Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:41 PM GMT

PDB ID	:	3UMM
Title	:	Formylglycinamide ribonucleotide amidotransferase from Salmonella typhimurium: Role of the ATP complexation and glutaminase domain in catalytic coupling
Authors	:	Anand, R.; Morar, M.; Tanwar, A.S.; Panjikar, S.
Deposited on	:	2011-11-14
Resolution	:	3.20 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:

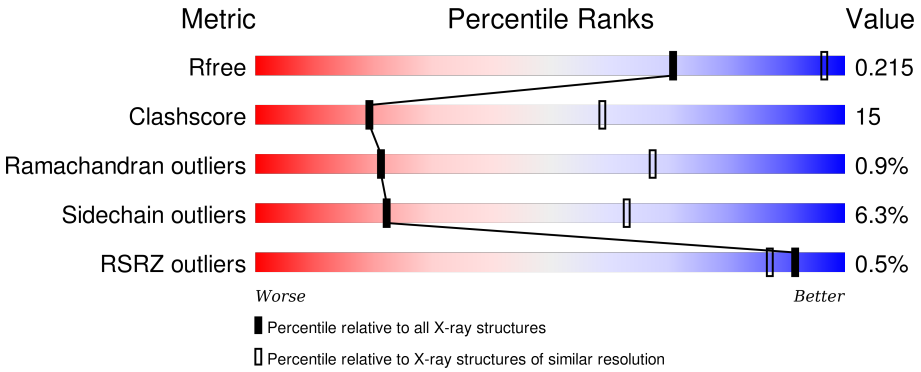
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.20 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))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	1303	67% 29%

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
1	CYG	A	1135	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	A	2005	-	-	-	X
4	MG	A	2006	-	-	-	X
4	MG	A	2008	-	-	-	X
5	SO4	A	2009	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10462 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.

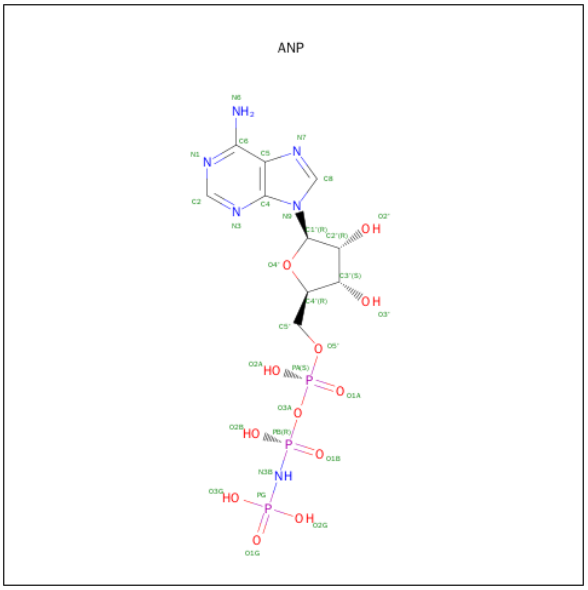
- Molecule 1 is a protein called Phosphoribosylformylglycinamidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1285	Total	C	N	O	S	0	0	0
			9909	6216	1769	1876	48			

There are 8 discrepancies between the modelled and reference sequences:

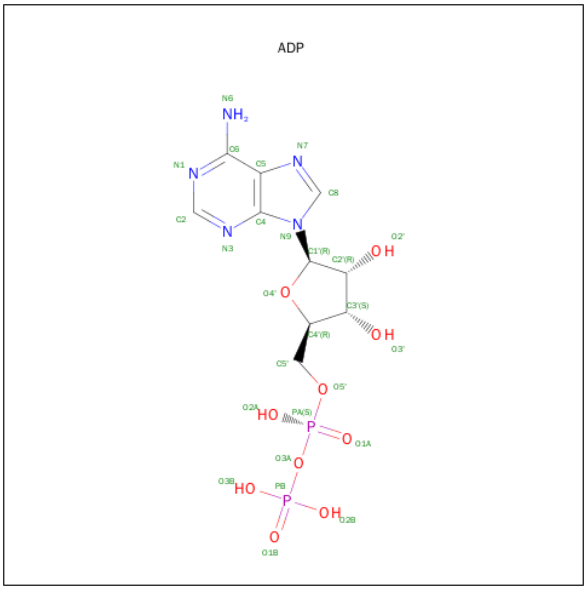
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP P74881
A	-6	LEU	-	EXPRESSION TAG	UNP P74881
A	-5	VAL	-	EXPRESSION TAG	UNP P74881
A	-4	PRO	-	EXPRESSION TAG	UNP P74881
A	-3	ARG	-	EXPRESSION TAG	UNP P74881
A	-2	GLY	-	EXPRESSION TAG	UNP P74881
A	-1	SER	-	EXPRESSION TAG	UNP P74881
A	0	HIS	-	EXPRESSION TAG	UNP P74881

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

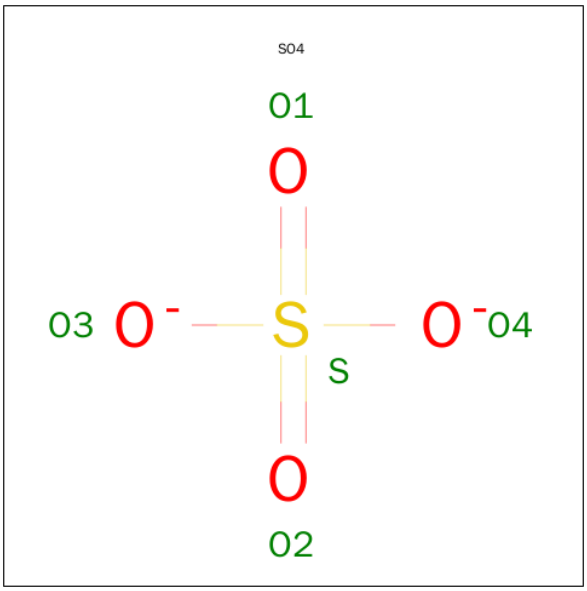


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	0
			3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is water.

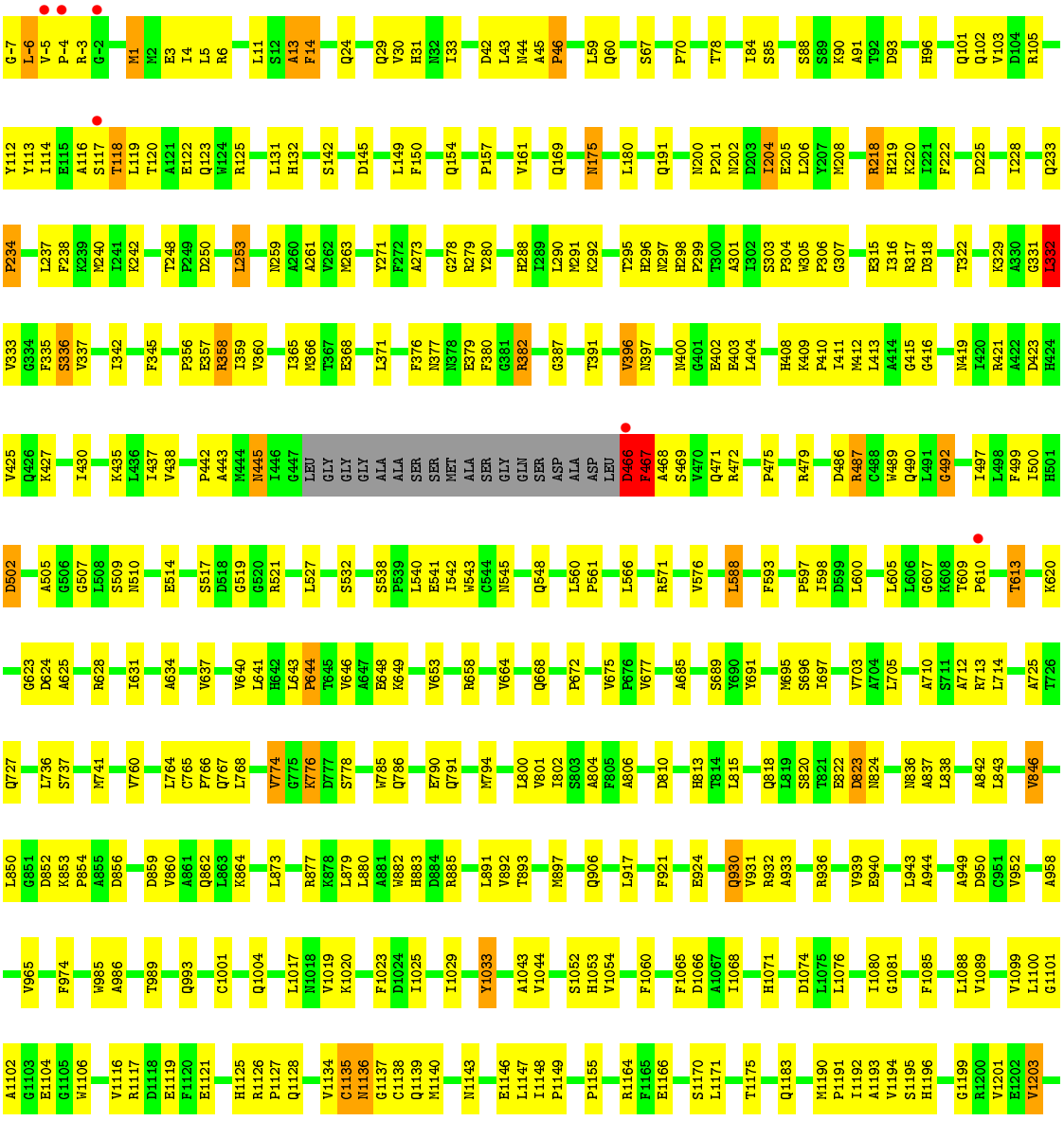
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	482	Total O 482 482	0	0

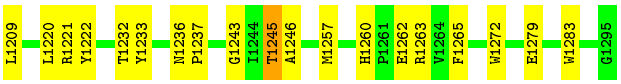
3 Residue-property plots (i)

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: Phosphoribosylformylglycinamidine synthase

Chain A:




L1209
L1220
R1221
Y1222
T1232
Y1233
N1236
P1237
G1243
I1244
T1245
A1246
M1257
H1260
P1261
E1262
R1263
V1264
F1265
W1272
E1279
W1283
G1295

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	148.68Å 148.68Å 142.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.20 19.97 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.98-3.20) 98.4 (19.97-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 3.22Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.276 0.216 , 0.215	Depositor DCC
R_{free} test set	1031 reflections (3.57%)	DCC
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 30.2	EDS
Estimated twinning fraction	0.030 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 28855 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	10462	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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: ANP, MG, CYG, SO4, ADP

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	0.42	0/10106	0.67	3/13716 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	466	ASP	C-N-CA	10.45	147.82	121.70
1	A	332	LEU	CA-CB-CG	6.56	130.39	115.30
1	A	466	ASP	CB-CG-OD2	5.22	123.00	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1135	CYG	Mainchain
1	A	466	ASP	Peptide

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	9909	0	9694	297	0
2	A	31	0	13	3	0
3	A	27	0	11	0	0
4	A	3	0	0	0	0
5	A	10	0	0	5	0
6	A	482	0	0	3	0
All	All	10462	0	9718	298	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 15.

All (298) 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:13:ALA:HB3	5:A:2009:SO4:O4	1.03	1.19
1:A:13:ALA:CB	5:A:2009:SO4:O4	1.96	1.13
1:A:466:ASP:C	6:A:1335:HOH:O	2.06	0.93
1:A:336:SER:HB2	1:A:411:ILE:HB	1.51	0.93
1:A:387:GLY:HA2	1:A:697:ILE:HD12	1.51	0.92
1:A:628:ARG:HA	1:A:631:ILE:HD13	1.52	0.90
1:A:120:THR:H	1:A:123:GLN:HE21	1.22	0.86
1:A:358:ARG:HD3	1:A:358:ARG:H	1.39	0.86
1:A:466:ASP:CA	6:A:1335:HOH:O	2.24	0.85
1:A:487:ARG:HG2	1:A:566:LEU:HD22	1.57	0.83
1:A:329:LYS:HZ3	1:A:685:ALA:HA	1.44	0.81
1:A:1076:LEU:HD23	1:A:1116:VAL:HG21	1.61	0.81
1:A:1175:THR:HG21	1:A:1221:ARG:HE	1.46	0.80
1:A:119:LEU:HB3	1:A:123:GLN:HB2	1.62	0.80
1:A:5:LEU:HD22	1:A:59:LEU:HD12	1.65	0.78
1:A:305:TRP:HB3	1:A:306:PRO:HD3	1.65	0.76
1:A:609:THR:HB	1:A:610:PRO:HD2	1.68	0.75
1:A:443:ALA:HB1	1:A:545:ASN:HD21	1.52	0.75
1:A:859:ASP:HB3	1:A:862:GLN:HB2	1.68	0.74
1:A:120:THR:HG23	1:A:123:GLN:HE21	1.52	0.74
1:A:1135:CYG:HB13	1:A:1136:ASN:HB2	1.70	0.73
1:A:329:LYS:NZ	1:A:685:ALA:HA	2.03	0.73
1:A:408:HIS:CD2	1:A:794:MET:HG2	2.24	0.72
1:A:466:ASP:HB2	1:A:467:PHE:HB2	1.71	0.72
1:A:510:ASN:O	1:A:514:GLU:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:LEU:HB2	1:A:598:ILE:HB	1.73	0.71
1:A:1106:TRP:CD2	1:A:1140:MET:HG3	2.27	0.70
1:A:443:ALA:HB1	1:A:545:ASN:ND2	2.06	0.70
1:A:1221:ARG:HA	1:A:1243:GLY:O	1.91	0.70
1:A:13:ALA:HB3	5:A:2009:SO4:S	2.29	0.69
1:A:466:ASP:HB2	1:A:467:PHE:CB	2.23	0.69
1:A:631:ILE:H	1:A:631:ILE:HD12	1.56	0.69
1:A:1262:GLU:O	1:A:1265:PHE:HD2	1.76	0.68
1:A:885:ARG:NH2	1:A:924:GLU:HB2	2.09	0.68
1:A:931:VAL:HG11	1:A:939:VAL:HG11	1.78	0.66
1:A:356:PRO:HG3	1:A:785:TRP:HB3	1.78	0.66
1:A:142:SER:O	1:A:145:ASP:HB2	1.95	0.66
1:A:84:ILE:HG13	1:A:105:ARG:NH1	2.11	0.66
1:A:823:ASP:HB3	1:A:933:ALA:CB	2.26	0.66
1:A:14:PHE:HB3	5:A:2009:SO4:O2	1.96	0.65
1:A:1121:GLU:HG2	1:A:1125:HIS:CD2	2.32	0.65
1:A:1236:ASN:ND2	1:A:1243:GLY:HA2	2.12	0.65
1:A:541:GLU:O	1:A:545:ASN:HB3	1.96	0.65
1:A:175:ASN:ND2	1:A:180:LEU:HB2	2.11	0.65
1:A:588:LEU:HD12	1:A:598:ILE:HD12	1.79	0.65
1:A:-6:LEU:HG	1:A:1:MET:SD	2.36	0.64
1:A:1126:ARG:HG3	1:A:1127:PRO:HD2	1.79	0.64
1:A:1262:GLU:HG2	1:A:1263:ARG:N	2.12	0.64
1:A:396:VAL:HG21	1:A:850:LEU:HD13	1.78	0.64
1:A:1004:GLN:NE2	1:A:1233:TYR:H	1.95	0.64
1:A:120:THR:H	1:A:123:GLN:NE2	1.92	0.64
1:A:218:ARG:HH21	1:A:220:LYS:HE2	1.63	0.64
1:A:1135:CYG:O	1:A:1137:GLY:N	2.30	0.63
1:A:486:ASP:HA	1:A:489:TRP:NE1	2.13	0.63
1:A:1222:TYR:OH	1:A:1245:THR:HG21	1.97	0.63
1:A:609:THR:HB	1:A:610:PRO:CD	2.29	0.63
1:A:885:ARG:HH21	1:A:924:GLU:HB2	1.64	0.62
1:A:337:VAL:HG23	1:A:391:THR:HG22	1.81	0.62
1:A:637:VAL:HG22	1:A:891:LEU:CD2	2.28	0.62
1:A:435:LYS:HG3	1:A:560:LEU:HD22	1.82	0.62
1:A:357:GLU:H	1:A:358:ARG:HH11	1.48	0.62
1:A:11:LEU:HD11	1:A:112:TYR:HE1	1.65	0.61
1:A:161:VAL:O	1:A:200:ASN:HB3	2.00	0.61
1:A:696:SER:OG	1:A:804:ALA:HB3	2.00	0.61
1:A:430:ILE:HD12	1:A:519:GLY:HA3	1.82	0.61
1:A:356:PRO:HD2	1:A:359:ILE:HD11	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-7:GLY:HA3	1:A:4:ILE:H	1.65	0.61
1:A:157:PRO:HA	1:A:593:PHE:CE2	2.35	0.60
1:A:1220:LEU:HB2	1:A:1246:ALA:HB3	1.83	0.60
1:A:815:LEU:HD21	1:A:879:LEU:HB2	1.83	0.60
1:A:332:LEU:HD12	1:A:695:MET:SD	2.42	0.60
1:A:161:VAL:HG21	1:A:206:LEU:HD22	1.83	0.60
1:A:315:GLU:HG3	1:A:415:GLY:HA2	1.84	0.60
1:A:396:VAL:HG22	1:A:850:LEU:HB2	1.83	0.59
1:A:96:HIS:HE1	1:A:103:VAL:O	1.84	0.59
1:A:986:ALA:O	1:A:989:THR:HG22	2.01	0.59
1:A:357:GLU:H	1:A:358:ARG:NH1	2.00	0.59
1:A:317:ARG:HH22	1:A:548:GLN:NE2	2.01	0.59
1:A:466:ASP:N	6:A:1335:HOH:O	2.33	0.59
1:A:1044:VAL:HA	1:A:1089:VAL:CG1	2.33	0.58
1:A:527:LEU:HB2	1:A:588:LEU:HD22	1.85	0.58
1:A:118:THR:H	1:A:119:LEU:HD12	1.69	0.58
1:A:120:THR:HG23	1:A:123:GLN:NE2	2.19	0.58
1:A:466:ASP:N	1:A:468:ALA:H	2.01	0.58
1:A:631:ILE:N	1:A:631:ILE:HD12	2.18	0.58
1:A:943:LEU:HD13	1:A:952:VAL:HG21	1.85	0.58
1:A:1033:TYR:N	1:A:1033:TYR:CD2	2.72	0.58
1:A:640:VAL:HG21	1:A:921:PHE:CE1	2.38	0.58
1:A:238:PHE:HE2	1:A:242:LYS:HE3	1.68	0.57
1:A:1071:HIS:O	1:A:1074:ASP:HB2	2.04	0.57
1:A:329:LYS:NZ	1:A:419:ASN:HD21	2.02	0.57
1:A:1196:HIS:CD2	1:A:1199:GLY:HA3	2.40	0.57
1:A:358:ARG:HD3	1:A:358:ARG:N	2.15	0.57
1:A:815:LEU:CD2	1:A:879:LEU:HB2	2.35	0.56
1:A:14:PHE:HD2	5:A:2009:SO4:O3	1.89	0.56
1:A:317:ARG:HH22	1:A:548:GLN:HE22	1.53	0.56
1:A:78:THR:HB	1:A:149:LEU:HD11	1.87	0.56
1:A:736:LEU:HG	1:A:802:ILE:HG23	1.87	0.56
1:A:823:ASP:HB3	1:A:933:ALA:HB2	1.86	0.55
1:A:1138:CYS:HB2	1:A:1257:MET:O	2.06	0.55
1:A:1060:PHE:O	1:A:1065:PHE:HB2	2.05	0.55
1:A:204:ILE:HD11	1:A:543:TRP:CD1	2.42	0.55
1:A:658:ARG:HD2	1:A:668:GLN:OE1	2.07	0.55
1:A:261:ALA:HB2	1:A:774:VAL:HG13	1.88	0.55
1:A:238:PHE:CE2	1:A:242:LYS:HE3	2.42	0.55
1:A:843:LEU:HD21	1:A:917:LEU:HD21	1.89	0.55
1:A:30:VAL:HA	1:A:116:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LEU:HD13	1:A:794:MET:HE1	1.89	0.54
1:A:1192:ILE:HG13	1:A:1193:ALA:H	1.72	0.54
1:A:-6:LEU:HG	1:A:1:MET:CE	2.36	0.54
1:A:640:VAL:HG21	1:A:921:PHE:HE1	1.71	0.54
1:A:824:ASN:HD21	1:A:958:ALA:H	1.54	0.54
1:A:301:ALA:HB2	1:A:410:PRO:HD2	1.90	0.53
1:A:33:ILE:HG13	1:A:114:ILE:HG12	1.89	0.53
1:A:288:HIS:O	1:A:419:ASN:HA	2.08	0.53
1:A:823:ASP:HB3	1:A:933:ALA:HB3	1.91	0.53
1:A:29:GLN:HG3	1:A:31:HIS:HE1	1.73	0.53
1:A:175:ASN:HD22	1:A:180:LEU:HB2	1.72	0.53
1:A:517:SER:C	1:A:519:GLY:H	2.09	0.53
1:A:1033:TYR:HD2	1:A:1033:TYR:H	1.56	0.53
1:A:204:ILE:HD13	1:A:540:LEU:HA	1.89	0.53
1:A:1192:ILE:HG13	1:A:1193:ALA:N	2.23	0.53
1:A:989:THR:O	1:A:993:GLN:HG3	2.08	0.53
1:A:637:VAL:HG22	1:A:891:LEU:HD21	1.89	0.52
1:A:1134:VAL:O	1:A:1135:CYG:O	2.26	0.52
1:A:737:SER:HB2	1:A:774:VAL:HG23	1.92	0.52
1:A:497:ILE:HG21	1:A:500:ILE:HB	1.91	0.52
1:A:1135:CYG:O	1:A:1138:CYS:N	2.37	0.52
1:A:1004:GLN:NE2	1:A:1232:THR:HG23	2.25	0.52
1:A:1023:PHE:CE1	1:A:1025:ILE:HG22	2.44	0.52
1:A:675:VAL:HG12	1:A:677:VAL:HG13	1.91	0.52
1:A:906:GLN:OE1	1:A:965:VAL:HB	2.10	0.52
1:A:91:ALA:HB2	1:A:1099:VAL:HG11	1.92	0.52
1:A:893:THR:O	1:A:897:MET:HG3	2.09	0.51
1:A:396:VAL:CG2	1:A:850:LEU:HB2	2.40	0.51
1:A:219:HIS:HE1	2:A:2001:ANP:O2A	1.94	0.51
1:A:1135:CYG:O	1:A:1136:ASN:C	2.49	0.51
1:A:873:LEU:HD13	1:A:879:LEU:HD21	1.93	0.51
1:A:225:ASP:HB2	1:A:613:THR:HG23	1.93	0.51
1:A:-5:VAL:HG12	1:A:-4:PRO:HD2	1.94	0.50
1:A:-7:GLY:O	1:A:3:GLU:HG3	2.11	0.50
1:A:1033:TYR:HD2	1:A:1033:TYR:N	2.10	0.50
1:A:1019:VAL:CG1	1:A:1020:LYS:N	2.74	0.50
1:A:202:ASN:HB2	1:A:205:GLU:HG3	1.94	0.50
1:A:201:PRO:HB2	1:A:206:LEU:HD13	1.94	0.49
1:A:765:CYS:HB2	1:A:766:PRO:HD3	1.93	0.49
1:A:413:LEU:HD13	1:A:801:VAL:HG11	1.93	0.49
1:A:1052:SER:O	1:A:1054:VAL:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ASN:HA	2:A:2001:ANP:O1B	2.13	0.49
1:A:1139:GLN:O	1:A:1143:ASN:ND2	2.46	0.49
1:A:304:PRO:HB2	1:A:368:GLU:HB2	1.95	0.49
1:A:218:ARG:NH2	1:A:220:LYS:HE2	2.26	0.49
1:A:648:GLU:HB2	1:A:985:TRP:CE3	2.48	0.49
1:A:725:ALA:HB2	1:A:882:TRP:CD1	2.47	0.49
1:A:445:ASN:HD22	1:A:445:ASN:C	2.16	0.49
1:A:228:ILE:HD13	1:A:233:GLN:HG3	1.94	0.49
1:A:1019:VAL:HG12	1:A:1020:LYS:N	2.28	0.48
1:A:337:VAL:O	1:A:391:THR:HA	2.13	0.48
1:A:1135:CYG:HB3	1:A:1260:HIS:CE1	2.49	0.48
1:A:161:VAL:HB	1:A:201:PRO:HG2	1.93	0.48
1:A:1101:GLY:O	1:A:1104:GLU:HB2	2.14	0.48
1:A:1236:ASN:HD21	1:A:1243:GLY:HA2	1.76	0.48
1:A:301:ALA:O	1:A:360:VAL:HG22	2.13	0.48
1:A:486:ASP:O	1:A:490:GLN:HG3	2.13	0.48
1:A:710:ALA:HA	1:A:856:ASP:OD1	2.14	0.48
1:A:278:GLY:O	1:A:1068:ILE:HG23	2.14	0.48
1:A:295:THR:HB	1:A:297:ASN:HD21	1.79	0.48
1:A:1166:GLU:O	1:A:1195:SER:HA	2.14	0.48
1:A:400:ASN:HB3	1:A:403:GLU:OE1	2.14	0.47
1:A:842:ALA:O	1:A:846:VAL:HB	2.14	0.47
1:A:471:GLN:HE21	1:A:472:ARG:H	1.61	0.47
1:A:1194:VAL:HG13	1:A:1196:HIS:CE1	2.49	0.47
1:A:1080:ILE:HG22	1:A:1081:GLY:N	2.30	0.47
1:A:466:ASP:CB	1:A:467:PHE:HB2	2.41	0.47
1:A:631:ILE:HG21	1:A:917:LEU:HD21	1.97	0.47
1:A:29:GLN:HG3	1:A:31:HIS:CE1	2.50	0.47
1:A:1170:SER:HB2	1:A:1194:VAL:HG21	1.96	0.47
1:A:936:ARG:O	1:A:940:GLU:HG3	2.15	0.47
1:A:1088:LEU:HG	1:A:1089:VAL:N	2.29	0.46
1:A:411:ILE:HG12	1:A:741:MET:HG2	1.97	0.46
1:A:637:VAL:HG22	1:A:891:LEU:HD22	1.96	0.46
1:A:379:GLU:HB3	1:A:475:PRO:HB2	1.96	0.46
1:A:1101:GLY:HA3	1:A:1104:GLU:HG3	1.97	0.46
1:A:1203:VAL:HG21	1:A:1209:LEU:HB2	1.97	0.46
1:A:689:SER:HG	1:A:691:TYR:HD2	1.63	0.46
1:A:427:LYS:HB3	1:A:499:PHE:CD1	2.50	0.46
1:A:605:LEU:C	1:A:607:GLY:H	2.19	0.46
1:A:712:ALA:HA	1:A:800:LEU:HD23	1.97	0.46
1:A:837:ALA:HB1	1:A:853:LYS:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:HIS:HB3	1:A:299:PRO:HD3	1.96	0.46
1:A:944:ALA:HA	1:A:949:ALA:HB2	1.97	0.46
1:A:471:GLN:NE2	1:A:472:ARG:H	2.13	0.46
1:A:880:LEU:HB2	1:A:930:GLN:O	2.15	0.45
1:A:335:PHE:CD1	1:A:366:MET:HE1	2.51	0.45
1:A:387:GLY:HA2	1:A:697:ILE:CD1	2.35	0.45
1:A:880:LEU:HD11	1:A:932:ARG:HG2	1.98	0.45
1:A:335:PHE:HB3	1:A:366:MET:HE3	1.97	0.45
1:A:380:PHE:O	1:A:479:ARG:HD3	2.17	0.45
1:A:90:LYS:O	1:A:93:ASP:HB2	2.16	0.45
1:A:767:GLN:HB3	1:A:860:VAL:HG11	1.98	0.45
1:A:1194:VAL:HG11	1:A:1237:PRO:HG3	1.99	0.45
2:A:2001:ANP:O5'	2:A:2001:ANP:H8	2.17	0.45
1:A:296:HIS:HD2	1:A:307:GLY:O	2.00	0.45
1:A:813:HIS:CD2	1:A:877:ARG:HD3	2.52	0.45
1:A:437:ILE:HG22	1:A:438:VAL:N	2.32	0.45
1:A:116:ALA:HB1	1:A:119:LEU:HD11	1.98	0.45
1:A:517:SER:C	1:A:519:GLY:N	2.70	0.45
1:A:1134:VAL:HG12	1:A:1135:CYG:N	2.32	0.45
1:A:1222:TYR:CZ	1:A:1245:THR:HG21	2.52	0.45
1:A:1135:CYG:C	1:A:1137:GLY:N	2.81	0.45
1:A:815:LEU:HD12	1:A:815:LEU:N	2.32	0.44
1:A:377:ASN:OD1	1:A:382:ARG:HD2	2.17	0.44
1:A:332:LEU:HD13	1:A:416:GLY:HA2	1.98	0.44
1:A:208:MET:HG3	1:A:509:SER:O	2.16	0.44
1:A:220:LYS:NZ	1:A:220:LYS:HB3	2.32	0.44
1:A:292:LYS:HB3	1:A:315:GLU:OE2	2.18	0.44
1:A:44:ASN:OD1	1:A:45:ALA:N	2.50	0.44
1:A:119:LEU:N	1:A:119:LEU:HD12	2.32	0.44
1:A:421:ARG:NH1	1:A:492:GLY:HA2	2.33	0.44
1:A:297:ASN:OD1	1:A:411:ILE:HA	2.17	0.44
1:A:741:MET:SD	1:A:778:SER:HB2	2.58	0.44
1:A:271:TYR:CZ	1:A:280:TYR:HB3	2.53	0.44
1:A:643:LEU:HD12	1:A:644:PRO:HD2	1.98	0.44
1:A:472:ARG:O	1:A:548:GLN:HG3	2.18	0.44
1:A:342:ILE:HB	1:A:345:PHE:HB3	1.99	0.44
1:A:1043:ALA:HB2	1:A:1085:PHE:CD2	2.53	0.44
1:A:672:PRO:HG3	1:A:1272:TRP:NE1	2.32	0.44
1:A:120:THR:N	1:A:123:GLN:HE21	2.03	0.44
1:A:259:ASN:ND2	1:A:502:ASP:HB3	2.33	0.44
1:A:760:VAL:O	1:A:765:CYS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1155:PRO:CB	1:A:1201:VAL:HG13	2.48	0.44
1:A:1044:VAL:HA	1:A:1089:VAL:HG13	1.99	0.43
1:A:316:ILE:HD13	1:A:380:PHE:CD2	2.53	0.43
1:A:45:ALA:HB1	1:A:46:PRO:HD2	1.99	0.43
1:A:634:ALA:HA	1:A:974:PHE:HE1	1.84	0.43
1:A:376:PHE:CD1	1:A:475:PRO:HG3	2.53	0.43
1:A:631:ILE:H	1:A:631:ILE:CD1	2.29	0.43
1:A:625:ALA:HA	1:A:852:ASP:HB2	2.00	0.43
1:A:298:HIS:HB2	1:A:409:LYS:HE3	2.01	0.43
1:A:120:THR:OG1	1:A:122:GLU:HB2	2.19	0.43
1:A:736:LEU:HG	1:A:802:ILE:CG2	2.49	0.43
1:A:1099:VAL:O	1:A:1100:LEU:HB2	2.19	0.42
1:A:930:GLN:HE21	1:A:930:GLN:HB3	1.63	0.42
1:A:273:ALA:HA	1:A:280:TYR:HA	2.01	0.42
1:A:253:LEU:HB3	1:A:425:VAL:HG11	2.01	0.42
1:A:1192:ILE:HD12	1:A:1283:TRP:CE2	2.53	0.42
1:A:786:GLN:OE1	1:A:786:GLN:HA	2.19	0.42
1:A:437:ILE:HG12	1:A:576:VAL:HG12	2.01	0.42
1:A:658:ARG:O	1:A:664:VAL:HG11	2.19	0.42
1:A:637:VAL:O	1:A:641:LEU:HG	2.20	0.42
1:A:768:LEU:CD2	1:A:864:LYS:HB2	2.49	0.42
1:A:70:PRO:HB3	1:A:113:TYR:CZ	2.54	0.42
1:A:379:GLU:OE2	1:A:475:PRO:HD2	2.19	0.42
1:A:42:ASP:HB2	1:A:150:PHE:CD1	2.55	0.42
1:A:331:GLY:HA2	1:A:416:GLY:HA3	2.02	0.42
1:A:1017:LEU:HD22	1:A:1191:PRO:HB3	2.02	0.42
1:A:114:ILE:HD11	1:A:131:LEU:HD11	2.02	0.42
1:A:154:GLN:HA	1:A:154:GLN:OE1	2.20	0.42
1:A:560:LEU:HA	1:A:560:LEU:HD12	1.85	0.41
1:A:560:LEU:N	1:A:561:PRO:CD	2.83	0.41
1:A:1192:ILE:CG1	1:A:1193:ALA:N	2.83	0.41
1:A:397:ASN:HA	1:A:402:GLU:HA	2.02	0.41
1:A:646:VAL:HG13	1:A:892:VAL:HG11	2.02	0.41
1:A:295:THR:HB	1:A:297:ASN:ND2	2.35	0.41
1:A:333:VAL:O	1:A:387:GLY:HA3	2.19	0.41
1:A:486:ASP:HA	1:A:489:TRP:CD1	2.54	0.41
1:A:11:LEU:HD11	1:A:112:TYR:CE1	2.52	0.41
1:A:228:ILE:HD13	1:A:233:GLN:CG	2.50	0.41
1:A:538:SER:OG	1:A:541:GLU:HG3	2.20	0.41
1:A:1001:CYS:HB3	1:A:1233:TYR:CD2	2.55	0.41
1:A:1081:GLY:HA2	1:A:1119:GLU:OE2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LEU:HD22	1:A:322:THR:HG21	2.01	0.41
1:A:233:GLN:HA	1:A:234:PRO:HD3	1.79	0.41
1:A:838:LEU:HD23	1:A:838:LEU:HA	1.85	0.41
1:A:1102:ALA:HB1	1:A:1139:GLN:OE1	2.21	0.41
1:A:786:GLN:NE2	1:A:791:GLN:HG2	2.35	0.41
1:A:649:LYS:O	1:A:653:VAL:HG23	2.20	0.41
1:A:1146:GLU:HG3	1:A:1147:LEU:HD13	2.02	0.41
1:A:713:ARG:HG2	1:A:764:LEU:HD22	2.01	0.41
1:A:85:SER:O	1:A:88:SER:HB3	2.20	0.41
1:A:1148:ILE:HA	1:A:1149:PRO:HD3	1.85	0.41
1:A:538:SER:O	1:A:542:ILE:HG13	2.20	0.41
1:A:237:LEU:HD23	1:A:240:MET:CE	2.50	0.41
1:A:263:MET:HE1	1:A:806:ALA:HA	2.02	0.41
1:A:303:SER:O	1:A:306:PRO:HD2	2.19	0.41
1:A:365:ILE:HD13	1:A:410:PRO:HG3	2.03	0.41
1:A:882:TRP:CG	1:A:883:HIS:N	2.89	0.41
1:A:1017:LEU:CD2	1:A:1171:LEU:HB2	2.51	0.41
1:A:371:LEU:HD21	1:A:1164:ARG:HD2	2.02	0.41
1:A:356:PRO:HB2	1:A:359:ILE:HG12	2.03	0.41
1:A:703:VAL:HG21	1:A:714:LEU:HD12	2.02	0.41
1:A:727:GLN:OE1	1:A:810:ASP:HB3	2.21	0.40
1:A:776:LYS:HD2	1:A:776:LYS:HA	1.81	0.40
1:A:305:TRP:HB3	1:A:306:PRO:CD	2.44	0.40
1:A:396:VAL:HG11	1:A:705:LEU:HD13	2.02	0.40
1:A:1128:GLN:OE1	1:A:1128:GLN:HA	2.21	0.40
1:A:820:SER:OG	1:A:822:GLU:HG2	2.22	0.40
1:A:505:ALA:C	1:A:507:GLY:H	2.24	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	1280/1303 (98%)	1152 (90%)	116 (9%)	12 (1%)	21 67

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	ALA
1	A	117	SER
1	A	623	GLY
1	A	1053	HIS
1	A	1136	ASN
1	A	467	PHE
1	A	-6	LEU
1	A	836	ASN
1	A	818	GLN
1	A	423	ASP
1	A	492	GLY
1	A	234	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1030/1040 (99%)	965 (94%)	65 (6%)	22 63

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	ARG
1	A	1	MET
1	A	6	ARG
1	A	14	PHE
1	A	24	GLN
1	A	43	LEU
1	A	46	PRO
1	A	60	GLN
1	A	67	SER

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Mol	Chain	Res	Type
1	A	101	GLN
1	A	102	GLN
1	A	118	THR
1	A	125	ARG
1	A	132	HIS
1	A	169	GLN
1	A	175	ASN
1	A	191	GLN
1	A	204	ILE
1	A	218	ARG
1	A	222	PHE
1	A	248	THR
1	A	250	ASP
1	A	253	LEU
1	A	279	ARG
1	A	291	MET
1	A	318	ASP
1	A	332	LEU
1	A	336	SER
1	A	358	ARG
1	A	382	ARG
1	A	396	VAL
1	A	412	MET
1	A	442	PRO
1	A	445	ASN
1	A	467	PHE
1	A	469	SER
1	A	487	ARG
1	A	502	ASP
1	A	521	ARG
1	A	532	SER
1	A	571	ARG
1	A	588	LEU
1	A	597	PRO
1	A	600	LEU
1	A	613	THR
1	A	620	LYS
1	A	624	ASP
1	A	644	PRO
1	A	774	VAL
1	A	776	LYS
1	A	790	GLU

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Mol	Chain	Res	Type
1	A	823	ASP
1	A	846	VAL
1	A	854	PRO
1	A	930	GLN
1	A	950	ASP
1	A	1029	ILE
1	A	1033	TYR
1	A	1066	ASP
1	A	1117	ARG
1	A	1183	GLN
1	A	1190	MET
1	A	1203	VAL
1	A	1245	THR
1	A	1279	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	31	HIS
1	A	39	HIS
1	A	52	GLN
1	A	96	HIS
1	A	123	GLN
1	A	175	ASN
1	A	219	HIS
1	A	259	ASN
1	A	296	HIS
1	A	339	ASN
1	A	408	HIS
1	A	419	ASN
1	A	426	GLN
1	A	445	ASN
1	A	471	GLN
1	A	501	HIS
1	A	545	ASN
1	A	548	GLN
1	A	559	GLN
1	A	589	HIS
1	A	627	ASN
1	A	739	ASN
1	A	824	ASN

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Mol	Chain	Res	Type
1	A	1004	GLN
1	A	1018	ASN
1	A	1026	ASN
1	A	1125	HIS
1	A	1143	ASN
1	A	1176	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	CYG	A	1135	1	10,14,15	0.66	0	6,17,19	6.83	4 (66%)

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
1	CYG	A	1135	1	-	0/10/16/18	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1135	CYG	OE2-CD1-CG1	-12.95	115.02	123.94
1	A	1135	CYG	O-C-CA	-5.19	111.97	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1135	CYG	CB1-CG1-CD1	-3.23	108.34	113.12
1	A	1135	CYG	CG1-CD1-SG	8.54	121.03	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1135	CYG	8	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ANP	A	2001	-	27,33,33	6.11	10 (37%)	30,52,52	4.27	10 (33%)
5	SO4	A	2002	-	4,4,4	0.62	0	6,6,6	0.20	0
3	ADP	A	2005	4	22,29,29	2.29	4 (18%)	27,45,45	2.01	6 (22%)
5	SO4	A	2009	-	4,4,4	0.62	0	6,6,6	0.20	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
2	ANP	A	2001	-	-	0/12/38/38	0/3/3/3
5	SO4	A	2002	-	-	0/0/0/0	0/0/0/0
3	ADP	A	2005	4	-	0/12/32/32	0/3/3/3
5	SO4	A	2009	-	-	0/0/0/0	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2005	ADP	O4'-C4'	-7.67	1.27	1.45
3	A	2005	ADP	O3'-C3'	-4.89	1.31	1.43
3	A	2005	ADP	C6-N6	-2.19	1.28	1.34
3	A	2005	ADP	PB-O2B	-2.12	1.47	1.54
2	A	2001	ANP	C4-N3	2.17	1.38	1.35
2	A	2001	ANP	C2-N1	2.38	1.38	1.33
2	A	2001	ANP	O4'-C1'	2.90	1.44	1.41
2	A	2001	ANP	C2-N3	2.99	1.37	1.32
2	A	2001	ANP	C5'-C4'	3.10	1.61	1.51
2	A	2001	ANP	PG-O3G	4.08	1.68	1.56
2	A	2001	ANP	PA-O1A	4.85	1.68	1.51
2	A	2001	ANP	PB-O3A	11.87	1.73	1.59
2	A	2001	ANP	PB-O1B	18.36	1.67	1.46
2	A	2001	ANP	PG-O1G	20.94	1.70	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	ANP	O1B-PB-N3B	-11.95	93.57	111.90
2	A	2001	ANP	N3-C2-N1	-7.41	123.22	128.89
2	A	2001	ANP	O5'-PA-O1A	-7.23	81.54	109.62
3	A	2005	ADP	N3-C2-N1	-6.77	123.71	128.89
2	A	2001	ANP	PA-O3A-PB	-3.65	120.44	132.67
2	A	2001	ANP	C5'-C4'-C3'	-2.37	105.82	115.21
3	A	2005	ADP	O2B-PB-O1B	2.00	117.03	110.58
3	A	2005	ADP	O4'-C4'-C5'	2.06	116.67	109.32
3	A	2005	ADP	C4-C5-N7	2.46	111.74	109.48
2	A	2001	ANP	C4-C5-N7	2.73	111.99	109.48
2	A	2001	ANP	O2B-PB-O3A	3.17	119.47	105.09
3	A	2005	ADP	C2-N1-C6	3.38	124.80	118.77
3	A	2005	ADP	C4'-O4'-C1'	4.08	114.20	109.72
2	A	2001	ANP	O3A-PB-N3B	4.27	118.19	106.44
2	A	2001	ANP	O5'-C5'-C4'	5.36	128.87	109.12
2	A	2001	ANP	O3A-PA-O5'	13.66	139.18	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	ANP	3	0
5	A	2009	SO4	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1284/1303 (98%)	-0.62	6 (0%) 91 87	11, 28, 52, 95	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-4	PRO	5.3
1	A	466	ASP	4.4
1	A	-2	GLY	2.5
1	A	610	PRO	2.4
1	A	-5	VAL	2.4
1	A	117	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	CYG	A	1135	15/16	0.95	0.17	-	43,45,46,48	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	MG	A	2006	1/1	0.86	0.26	5.85	30,30,30,30	0
3	ADP	A	2005	27/27	0.92	0.28	5.69	30,30,30,30	18
4	MG	A	2008	1/1	0.95	0.19	3.08	30,30,30,30	0
2	ANP	A	2001	31/31	0.93	0.21	1.21	30,30,30,30	0
5	SO4	A	2002	5/5	0.96	0.13	-0.98	30,30,30,30	0
5	SO4	A	2009	5/5	0.77	0.59	-	30,30,30,30	0
4	MG	A	2007	1/1	0.95	0.39	-	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.