PHE:CD1	2.73	0.41
1:C:27:LEU:HD21	1:C:295:THR:HG21	2.02	0.41
1:D:114:LEU:O	1:D:118:VAL:HG12	2.21	0.41
1:A:338:GLU:HG2	1:A:340:ARG:NH1	2.36	0.40
1:B:144:GLN:HG3	1:B:152:PRO:O	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	346/352 (98%)	335 (97%)	10 (3%)	1 (0%)	46 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	345/352 (98%)	339 (98%)	6 (2%)	0	100 100
1	C	323/352 (92%)	303 (94%)	19 (6%)	1 (0%)	46 29
1	D	332/352 (94%)	314 (95%)	15 (4%)	3 (1%)	21 7
All	All	1346/1408 (96%)	1291 (96%)	50 (4%)	5 (0%)	39 23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	188	LYS
1	A	73	ALA
1	C	313	PRO
1	D	150	ASP
1	D	68	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	282/285 (99%)	265 (94%)	17 (6%)	24 8
1	B	281/285 (99%)	261 (93%)	20 (7%)	18 6
1	C	272/285 (95%)	235 (86%)	37 (14%)	5 1
1	D	274/285 (96%)	240 (88%)	34 (12%)	6 1
All	All	1109/1140 (97%)	1001 (90%)	108 (10%)	10 2

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	69	LYS
1	A	74	THR
1	A	80	ARG
1	A	87	LEU
1	A	88	LYS

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Mol	Chain	Res	Type
1	A	106	SER
1	A	134	LYS
1	A	147	HIS
1	A	188	LYS
1	A	246	ASN
1	A	276	VAL
1	A	283	GLU
1	A	302	LYS
1	A	305	LYS
1	A	315	LEU
1	A	335	LYS
1	B	7	GLU
1	B	82	SER
1	B	83	SER
1	B	88	LYS
1	B	114	LEU
1	B	134	LYS
1	B	191	GLN
1	B	204	ASN
1	B	209	LYS
1	B	228	ASP
1	B	239	LYS
1	B	244	ARG
1	B	250	LYS
1	B	281	LYS
1	B	302	LYS
1	B	315	LEU
1	B	320	LYS
1	B	331	GLN
1	B	335	LYS
1	B	338	GLU
1	C	6	VAL
1	C	11	VAL
1	C	14	ARG
1	C	69	LYS
1	C	72	TRP
1	C	85	MET
1	C	88	LYS
1	C	98	LEU
1	C	114	LEU
1	C	123	GLU
1	C	124	SER

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Mol	Chain	Res	Type
1	C	126	ILE
1	C	128	LEU
1	C	134	LYS
1	C	144	GLN
1	C	147	HIS
1	C	149	LEU
1	C	163	LEU
1	C	174	GLU
1	C	194	ARG
1	C	201	SER
1	C	204	ASN
1	C	228	ASP
1	C	236	LEU
1	C	239	LYS
1	C	263	THR
1	C	266	LYS
1	C	275	ARG
1	C	282	SER
1	C	284	VAL
1	C	314	GLN
1	C	316	THR
1	C	319	LEU
1	C	320	LYS
1	C	346	GLU
1	C	348	VAL
1	C	349	GLU
1	D	7	GLU
1	D	10	SER
1	D	14	ARG
1	D	40	SER
1	D	50	VAL
1	D	57	ASP
1	D	64	MET
1	D	69	LYS
1	D	91	ASP
1	D	94	SER
1	D	102	VAL
1	D	106	SER
1	D	108	ASN
1	D	118	VAL
1	D	121	SER
1	D	128	LEU

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Mol	Chain	Res	Type
1	D	142	THR
1	D	168	LEU
1	D	183	GLU
1	D	188	LYS
1	D	189	ILE
1	D	194	ARG
1	D	209	LYS
1	D	212	THR
1	D	236	LEU
1	D	239	LYS
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	250	LYS
1	D	276	VAL
1	D	312	GLU
1	D	314	GLN
1	D	327	THR
1	D	337	ILE

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

Mol	Chain	Res	Type
1	A	99	ASN
1	A	154	GLN
1	A	170	HIS
1	A	187	ASN
1	A	303	ASN
1	A	347	ASN
1	B	105	GLN
1	B	202	ASN
1	B	204	ASN
1	B	274	GLN
1	B	285	ASN
1	B	331	GLN
1	B	347	ASN
1	C	105	GLN
1	C	122	GLN
1	C	130	ASN
1	C	179	HIS
1	C	204	ASN
1	C	219	ASN
1	C	226	GLN

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Mol	Chain	Res	Type
1	C	285	ASN
1	C	303	ASN
1	C	314	GLN
1	C	339	GLN
1	C	347	ASN
1	D	108	ASN
1	D	144	GLN
1	D	285	ASN
1	D	303	ASN
1	D	331	GLN
1	D	339	GLN

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

8 ligands are modelled in this entry.

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	A	353	-	4,4,4	0.23	0	6,6,6	0.30	0
2	AIX	A	500	1	17,25,25	1.49	2 (11%)	20,36,36	0.95	1 (5%)
3	SO4	B	353	-	4,4,4	0.27	0	6,6,6	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	B	354	-	4,4,4	0.09	0	6,6,6	0.27	0
3	SO4	C	353	-	4,4,4	0.23	0	6,6,6	0.16	0
3	SO4	C	354	-	4,4,4	0.18	0	6,6,6	0.07	0
3	SO4	C	355	-	4,4,4	0.24	0	6,6,6	0.21	0
4	AIC	D	501	-	22,26,26	1.73	6 (27%)	32,40,40	2.51	9 (28%)

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	A	353	-	-	0/0/0/0	0/0/0/0
2	AIX	A	500	1	-	0/12/37/37	0/2/2/2
3	SO4	B	353	-	-	0/0/0/0	0/0/0/0
3	SO4	B	354	-	-	0/0/0/0	0/0/0/0
3	SO4	C	353	-	-	0/0/0/0	0/0/0/0
3	SO4	C	354	-	-	0/0/0/0	0/0/0/0
3	SO4	C	355	-	-	0/0/0/0	0/0/0/0
4	AIC	D	501	-	-	0/12/47/47	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	AIX	C6-S1	-4.39	1.76	1.85
4	D	501	AIC	C6-S1	-3.66	1.77	1.85
4	D	501	AIC	C15-N3	-3.32	1.30	1.37
4	D	501	AIC	C12-N3	-3.31	1.44	1.47
2	A	500	AIX	C5-C4	-3.31	1.48	1.52
4	D	501	AIC	C13-S1	-2.93	1.76	1.81
4	D	501	AIC	C5-C4	-2.69	1.49	1.52
4	D	501	AIC	C4-C3	-2.50	1.49	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	501	AIC	S1-C13-N3	-8.06	94.18	105.09
4	D	501	AIC	C14-C13-N3	-3.82	83.06	87.98
4	D	501	AIC	C6-C12-N3	-3.41	101.31	106.45
4	D	501	AIC	C13-C14-N1	-3.14	111.26	118.21
2	A	500	AIX	C13-C14-N1	2.02	114.28	109.57
4	D	501	AIC	O4-C15-N3	2.96	135.89	131.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	501	AIC	C6-S1-C13	3.30	101.35	94.06
4	D	501	AIC	C12-N3-C15	3.69	134.67	125.99
4	D	501	AIC	C13-N3-C15	4.15	99.31	93.89
4	D	501	AIC	C13-N3-C12	6.40	123.85	117.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	355	SO4	2	0
4	D	501	AIC	3	0

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	348/352 (98%)	0.19	15 (4%)	39	32	19, 30, 56, 87	0
1	B	347/352 (98%)	-0.03	8 (2%)	64	59	21, 32, 53, 71	0
1	C	330/352 (93%)	0.52	28 (8%)	13	10	29, 47, 75, 103	0
1	D	333/352 (94%)	0.25	27 (8%)	15	11	22, 40, 72, 96	0
All	All	1358/1408 (96%)	0.23	78 (5%)	27	22	19, 37, 68, 103	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	ALA	8.4
1	C	72	TRP	8.1
1	C	86	PHE	7.3
1	C	352	GLY	6.1
1	A	75	GLY	6.1
1	C	152	PRO	6.0
1	C	69	LYS	5.8
1	C	88	LYS	5.6
1	D	187	ASN	5.2
1	A	80	ARG	5.1
1	A	77	PRO	5.0
1	C	84	VAL	4.9
1	A	74	THR	4.7
1	A	76	ASN	4.5
1	D	188	LYS	4.5
1	D	69	LYS	4.4
1	C	155	PHE	4.1
1	D	93	VAL	4.1
1	A	73	ALA	4.0
1	D	155	PHE	4.0
1	A	352	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	89	PRO	3.9
1	D	66	THR	3.7
1	C	228	ASP	3.7
1	D	185	THR	3.7
1	B	352	GLY	3.7
1	D	189	ILE	3.6
1	A	72	TRP	3.5
1	D	92	GLN	3.4
1	D	70	ASP	3.3
1	A	334	GLY	3.3
1	B	8	ALA	3.2
1	C	67	VAL	3.2
1	B	164	LEU	3.2
1	D	64	MET	3.2
1	D	186	PHE	3.1
1	C	44	ILE	3.0
1	B	75	GLY	3.0
1	D	68	GLY	3.0
1	D	89	PRO	3.0
1	C	191	GLN	2.9
1	D	149	LEU	2.9
1	C	90	GLY	2.8
1	D	152	PRO	2.8
1	A	44	ILE	2.8
1	A	164	LEU	2.7
1	D	71	ALA	2.7
1	D	91	ASP	2.7
1	D	216	ALA	2.6
1	C	349	GLU	2.6
1	B	44	ILE	2.6
1	C	46	THR	2.6
1	D	190	ARG	2.6
1	C	68	GLY	2.5
1	C	91	ASP	2.5
1	C	201	SER	2.5
1	D	65	VAL	2.5
1	C	185	THR	2.4
1	C	333	ASN	2.4
1	D	215	GLY	2.4
1	C	239	LYS	2.4
1	C	202	ASN	2.3
1	C	164	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	42	THR	2.3
1	D	164	LEU	2.2
1	D	95	VAL	2.2
1	C	351	GLY	2.2
1	D	41	LEU	2.2
1	C	71	ALA	2.1
1	A	49	VAL	2.1
1	A	221	VAL	2.1
1	D	44	ILE	2.1
1	C	31	ASN	2.1
1	B	41	LEU	2.0
1	D	192	PRO	2.0
1	C	150	ASP	2.0
1	A	234	VAL	2.0
1	B	162	ALA	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
4	AIC	D	501	24/24	0.90	0.21	12.20	39,64,82,85	0
3	SO4	C	355	5/5	0.94	0.26	3.18	67,69,74,75	0
3	SO4	B	354	5/5	0.92	0.11	0.85	53,57,65,69	0
3	SO4	C	354	5/5	0.90	0.11	-1.04	93,98,102,103	0
2	AIX	A	500	24/24	0.96	0.08	-1.20	28,41,50,64	0
3	SO4	B	353	5/5	0.93	0.09	-1.21	42,43,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	A	353	5/5	0.98	0.11	-	45,49,57,62	0
3	SO4	C	353	5/5	0.97	0.13	-	52,55,61,63	0

6.5 Other polymers (i)

There are no such residues in this entry.