Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2021 – 09:25 PM EDT

PDB ID	:	3HB9
Title	:	Crystal Structure of S. aureus Pyruvate Carboxylase A610T Mutant
Authors	:	Tong, L.; Yu, L.P.C.
Deposited on	:	2009-05-04
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

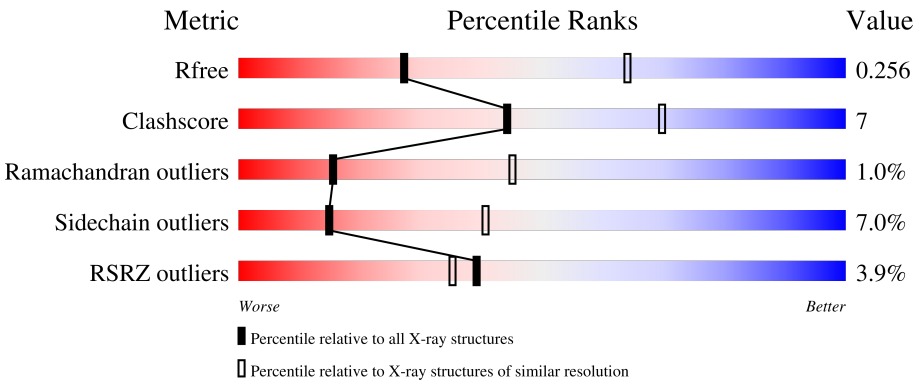
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1150	4% 79% 17% • •
1	B	1150	4% 75% 16% • 7%
1	C	1150	3% 74% 16% • 7%
1	D	1150	3% 70% 14% • 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 33840 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.

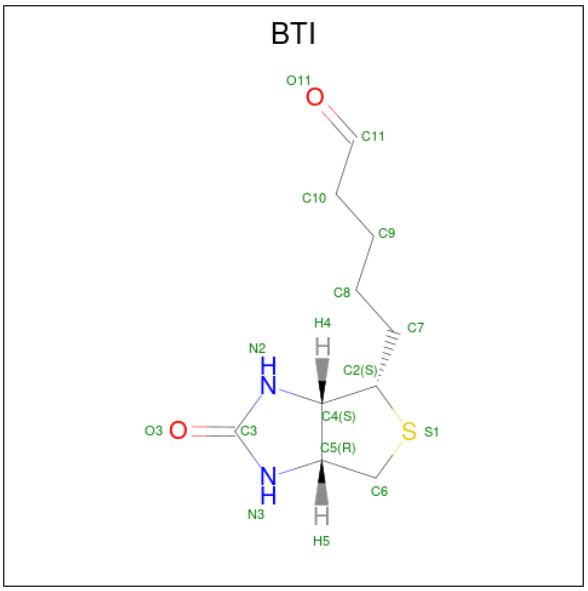
- Molecule 1 is a protein called Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1133	8942	5665	1505	1742	30	0	0	0
1	B	1074	8467	5366	1427	1645	29	0	0	0
1	C	1067	8443	5351	1421	1641	30	0	0	0
1	D	993	7870	4995	1326	1521	28	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

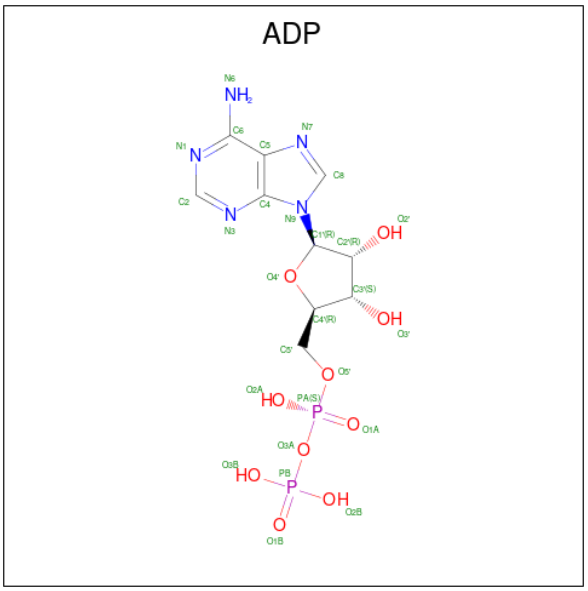
Chain	Residue	Modelled	Actual	Comment	Reference
A	610	THR	ALA	engineered mutation	UNP Q99UY8
B	610	THR	ALA	engineered mutation	UNP Q99UY8
C	610	THR	ALA	engineered mutation	UNP Q99UY8
D	610	THR	ALA	engineered mutation	UNP Q99UY8

- Molecule 2 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: $C_{10}H_{16}N_2O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	15	10	2	2	1	0	0
			Total	C	N	O	S		
2	B	1	15	10	2	2	1	0	0
			Total	C	N	O	S		
2	C	1	15	10	2	2	1	0	0
			Total	C	N	O	S		
2	C	1	15	10	2	2	1	0	0

- 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
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	C	1	27	10	5	10	2	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

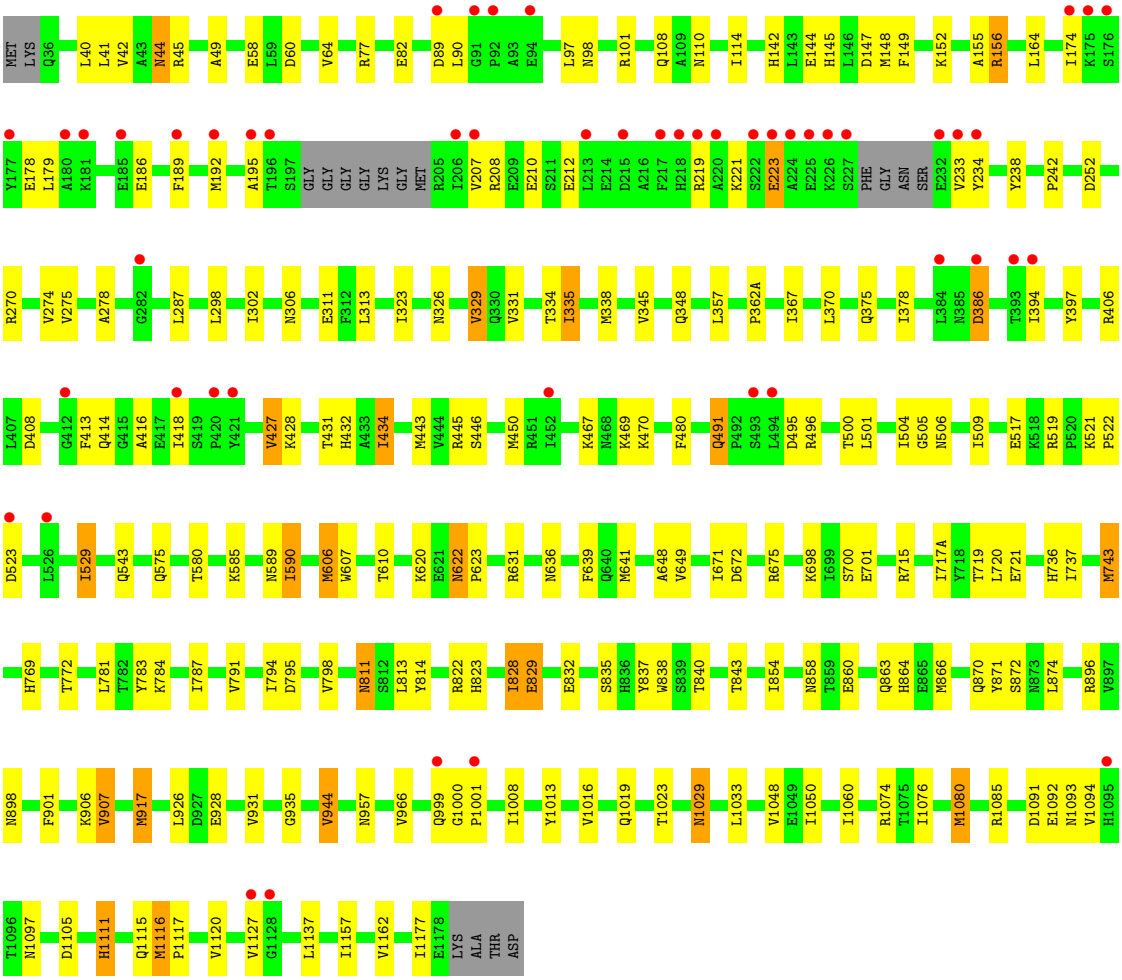
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
4	A	1	1	1	0	0
			Total	Mn		
4	B	1	1	1	0	0
			Total	Mn		
4	C	1	1	1	0	0
			Total	Mn		
4	D	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

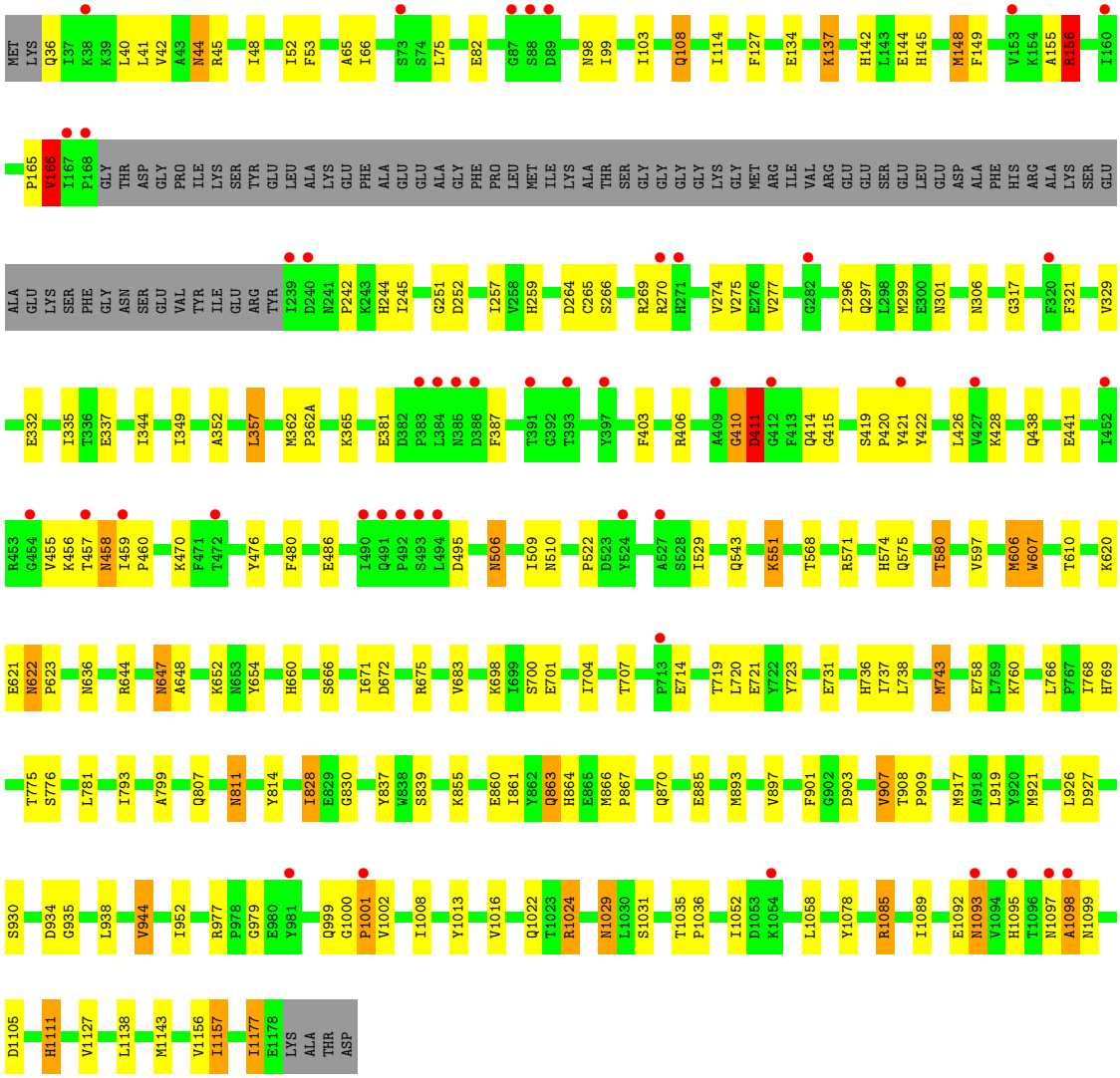
• Molecule 1: Pyruvate carboxylase

Chain A:



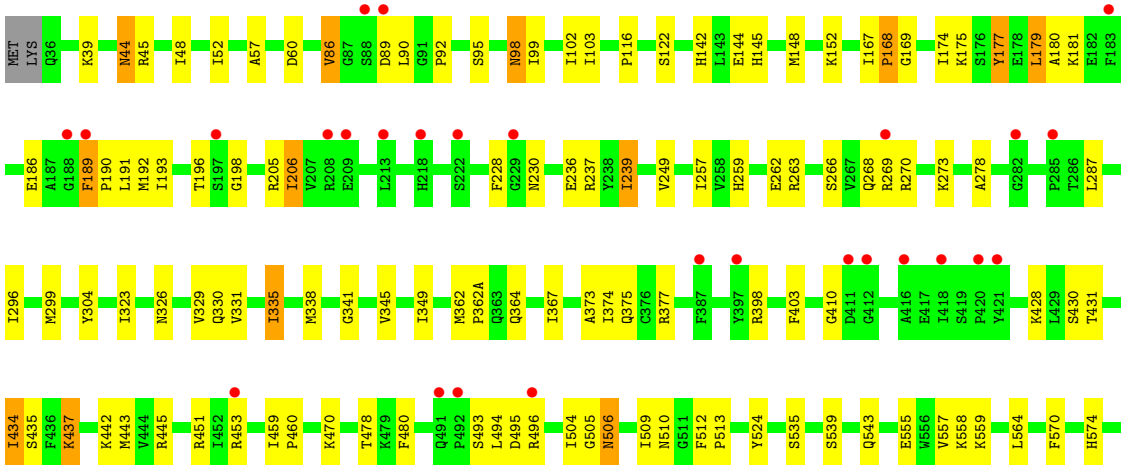
• Molecule 1: Pyruvate carboxylase

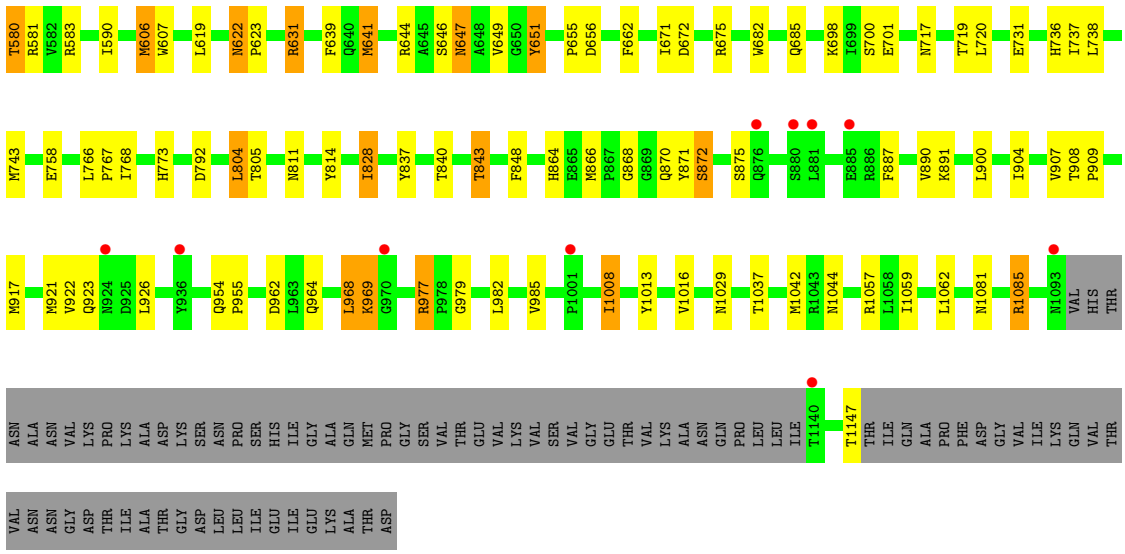
Chain B:



- Molecule 1: Pyruvate carboxylase

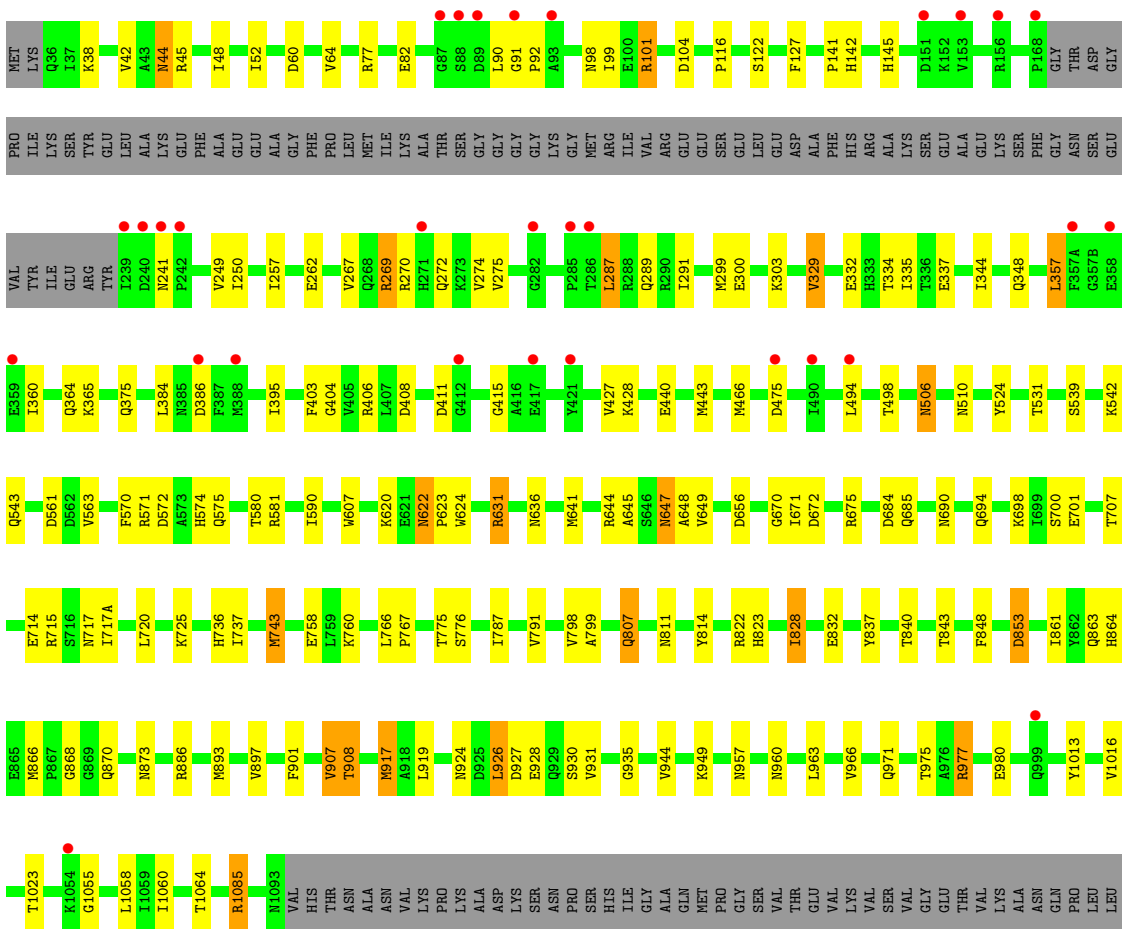
Chain C:

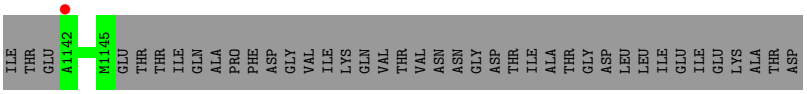




- Molecule 1: Pyruvate carboxylase

Chain D:




ILE
THR
GLU
A1142
M1145
GLU
THR
THR
ILE
GLN
ALA
PRO
PHE
ASP
GLY
VAL
ILE
LYS
GLN
VAL
THR
VAL
ASN
ASN
GLY
ASP
THR
ILE
ALA
THR
GLY
ASP
LEU
LEU
ILE
GLU
ILE
GLU
LYS
ALA
THR
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.57Å 256.76Å 126.48Å 90.00° 109.65° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.58 – 2.82	Depositor EDS
% Data completeness (in resolution range)	92.8 (30.00-2.90) 90.1 (29.58-2.82)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.266 0.213 , 0.256	Depositor DCC
R_{free} test set	6262 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	51.8	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 30.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	33840	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MN, BTI

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	0.34	0/9110	0.50	0/12324
1	B	0.33	0/8627	0.49	0/11678
1	C	0.33	0/8605	0.49	0/11630
1	D	0.33	0/8021	0.50	0/10848
All	All	0.33	0/34363	0.49	0/46480

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8942	0	8872	118	0
1	B	8467	0	8413	115	0
1	C	8443	0	8352	118	0
1	D	7870	0	7808	102	0
2	A	15	0	15	1	0
2	B	15	0	15	1	0
2	C	30	0	31	1	0
3	A	27	0	12	0	0
3	C	27	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	33840	0	33530	444	0

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

All (444) 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:B:1024:ARG:HG3	1:B:1024:ARG:HH11	1.13	1.14
1:D:1085:ARG:HG2	1:D:1085:ARG:HH11	1.21	1.05
1:C:44:ASN:HD22	1:C:45:ARG:H	1.00	0.99
1:B:1000:GLY:H	1:B:1001:PRO:HD3	1.28	0.94
1:C:700:SER:H	1:C:736:HIS:HD2	1.16	0.94
1:A:44:ASN:HD22	1:A:45:ARG:H	1.13	0.93
1:B:1024:ARG:HG3	1:B:1024:ARG:NH1	1.90	0.85
1:D:44:ASN:HD22	1:D:45:ARG:H	1.24	0.84
1:A:700:SER:H	1:A:736:HIS:HD2	1.27	0.82
1:D:644:ARG:HH21	1:D:908:THR:HB	1.44	0.81
1:B:700:SER:H	1:B:736:HIS:HD2	1.25	0.81
1:D:700:SER:H	1:D:736:HIS:HD2	1.28	0.81
1:D:101:ARG:HG2	1:D:101:ARG:HH21	1.46	0.81
1:A:329:VAL:HG22	1:A:348:GLN:HE22	1.47	0.79
1:A:590:ILE:HG12	1:A:837:TYR:CE2	2.18	0.78
1:B:644:ARG:HH11	1:B:647:ASN:HD21	1.32	0.77
1:B:410:GLY:O	1:B:411:ASP:HB2	1.83	0.77
1:C:98:ASN:O	1:C:102:ILE:HG12	1.86	0.76
1:A:811:ASN:HD22	1:A:811:ASN:H	1.31	0.76
1:B:917:MET:HG2	1:B:944:VAL:HG11	1.66	0.76
1:C:700:SER:H	1:C:736:HIS:CD2	2.03	0.76
1:B:1024:ARG:HH11	1:B:1024:ARG:CG	1.94	0.76
1:A:864:HIS:HD2	1:A:866:MET:H	1.34	0.75
1:A:164:LEU:HD11	1:A:298:LEU:HB2	1.68	0.74
1:A:1115:GLN:CD	1:A:1115:GLN:H	1.92	0.73
1:B:48:ILE:O	1:B:52:ILE:HG12	1.89	0.73
1:B:44:ASN:HD22	1:B:45:ARG:H	1.35	0.72
1:C:44:ASN:ND2	1:C:45:ARG:H	1.82	0.72
1:D:743:MET:HG3	1:D:907:VAL:HG13	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ARG:HE	1:B:166:VAL:HG21	1.53	0.71
1:B:551:LYS:HD3	1:B:551:LYS:H	1.54	0.71
1:B:644:ARG:HD2	1:B:647:ASN:HD21	1.52	0.71
1:D:644:ARG:HH11	1:D:647:ASN:HD21	1.38	0.71
1:D:720:LEU:HD21	1:D:758:GLU:HG3	1.71	0.71
1:A:335:ILE:HD13	1:A:375:GLN:HB2	1.74	0.70
1:C:590:ILE:HG12	1:C:837:TYR:CE2	2.27	0.70
1:A:999:GLN:HG2	1:A:1001:PRO:HD2	1.74	0.69
1:D:864:HIS:HD2	1:D:866:MET:H	1.40	0.69
1:C:672:ASP:HA	1:C:698:LYS:HD2	1.74	0.69
1:D:776:SER:HB3	1:D:861:ILE:HD11	1.73	0.69
1:C:48:ILE:O	1:C:52:ILE:HG12	1.91	0.69
1:D:48:ILE:O	1:D:52:ILE:HG12	1.92	0.69
1:B:811:ASN:H	1:B:811:ASN:HD22	1.40	0.69
1:B:1000:GLY:N	1:B:1001:PRO:HD3	2.06	0.68
1:D:917:MET:HG2	1:D:944:VAL:HG21	1.76	0.68
1:D:44:ASN:HD22	1:D:45:ARG:N	1.91	0.68
1:B:458:ASN:HD22	1:B:458:ASN:H	1.42	0.66
1:D:90:LEU:HD11	1:D:98:ASN:HD22	1.59	0.66
1:C:864:HIS:HD2	1:C:866:MET:H	1.43	0.66
1:D:644:ARG:NH2	1:D:908:THR:HB	2.10	0.66
1:D:1085:ARG:HH11	1:D:1085:ARG:CG	2.05	0.66
1:A:44:ASN:ND2	1:A:45:ARG:H	1.90	0.65
1:A:898:ASN:ND2	1:A:906:LYS:HE3	2.11	0.65
1:A:701:GLU:HG2	1:A:737:ILE:HB	1.78	0.65
1:A:144:GLU:O	1:A:148:MET:HB2	1.98	0.64
1:A:491:GLN:H	1:A:491:GLN:HE21	1.45	0.64
1:B:142:HIS:H	1:B:145:HIS:HD2	1.46	0.64
1:B:864:HIS:HD2	1:B:866:MET:H	1.47	0.63
1:C:326:ASN:HD22	1:C:330:GLN:NE2	1.97	0.63
1:D:1085:ARG:HG2	1:D:1085:ARG:NH1	2.01	0.63
1:C:641:MET:HG2	1:C:671:ILE:HG21	1.81	0.62
1:A:313:LEU:HD13	1:A:323:ILE:HG13	1.81	0.62
1:B:672:ASP:HA	1:B:698:LYS:HD2	1.82	0.62
1:A:620:LYS:HG2	1:A:1023:THR:HG21	1.81	0.62
1:A:901:PHE:HZ	1:A:917:MET:HG3	1.65	0.62
1:D:269:ARG:HD2	1:D:270:ARG:HG3	1.82	0.62
1:C:574:HIS:HD2	1:C:580:THR:HA	1.65	0.61
1:A:935:GLY:HA3	1:A:966:VAL:HG13	1.82	0.61
1:B:675:ARG:HA	1:B:701:GLU:HB2	1.82	0.61
1:B:901:PHE:HZ	1:B:917:MET:HG3	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:ILE:HD11	1:D:344:ILE:HG23	1.83	0.61
1:C:434:ILE:HD13	1:C:434:ILE:H	1.66	0.61
1:D:329:VAL:HG22	1:D:348:GLN:HE22	1.66	0.60
1:D:814:TYR:CE2	1:D:828:ILE:HG12	2.36	0.60
1:B:1105:ASP:H	1:B:1111:HIS:HD2	1.49	0.60
1:D:960:ASN:HD22	1:D:963:LEU:H	1.46	0.60
1:C:814:TYR:CE2	1:C:828:ILE:HG12	2.35	0.60
1:D:935:GLY:HA3	1:D:966:VAL:HG13	1.83	0.60
1:C:335:ILE:HD13	1:C:375:GLN:HB2	1.84	0.60
1:B:644:ARG:HD2	1:B:647:ASN:ND2	2.16	0.59
1:D:337:GLU:HG2	1:D:344:ILE:HG12	1.82	0.59
1:A:64:VAL:HG22	1:A:82:GLU:HB2	1.85	0.59
1:B:1105:ASP:H	1:B:1111:HIS:CD2	2.19	0.59
1:B:337:GLU:HG2	1:B:344:ILE:HG12	1.84	0.59
1:C:403:PHE:O	1:C:442:LYS:HE3	2.03	0.59
1:B:543:GLN:HE22	1:B:636:ASN:HA	1.68	0.59
1:D:901:PHE:HZ	1:D:917:MET:HG3	1.68	0.59
1:D:539:SER:HA	1:D:543:GLN:HG3	1.84	0.59
1:A:145:HIS:HE1	1:A:302:ILE:O	1.85	0.58
1:A:311:GLU:OE1	1:A:326:ASN:ND2	2.36	0.58
1:D:1058:LEU:HD23	1:D:1060:ILE:HD11	1.85	0.58
1:B:743:MET:HG3	1:B:907:VAL:HG13	1.85	0.58
1:C:871:TYR:O	1:C:872:SER:HB2	2.03	0.58
1:A:901:PHE:CZ	1:A:917:MET:HG3	2.38	0.58
1:C:647:ASN:OD1	1:C:647:ASN:N	2.37	0.58
1:C:86:VAL:HG11	1:C:102:ILE:HD13	1.85	0.58
1:B:299:MET:HA	1:B:299:MET:HE2	1.85	0.58
1:C:44:ASN:HD22	1:C:45:ARG:N	1.85	0.58
1:B:1000:GLY:H	1:B:1001:PRO:CD	2.11	0.58
1:D:543:GLN:HE21	1:D:636:ASN:HA	1.67	0.58
1:D:949:LYS:HE3	1:D:971:GLN:OE1	2.04	0.58
1:C:1059:ILE:H	1:C:1081:ASN:HD21	1.52	0.57
1:A:142:HIS:H	1:A:145:HIS:HD2	1.51	0.57
1:B:144:GLU:O	1:B:148:MET:HB3	2.04	0.57
1:A:622:ASN:HD22	1:A:623:PRO:HD2	1.70	0.57
1:A:672:ASP:HA	1:A:698:LYS:HD2	1.86	0.57
1:D:935:GLY:HA3	1:D:966:VAL:CG1	2.35	0.57
1:C:398:ARG:HB3	1:C:451:ARG:HB2	1.85	0.57
1:D:901:PHE:CZ	1:D:917:MET:HG3	2.40	0.57
1:C:656:ASP:OD1	1:C:977:ARG:NH2	2.37	0.57
1:D:590:ILE:HG12	1:D:837:TYR:CE2	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ASP:HB3	1:B:357:LEU:HD23	1.86	0.56
1:B:1095:HIS:HB3	1:B:1098:ALA:HB3	1.85	0.56
1:D:647:ASN:HD22	1:D:647:ASN:C	2.07	0.56
1:A:675:ARG:HA	1:A:701:GLU:HB2	1.87	0.56
1:C:644:ARG:HD2	1:C:647:ASN:OD1	2.04	0.56
1:B:935:GLY:HA2	1:B:938:LEU:HD12	1.86	0.56
1:D:622:ASN:ND2	1:D:624:TRP:H	2.04	0.56
1:A:575:GLN:NE2	1:A:610:THR:H	2.02	0.56
1:B:622:ASN:HD22	1:B:623:PRO:HD2	1.70	0.56
1:D:357:LEU:HA	1:D:360:ILE:HB	1.88	0.56
1:A:606:MET:HE1	1:A:639:PHE:HB3	1.86	0.56
1:A:1105:ASP:H	1:A:1111:HIS:HD2	1.53	0.56
1:C:174:ILE:HG21	1:C:180:ALA:HB2	1.87	0.56
1:D:287:LEU:HD22	1:D:291:ILE:HD11	1.88	0.56
1:D:506:ASN:ND2	1:D:510:ASN:HD22	2.04	0.56
1:D:44:ASN:ND2	1:D:45:ARG:H	2.00	0.55
1:D:101:ARG:HH21	1:D:101:ARG:CG	2.18	0.55
1:A:77:ARG:HH22	1:C:1057:ARG:HD2	1.71	0.55
1:A:446:SER:O	1:A:450:MET:HG2	2.05	0.55
1:C:152:LYS:H	1:C:196:THR:HG23	1.71	0.55
1:C:811:ASN:HD22	1:C:811:ASN:H	1.54	0.55
1:C:871:TYR:O	1:C:872:SER:CB	2.54	0.55
1:B:149:PHE:HA	1:B:155:ALA:HB2	1.88	0.55
1:C:622:ASN:HD22	1:C:623:PRO:HD2	1.70	0.55
1:C:651:TYR:HD1	1:C:651:TYR:H	1.53	0.55
1:D:408:ASP:HB2	1:D:428:LYS:HB3	1.89	0.55
1:D:701:GLU:HG2	1:D:737:ILE:HB	1.89	0.55
1:C:191:LEU:HD23	1:C:237:ARG:HA	1.87	0.54
1:D:675:ARG:HA	1:D:701:GLU:HB2	1.89	0.54
1:B:738:LEU:HD23	1:B:768:ILE:HG12	1.89	0.54
1:B:769:HIS:CD2	1:B:793:ILE:HB	2.42	0.54
1:C:169:GLY:HA2	1:C:236:GLU:HA	1.88	0.54
1:B:41:LEU:HB3	1:B:114:ILE:HG12	1.88	0.54
1:C:606:MET:HE1	1:C:639:PHE:HB3	1.90	0.54
1:C:375:GLN:NE2	1:C:428:LYS:HD3	2.23	0.54
1:C:453:ARG:HH11	1:C:453:ARG:HB2	1.73	0.54
1:A:791:VAL:O	1:A:822:ARG:NH2	2.36	0.54
1:C:338:MET:HE3	1:C:373:ALA:HB1	1.90	0.53
1:C:917:MET:O	1:C:921:MET:HB2	2.07	0.53
1:D:828:ILE:O	1:D:832:GLU:HG2	2.08	0.53
1:C:700:SER:N	1:C:736:HIS:HD2	1.97	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LEU:HD11	1:B:349:ILE:HD12	1.90	0.53
1:D:1013:TYR:HB3	1:D:1016:VAL:HB	1.89	0.53
1:A:811:ASN:H	1:A:811:ASN:ND2	2.02	0.53
1:D:571:ARG:HH11	1:D:575:GLN:NE2	2.06	0.53
1:D:840:THR:O	1:D:843:THR:HB	2.09	0.53
1:D:690:ASN:O	1:D:694:GLN:HG2	2.08	0.53
1:C:655:PRO:HG2	1:C:985:VAL:HG23	1.91	0.52
1:D:561:ASP:O	1:D:822:ARG:HD2	2.10	0.52
1:A:90:LEU:HD12	1:A:98:ASN:HD22	1.74	0.52
1:A:149:PHE:HA	1:A:155:ALA:HB2	1.90	0.52
1:A:278:ALA:HB3	1:A:335:ILE:HG23	1.91	0.52
1:C:494:LEU:HB3	1:C:496:ARG:NH1	2.24	0.52
1:A:345:VAL:O	1:A:348:GLN:HB2	2.10	0.52
1:C:570:PHE:O	1:C:574:HIS:HE1	1.92	0.52
1:A:828:ILE:HD12	1:A:829:GLU:H	1.74	0.52
1:B:1127:VAL:HA	1:B:1157:ILE:HG22	1.91	0.52
1:C:828:ILE:HD12	1:C:828:ILE:H	1.73	0.52
1:A:174:ILE:HD12	1:A:179:LEU:HD11	1.91	0.52
1:B:1052:ILE:HD11	1:B:1058:LEU:HG	1.92	0.52
1:B:1078:TYR:HB2	1:B:1085:ARG:HB3	1.91	0.52
1:C:144:GLU:O	1:C:148:MET:HB2	2.10	0.52
1:A:866:MET:HE2	1:A:870:GLN:HG2	1.91	0.52
1:B:867:PRO:O	1:B:870:GLN:HB2	2.10	0.52
1:B:1177:ILE:HD13	1:B:1177:ILE:N	2.25	0.52
1:C:890:VAL:HG22	1:C:922:VAL:HG21	1.92	0.52
1:B:860:GLU:O	1:B:863:GLN:HG2	2.11	0.51
1:C:539:SER:HA	1:C:543:GLN:HG3	1.92	0.51
1:A:575:GLN:HE22	1:A:610:THR:H	1.58	0.51
1:D:631:ARG:NH2	1:D:672:ASP:OD1	2.43	0.51
1:C:574:HIS:CD2	1:C:580:THR:HA	2.44	0.51
1:B:99:ILE:HG23	1:B:127:PHE:HD1	1.76	0.51
1:B:406:ARG:HD3	1:D:404:GLY:H	1.75	0.51
1:C:871:TYR:HE1	1:C:891:LYS:HD3	1.74	0.51
1:A:606:MET:HE1	1:A:671:ILE:HD13	1.92	0.51
1:C:335:ILE:HD11	1:C:374:ILE:C	2.30	0.51
1:A:274:VAL:HG12	1:A:275:VAL:HG23	1.93	0.51
1:B:1022:GLN:HE21	1:B:1022:GLN:HA	1.75	0.51
1:A:192:MET:HB2	1:A:238:TYR:HB2	1.91	0.51
1:A:717(A):ILE:HG12	1:A:957:ASN:OD1	2.11	0.51
1:D:334:THR:HB	1:D:375:GLN:NE2	2.25	0.51
1:B:814:TYR:CZ	1:B:828:ILE:HG12	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:VAL:HG22	1:D:82:GLU:HB2	1.93	0.51
1:D:977:ARG:HG3	1:D:980:GLU:HG3	1.93	0.51
1:A:207:VAL:HG13	1:A:212:GLU:HB3	1.92	0.51
1:C:505:GLY:O	1:C:509:ILE:HG12	2.10	0.50
1:B:909:PRO:HG2	1:B:952:ILE:HD12	1.93	0.50
1:C:701:GLU:HG2	1:C:737:ILE:HB	1.94	0.50
1:B:266:SER:HB2	1:B:476:TYR:HE2	1.75	0.50
1:B:411:ASP:HB3	1:B:426:LEU:HD23	1.94	0.50
1:B:244:HIS:HD2	1:B:265:CYS:HB2	1.77	0.50
1:C:116:PRO:HB2	1:C:122:SER:HA	1.94	0.50
1:A:329:VAL:HG22	1:A:348:GLN:NE2	2.20	0.50
1:B:381:GLU:HB3	1:B:387:PHE:HA	1.94	0.50
1:B:927:ASP:H	1:B:930:SER:HB2	1.77	0.50
1:B:406:ARG:HD3	1:D:403:PHE:HA	1.94	0.49
1:D:622:ASN:C	1:D:622:ASN:HD22	2.15	0.49
1:D:581:ARG:HG3	1:D:848:PHE:CG	2.47	0.49
1:A:370:LEU:O	1:A:432:HIS:HE1	1.95	0.49
1:B:42:VAL:HG12	1:B:44:ASN:H	1.77	0.49
1:B:720:LEU:HD21	1:B:758:GLU:HG3	1.95	0.49
1:B:1035:THR:HB	1:B:1036:PRO:HD3	1.94	0.49
1:C:1042:MET:HB3	1:C:1062:LEU:HD13	1.94	0.49
1:A:858:ASN:HD21	1:A:860:GLU:HB2	1.77	0.49
1:C:364:GLN:HA	1:C:367:ILE:HD12	1.93	0.49
1:B:652:LYS:HG2	1:B:654:TYR:CZ	2.48	0.49
1:A:313:LEU:HB2	1:A:323:ILE:HD11	1.94	0.49
1:D:622:ASN:HD22	1:D:623:PRO:N	2.11	0.49
1:A:1116:MET:HB2	1:A:1117:PRO:CD	2.43	0.48
1:B:811:ASN:H	1:B:811:ASN:ND2	2.07	0.48
1:C:99:ILE:O	1:C:103:ILE:HG12	2.13	0.48
1:C:583:ARG:HG2	1:C:619:LEU:HD22	1.95	0.48
1:A:335:ILE:HD12	1:A:338:MET:HE2	1.96	0.48
1:A:1013:TYR:HB3	1:A:1016:VAL:HB	1.94	0.48
1:D:99:ILE:HG23	1:D:127:PHE:HD1	1.77	0.48
1:D:811:ASN:H	1:D:811:ASN:HD22	1.61	0.48
1:A:814:TYR:CE2	1:A:828:ILE:HG12	2.48	0.48
1:A:278:ALA:CB	1:A:335:ILE:HG23	2.44	0.48
1:B:1029:ASN:C	1:B:1029:ASN:HD22	2.17	0.48
1:A:413:PHE:HE1	1:A:416:ALA:HB3	1.77	0.48
1:A:434:ILE:HG12	1:C:341:GLY:O	2.13	0.48
1:A:1033:LEU:HD23	1:A:1050:ILE:HD12	1.95	0.48
1:B:1013:TYR:HB3	1:B:1016:VAL:HB	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:572:ASP:HB3	1:D:807:GLN:NE2	2.27	0.48
1:D:672:ASP:HA	1:D:698:LYS:HD2	1.95	0.48
1:A:431:THR:HG21	1:A:443:MET:HA	1.96	0.48
1:A:590:ILE:HD11	1:A:838:TRP:CZ2	2.48	0.48
1:B:266:SER:HB2	1:B:476:TYR:CE2	2.49	0.48
1:D:631:ARG:HG2	1:D:670:GLY:HA3	1.96	0.48
1:A:585:LYS:HE2	1:A:589:ASN:HD21	1.78	0.48
1:A:41:LEU:HB3	1:A:114:ILE:HG12	1.95	0.48
1:B:529:ILE:HG12	1:B:837:TYR:HE1	1.79	0.48
1:A:42:VAL:HG11	1:A:49:ALA:HA	1.96	0.47
1:B:893:MET:O	1:B:897:VAL:HG23	2.14	0.47
1:D:274:VAL:HG12	1:D:275:VAL:HG23	1.96	0.47
1:A:394:ILE:HD11	1:A:418:ILE:HD11	1.95	0.47
1:A:219:ARG:HB3	1:A:223:GLU:HB2	1.95	0.47
1:C:174:ILE:HG23	1:C:179:LEU:HB3	1.96	0.47
1:D:787:ILE:HA	1:D:791:VAL:HG12	1.96	0.47
1:A:470:LYS:HB3	1:A:480:PHE:HE1	1.80	0.47
1:C:331:VAL:HG12	1:C:428:LYS:HE2	1.97	0.47
1:C:606:MET:CE	1:C:639:PHE:HB3	2.45	0.47
1:D:563:VAL:HG21	1:D:787:ILE:HG12	1.96	0.47
1:A:189:PHE:HB3	1:A:208:ARG:HE	1.79	0.47
1:A:743:MET:HG3	1:A:907:VAL:HG13	1.97	0.47
1:C:142:HIS:HB2	1:C:145:HIS:CD2	2.49	0.47
1:C:1059:ILE:H	1:C:1081:ASN:ND2	2.13	0.47
1:A:378:ILE:HB	1:A:427:VAL:HG23	1.97	0.46
1:C:506:ASN:ND2	1:C:510:ASN:HD22	2.12	0.46
1:D:799:ALA:H	1:D:811:ASN:ND2	2.13	0.46
1:A:606:MET:CE	1:A:639:PHE:HB3	2.46	0.46
1:A:866:MET:CE	1:A:870:GLN:HG2	2.45	0.46
1:A:1060:ILE:HG12	1:A:1080:MET:HG2	1.96	0.46
1:C:1085:ARG:CG	1:C:1085:ARG:HH11	2.27	0.46
1:B:799:ALA:H	1:B:811:ASN:ND2	2.13	0.46
1:A:505:GLY:O	1:A:509:ILE:HG12	2.16	0.46
1:C:875:SER:HA	1:C:887:PHE:CE1	2.50	0.46
1:A:620:LYS:HB2	2:B:2000:BTI:H63	1.97	0.46
1:B:506:ASN:ND2	1:B:510:ASN:HD22	2.14	0.46
1:B:606:MET:HE3	1:B:607:TRP:HB2	1.97	0.46
1:B:977:ARG:HG2	1:B:979:GLY:H	1.81	0.46
1:C:263:ARG:HG2	1:C:278:ALA:HB2	1.97	0.46
1:B:666:SER:HB3	1:B:671:ILE:HD13	1.98	0.46
1:A:917:MET:HG2	1:A:944:VAL:HG11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:ILE:HD12	1:D:1085:ARG:HH22	1.81	0.46
1:D:645:ALA:HB1	1:D:685:GLN:O	2.16	0.46
1:A:1127:VAL:HA	1:A:1157:ILE:HG22	1.98	0.46
1:C:675:ARG:HA	1:C:701:GLU:HB2	1.97	0.46
1:A:787:ILE:HA	1:A:791:VAL:HG12	1.97	0.46
2:A:2000:BTI:H63	1:B:620:LYS:CG	2.46	0.46
1:C:167:ILE:HG12	1:C:239:ILE:HD11	1.98	0.46
1:A:896:ARG:HD2	1:A:928:GLU:OE2	2.16	0.45
1:C:682:TRP:CE3	1:C:685:GLN:HG3	2.51	0.45
1:B:731:GLU:HG3	1:B:766:LEU:HD13	1.98	0.45
1:C:1013:TYR:HB3	1:C:1016:VAL:HB	1.99	0.45
1:B:406:ARG:HA	1:B:406:ARG:CZ	2.46	0.45
1:B:701:GLU:HG2	1:B:737:ILE:HB	1.98	0.45
1:D:543:GLN:NE2	1:D:636:ASN:HA	2.31	0.45
1:B:99:ILE:H	1:B:99:ILE:HD12	1.81	0.45
1:B:165:PRO:HG2	1:B:321:PHE:HA	1.99	0.45
1:C:662:PHE:HA	1:C:1008:ILE:HD13	1.98	0.45
1:C:921:MET:HG3	1:C:926:LEU:HD23	1.98	0.45
1:D:275:VAL:HG11	1:D:466:MET:HE1	1.97	0.45
1:A:543:GLN:HE22	1:A:636:ASN:HA	1.81	0.45
1:B:700:SER:H	1:B:736:HIS:CD2	2.17	0.45
1:C:504:ILE:HD12	1:C:1037:THR:HG22	1.99	0.45
1:D:332:GLU:O	1:D:335:ILE:HG22	2.15	0.45
1:A:362(A):PRO:HG2	1:A:367:ILE:HG12	1.98	0.45
1:C:152:LYS:HE3	1:C:198:GLY:H	1.81	0.45
1:A:1120:VAL:HG21	1:A:1162:VAL:HB	1.99	0.45
1:A:811:ASN:ND2	1:A:811:ASN:N	2.65	0.45
1:D:924:ASN:HB2	1:D:926:LEU:HD22	1.97	0.44
1:A:840:THR:O	1:A:843:THR:HB	2.17	0.44
1:B:459:ILE:N	1:B:460:PRO:HD2	2.32	0.44
1:D:927:ASP:HB3	1:D:930:SER:H	1.82	0.44
1:A:521:LYS:HA	1:A:522:PRO:HD3	1.86	0.44
1:A:935:GLY:HA3	1:A:966:VAL:CG1	2.46	0.44
1:D:524:TYR:CD2	1:D:843:THR:HG22	2.52	0.44
1:B:814:TYR:CE2	1:B:828:ILE:HG12	2.52	0.44
1:D:116:PRO:HB2	1:D:122:SER:HA	1.98	0.44
1:D:717(A):ILE:HG13	1:D:957:ASN:OD1	2.17	0.44
1:A:500:THR:O	1:A:504:ILE:HG12	2.17	0.44
1:C:504:ILE:HG21	1:C:1042:MET:CE	2.48	0.44
1:B:53:PHE:CZ	1:B:65:ALA:HB2	2.53	0.44
1:B:251:GLY:O	1:B:306:ASN:N	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:ILE:HG21	1:B:723:TYR:HD2	1.83	0.44
1:B:864:HIS:CD2	1:B:866:MET:HG3	2.52	0.44
1:C:206:ILE:HD13	1:C:206:ILE:H	1.83	0.44
1:B:571:ARG:HH11	1:B:575:GLN:NE2	2.16	0.44
1:C:453:ARG:HB2	1:C:453:ARG:NH1	2.31	0.44
1:D:249:VAL:HG21	1:D:299:MET:HG3	2.00	0.44
1:D:443:MET:HG2	1:D:466:MET:SD	2.58	0.44
1:D:622:ASN:HD22	1:D:623:PRO:CD	2.30	0.44
1:D:622:ASN:HD22	1:D:623:PRO:HD2	1.83	0.44
2:C:2000:BTI:H63	1:D:620:LYS:HB2	2.00	0.44
1:A:828:ILE:O	1:A:832:GLU:HG2	2.18	0.43
1:A:1074:ARG:NH1	1:A:1091:ASP:OD2	2.47	0.43
1:C:459:ILE:HB	1:C:460:PRO:HD3	1.99	0.43
1:B:760:LYS:HG2	1:B:768:ILE:HD12	2.00	0.43
1:C:375:GLN:HG3	1:C:430:SER:OG	2.18	0.43
1:C:435:SER:HB2	1:C:437:LYS:HE3	2.00	0.43
1:D:257:ILE:HD13	1:D:300:GLU:HA	2.00	0.43
1:D:498:THR:OG1	1:D:1085:ARG:NH2	2.50	0.43
1:C:890:VAL:HA	1:C:922:VAL:HG21	2.00	0.43
1:C:964:GLN:O	1:C:968:LEU:HG	2.19	0.43
1:D:494:LEU:HD23	1:D:494:LEU:H	1.83	0.43
1:B:568:THR:OG1	1:B:807:GLN:HG3	2.18	0.43
1:A:719:THR:HG22	1:A:721:GLU:H	1.83	0.43
1:C:89:ASP:HB2	1:C:90:LEU:HD12	2.01	0.43
1:C:249:VAL:HG11	1:C:299:MET:HG3	2.00	0.43
1:C:773:HIS:ND1	1:C:805:THR:O	2.47	0.43
1:D:334:THR:HB	1:D:375:GLN:HE22	1.84	0.43
1:D:620:LYS:HG2	1:D:1023:THR:HG21	2.00	0.43
1:A:331:VAL:HG12	1:A:428:LYS:HD2	2.00	0.43
1:A:406:ARG:HA	1:A:406:ARG:NE	2.34	0.43
1:A:772:THR:HG22	1:A:783:TYR:CZ	2.54	0.43
1:B:621:GLU:HB2	1:B:1031:SER:HB3	2.01	0.43
1:C:259:HIS:HB3	1:C:296:ILE:HD11	2.00	0.43
1:C:437:LYS:H	1:C:437:LYS:HD3	1.83	0.43
1:A:1029:ASN:C	1:A:1029:ASN:HD22	2.22	0.43
1:C:335:ILE:HD11	1:C:374:ILE:O	2.19	0.43
1:C:606:MET:HE1	1:C:671:ILE:HD13	2.00	0.43
1:A:769:HIS:NE2	1:A:795:ASP:OD1	2.52	0.43
1:C:814:TYR:CZ	1:C:828:ILE:HG12	2.54	0.43
1:D:641:MET:HE2	1:D:671:ILE:HG21	2.00	0.43
1:A:811:ASN:HD22	1:A:811:ASN:N	2.08	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:HIS:CD2	1:B:296:ILE:HD11	2.54	0.43
1:B:574:HIS:CD2	1:B:580:THR:HA	2.54	0.43
1:C:558:LYS:HG3	1:C:767:PRO:HG3	2.01	0.43
1:C:840:THR:O	1:C:843:THR:HG22	2.19	0.43
1:A:58:GLU:HG3	1:C:445:ARG:HD3	2.01	0.42
1:A:864:HIS:CD2	1:A:866:MET:HG3	2.54	0.42
1:B:644:ARG:HH11	1:B:647:ASN:ND2	2.10	0.42
1:B:917:MET:O	1:B:921:MET:HB2	2.18	0.42
1:C:512:PHE:HA	1:C:513:PRO:HD2	1.85	0.42
1:C:738:LEU:HD23	1:C:768:ILE:HD12	2.01	0.42
1:D:893:MET:O	1:D:897:VAL:HG23	2.20	0.42
1:A:152:LYS:O	1:A:156:ARG:HB2	2.20	0.42
1:A:641:MET:HE2	1:A:671:ILE:HG21	2.01	0.42
1:A:794:ILE:CD1	1:A:813:LEU:HD21	2.49	0.42
1:C:731:GLU:HG3	1:C:766:LEU:HD13	2.01	0.42
1:C:720:LEU:HD21	1:C:758:GLU:HG3	2.00	0.42
1:A:195:ALA:HA	1:A:233:VAL:HA	2.01	0.42
1:A:854:ILE:HD11	1:A:872:SER:HB2	2.02	0.42
1:B:438:GLN:HA	1:B:441:GLU:HG2	2.00	0.42
1:B:776:SER:HB3	1:B:861:ILE:HD11	2.01	0.42
1:C:470:LYS:HB2	1:C:480:PHE:CE1	2.55	0.42
1:C:979:GLY:HA2	1:C:982:LEU:HD12	2.02	0.42
1:A:252:ASP:HB3	1:A:357:LEU:HG	2.00	0.42
1:A:445:ARG:HD3	1:C:57:ALA:HB1	2.00	0.42
1:B:470:LYS:HB2	1:B:480:PHE:HE1	1.84	0.42
1:C:145:HIS:CE1	1:C:304:TYR:HA	2.55	0.42
1:C:345:VAL:O	1:C:349:ILE:HG12	2.20	0.42
1:C:631:ARG:NH2	1:C:672:ASP:OD1	2.52	0.42
1:D:570:PHE:O	1:D:574:HIS:HE1	2.03	0.42
1:D:631:ARG:HA	1:D:631:ARG:HD3	1.71	0.42
1:A:408:ASP:HB2	1:A:428:LYS:HB3	2.02	0.42
1:B:103:ILE:HG21	1:B:134:GLU:HG3	2.01	0.42
1:B:297:GLN:O	1:B:301:ASN:HB2	2.20	0.42
1:B:458:ASN:H	1:B:458:ASN:ND2	2.12	0.42
1:B:597:VAL:HG22	1:B:830:GLY:HA3	2.02	0.42
1:B:251:GLY:HA3	1:B:257:ILE:HG13	2.02	0.41
1:B:403:PHE:HB2	1:D:406:ARG:NH1	2.34	0.41
1:B:574:HIS:HD2	1:B:580:THR:HA	1.84	0.41
1:B:1022:GLN:HA	1:B:1022:GLN:NE2	2.35	0.41
1:C:954:GLN:HA	1:C:955:PRO:HD3	1.92	0.41
1:D:334:THR:HG23	1:D:406:ARG:NH1	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:737:ILE:HG12	1:D:767:PRO:HG2	2.02	0.41
1:B:274:VAL:HG12	1:B:275:VAL:HG23	2.03	0.41
1:C:555:GLU:HA	1:C:558:LYS:HE3	2.02	0.41
1:B:332:GLU:O	1:B:335:ILE:HG22	2.20	0.41
1:A:529:ILE:HG21	1:A:589:ASN:HB3	2.03	0.41
1:A:1115:GLN:CD	1:A:1115:GLN:N	2.68	0.41
1:C:167:ILE:HA	1:C:168:PRO:HD2	1.83	0.41
1:C:268:GLN:HG2	1:C:273:LYS:HA	2.02	0.41
1:C:431:THR:HG21	1:C:443:MET:HA	2.01	0.41
1:D:853:ASP:OD2	1:D:853:ASP:N	2.53	0.41
1:A:631:ARG:O	1:A:631:ARG:HD3	2.20	0.41
1:B:44:ASN:ND2	1:B:45:ARG:H	2.08	0.41
1:C:557:VAL:HG13	1:C:564:LEU:HD12	2.02	0.41
1:A:719:THR:HG22	1:A:720:LEU:N	2.36	0.41
1:A:798:VAL:CG1	1:A:835:SER:HA	2.50	0.41
1:A:828:ILE:H	1:A:828:ILE:HG13	1.62	0.41
1:C:335:ILE:HD12	1:C:335:ILE:HA	1.78	0.41
1:C:524:TYR:CD2	1:C:843:THR:HG23	2.56	0.41
1:C:908:THR:HA	1:C:909:PRO:HA	1.82	0.41
1:D:101:ARG:CG	1:D:101:ARG:NH2	2.80	0.41
1:A:58:GLU:OE2	1:C:445:ARG:NH1	2.53	0.41
1:A:866:MET:CE	1:A:874:LEU:HD22	2.51	0.41
1:B:82:GLU:HA	1:D:1055:GLY:O	2.21	0.41
1:B:108:GLN:HE21	1:B:108:GLN:HB3	1.72	0.41
1:B:264:ASP:HB3	1:B:277:VAL:HB	2.02	0.41
1:B:362:MET:HA	1:B:362(A):PRO:HD3	1.94	0.41
1:C:266:SER:O	1:C:478:THR:HA	2.21	0.41
1:A:335:ILE:HD12	1:A:335:ILE:HA	1.82	0.40
1:C:362:MET:CE	1:C:362(A):PRO:HD2	2.52	0.40
1:D:828:ILE:H	1:D:828:ILE:HG13	1.59	0.40
1:A:501:LEU:HD21	1:A:1080:MET:HG3	2.03	0.40
1:B:1092:GLU:O	1:B:1093:ASN:C	2.59	0.40
1:C:1085:ARG:CG	1:C:1085:ARG:NH1	2.85	0.40
1:B:509:ILE:HD12	1:B:1089:ILE:HB	2.04	0.40
1:A:174:ILE:HG12	1:A:234:TYR:HA	2.04	0.40
1:A:1105:ASP:H	1:A:1111:HIS:CD2	2.37	0.40
1:B:419:SER:HA	1:B:420:PRO:HD3	1.90	0.40
1:B:1097:ASN:C	1:B:1099:ASN:H	2.25	0.40
1:C:581:ARG:HG3	1:C:848:PHE:CD2	2.56	0.40
1:D:141:PRO:HB2	1:D:145:HIS:HB2	2.02	0.40
1:D:142:HIS:H	1:D:145:HIS:HD2	1.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:656:ASP:OD2	1:D:977:ARG:NH2	2.54	0.40
1:B:137:LYS:HG2	1:B:352:ALA:HB1	2.03	0.40
1:C:269:ARG:HG3	1:C:270:ARG:N	2.36	0.40
1:D:42:VAL:HG21	1:D:52:ILE:HB	2.03	0.40
1:D:590:ILE:H	1:D:590:ILE:HG13	1.79	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	1127/1150 (98%)	1044 (93%)	74 (7%)	9 (1%)	19	51
1	B	1070/1150 (93%)	995 (93%)	60 (6%)	15 (1%)	11	36
1	C	1063/1150 (92%)	983 (92%)	69 (6%)	11 (1%)	15	45
1	D	987/1150 (86%)	928 (94%)	52 (5%)	7 (1%)	22	54
All	All	4247/4600 (92%)	3950 (93%)	255 (6%)	42 (1%)	15	45

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	ASP
1	A	1094	VAL
1	B	522	PRO
1	B	1001	PRO
1	B	1093	ASN
1	C	804	LEU
1	C	872	SER
1	D	870	GLN
1	A	397	TYR
1	A	648	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	411	ASP
1	B	415	GLY
1	C	92	PRO
1	C	168	PRO
1	C	868	GLY
1	C	969	LYS
1	D	364	GLN
1	D	868	GLY
1	A	178	GLU
1	A	1093	ASN
1	B	156	ARG
1	B	648	ALA
1	C	177	TYR
1	C	189	PHE
1	C	410	GLY
1	D	648	ALA
1	B	166	VAL
1	B	269	ARG
1	B	1098	ALA
1	C	493	SER
1	D	92	PRO
1	B	903	ASP
1	B	1002	VAL
1	A	210	GLU
1	A	242	PRO
1	B	270	ARG
1	B	410	GLY
1	A	1000	GLY
1	C	190	PRO
1	D	415	GLY
1	B	317	GLY
1	D	91	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	978/988 (99%)	911 (93%)	67 (7%)	15	41
1	B	929/988 (94%)	863 (93%)	66 (7%)	14	40
1	C	918/988 (93%)	855 (93%)	63 (7%)	15	41
1	D	860/988 (87%)	799 (93%)	61 (7%)	14	40
All	All	3685/3952 (93%)	3428 (93%)	257 (7%)	15	41

All (257) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	44	ASN
1	A	60	ASP
1	A	89	ASP
1	A	97	LEU
1	A	101	ARG
1	A	108	GLN
1	A	110	ASN
1	A	147	ASP
1	A	156	ARG
1	A	186	GLU
1	A	221	LYS
1	A	223	GLU
1	A	270	ARG
1	A	287	LEU
1	A	306	ASN
1	A	329	VAL
1	A	334	THR
1	A	335	ILE
1	A	386	ASP
1	A	414	GLN
1	A	427	VAL
1	A	434	ILE
1	A	467	LYS
1	A	469	LYS
1	A	491	GLN
1	A	495	ASP
1	A	496	ARG
1	A	506	ASN
1	A	517	GLU
1	A	519	ARG
1	A	523	ASP
1	A	529	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	580	THR
1	A	590	ILE
1	A	606	MET
1	A	607	TRP
1	A	622	ASN
1	A	649	VAL
1	A	715	ARG
1	A	743	MET
1	A	781	LEU
1	A	784	LYS
1	A	811	ASN
1	A	823	HIS
1	A	828	ILE
1	A	829	GLU
1	A	863	GLN
1	A	871	TYR
1	A	907	VAL
1	A	917	MET
1	A	926	LEU
1	A	931	VAL
1	A	944	VAL
1	A	1008	ILE
1	A	1019	GLN
1	A	1029	ASN
1	A	1048	VAL
1	A	1076	ILE
1	A	1080	MET
1	A	1085	ARG
1	A	1092	GLU
1	A	1097	ASN
1	A	1111	HIS
1	A	1116	MET
1	A	1137	LEU
1	A	1177	ILE
1	B	36	GLN
1	B	44	ASN
1	B	66	ILE
1	B	75	LEU
1	B	98	ASN
1	B	108	GLN
1	B	137	LYS
1	B	148	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	156	ARG
1	B	166	VAL
1	B	242	PRO
1	B	245	ILE
1	B	329	VAL
1	B	357	LEU
1	B	365	LYS
1	B	411	ASP
1	B	414	GLN
1	B	421	TYR
1	B	422	TYR
1	B	428	LYS
1	B	455	VAL
1	B	456	LYS
1	B	457	THR
1	B	458	ASN
1	B	486	GLU
1	B	495	ASP
1	B	506	ASN
1	B	551	LYS
1	B	580	THR
1	B	606	MET
1	B	607	TRP
1	B	610	THR
1	B	622	ASN
1	B	647	ASN
1	B	660	HIS
1	B	683	VAL
1	B	707	THR
1	B	714	GLU
1	B	719	THR
1	B	721	GLU
1	B	743	MET
1	B	775	THR
1	B	781	LEU
1	B	811	ASN
1	B	828	ILE
1	B	839	SER
1	B	855	LYS
1	B	863	GLN
1	B	885	GLU
1	B	907	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	908	THR
1	B	919	LEU
1	B	926	LEU
1	B	934	ASP
1	B	944	VAL
1	B	999	GLN
1	B	1008	ILE
1	B	1024	ARG
1	B	1029	ASN
1	B	1085	ARG
1	B	1111	HIS
1	B	1138	LEU
1	B	1143	MET
1	B	1156	VAL
1	B	1157	ILE
1	B	1177	ILE
1	C	39	LYS
1	C	44	ASN
1	C	60	ASP
1	C	86	VAL
1	C	95	SER
1	C	98	ASN
1	C	175	LYS
1	C	177	TYR
1	C	179	LEU
1	C	181	LYS
1	C	186	GLU
1	C	189	PHE
1	C	192	MET
1	C	193	ILE
1	C	205	ARG
1	C	206	ILE
1	C	228	PHE
1	C	230	ASN
1	C	239	ILE
1	C	257	ILE
1	C	262	GLU
1	C	287	LEU
1	C	323	ILE
1	C	329	VAL
1	C	335	ILE
1	C	377	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	434	ILE
1	C	437	LYS
1	C	495	ASP
1	C	506	ASN
1	C	535	SER
1	C	559	LYS
1	C	580	THR
1	C	606	MET
1	C	607	TRP
1	C	622	ASN
1	C	631	ARG
1	C	641	MET
1	C	646	SER
1	C	647	ASN
1	C	649	VAL
1	C	651	TYR
1	C	717	ASN
1	C	719	THR
1	C	743	MET
1	C	792	ASP
1	C	804	LEU
1	C	828	ILE
1	C	843	THR
1	C	870	GLN
1	C	900	LEU
1	C	904	ILE
1	C	907	VAL
1	C	923	GLN
1	C	962	ASP
1	C	968	LEU
1	C	969	LYS
1	C	977	ARG
1	C	1008	ILE
1	C	1029	ASN
1	C	1044	ASN
1	C	1085	ARG
1	C	1147	THR
1	D	38	LYS
1	D	44	ASN
1	D	60	ASP
1	D	77	ARG
1	D	101	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	104	ASP
1	D	241	ASN
1	D	262	GLU
1	D	267	VAL
1	D	269	ARG
1	D	272	GLN
1	D	287	LEU
1	D	289	GLN
1	D	303	LYS
1	D	329	VAL
1	D	357	LEU
1	D	365	LYS
1	D	384	LEU
1	D	386	ASP
1	D	411	ASP
1	D	427	VAL
1	D	440	GLU
1	D	475	ASP
1	D	506	ASN
1	D	531	THR
1	D	542	LYS
1	D	580	THR
1	D	607	TRP
1	D	622	ASN
1	D	631	ARG
1	D	647	ASN
1	D	649	VAL
1	D	684	ASP
1	D	707	THR
1	D	714	GLU
1	D	715	ARG
1	D	717	ASN
1	D	725	LYS
1	D	743	MET
1	D	760	LYS
1	D	766	LEU
1	D	775	THR
1	D	798	VAL
1	D	807	GLN
1	D	823	HIS
1	D	828	ILE
1	D	853	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	863	GLN
1	D	873	ASN
1	D	886	ARG
1	D	907	VAL
1	D	908	THR
1	D	917	MET
1	D	919	LEU
1	D	926	LEU
1	D	928	GLU
1	D	931	VAL
1	D	975	THR
1	D	977	ARG
1	D	1064	THR
1	D	1085	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	108	GLN
1	A	145	HIS
1	A	241	ASN
1	A	256	ASN
1	A	432	HIS
1	A	491	GLN
1	A	506	ASN
1	A	543	GLN
1	A	574	HIS
1	A	575	GLN
1	A	589	ASN
1	A	617	ASN
1	A	622	ASN
1	A	736	HIS
1	A	778	ASN
1	A	807	GLN
1	A	811	ASN
1	A	818	ASN
1	A	858	ASN
1	A	864	HIS
1	A	898	ASN
1	A	1005	GLN
1	A	1025	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1029	ASN
1	A	1044	ASN
1	A	1093	ASN
1	A	1099	ASN
1	A	1111	HIS
1	A	1150	GLN
1	B	44	ASN
1	B	69	ASN
1	B	98	ASN
1	B	108	GLN
1	B	126	GLN
1	B	145	HIS
1	B	256	ASN
1	B	364	GLN
1	B	385	ASN
1	B	414	GLN
1	B	432	HIS
1	B	458	ASN
1	B	506	ASN
1	B	543	GLN
1	B	574	HIS
1	B	575	GLN
1	B	589	ASN
1	B	617	ASN
1	B	622	ASN
1	B	647	ASN
1	B	685	GLN
1	B	736	HIS
1	B	773	HIS
1	B	778	ASN
1	B	811	ASN
1	B	818	ASN
1	B	858	ASN
1	B	864	HIS
1	B	876	GLN
1	B	877	GLN
1	B	898	ASN
1	B	923	GLN
1	B	960	ASN
1	B	999	GLN
1	B	1005	GLN
1	B	1022	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1025	ASN
1	B	1026	GLN
1	B	1029	ASN
1	B	1044	ASN
1	B	1111	HIS
1	C	44	ASN
1	C	98	ASN
1	C	145	HIS
1	C	230	ASN
1	C	330	GLN
1	C	375	GLN
1	C	506	ASN
1	C	515	ASN
1	C	574	HIS
1	C	575	GLN
1	C	589	ASN
1	C	622	ASN
1	C	717	ASN
1	C	736	HIS
1	C	778	ASN
1	C	807	GLN
1	C	811	ASN
1	C	858	ASN
1	C	864	HIS
1	C	870	GLN
1	C	873	ASN
1	C	898	ASN
1	C	923	GLN
1	C	971	GLN
1	C	1005	GLN
1	C	1019	GLN
1	C	1025	ASN
1	C	1029	ASN
1	C	1081	ASN
1	D	44	ASN
1	D	272	GLN
1	D	289	GLN
1	D	326	ASN
1	D	330	GLN
1	D	375	GLN
1	D	432	HIS
1	D	506	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	543	GLN
1	D	574	HIS
1	D	575	GLN
1	D	589	ASN
1	D	622	ASN
1	D	647	ASN
1	D	717	ASN
1	D	736	HIS
1	D	778	ASN
1	D	807	GLN
1	D	811	ASN
1	D	858	ASN
1	D	864	HIS
1	D	898	ASN
1	D	960	ASN
1	D	1005	GLN
1	D	1019	GLN
1	D	1025	ASN
1	D	1044	ASN
1	D	1083	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	BTI	A	2000	1	16,16,16	1.69	2 (12%)	21,21,21	2.22	4 (19%)
2	BTI	B	2000	1	16,16,16	1.69	2 (12%)	21,21,21	2.09	4 (19%)
3	ADP	C	2100	-	24,29,29	1.02	1 (4%)	29,45,45	1.34	4 (13%)
3	ADP	A	2100	-	24,29,29	1.01	1 (4%)	29,45,45	1.37	4 (13%)
2	BTI	C	1183	-	16,16,16	1.64	2 (12%)	21,21,21	2.31	5 (23%)
2	BTI	C	2000	1	16,16,16	1.66	2 (12%)	21,21,21	2.14	3 (14%)

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	BTI	A	2000	1	-	3/5/27/27	0/2/2/2
2	BTI	B	2000	1	-	3/5/27/27	0/2/2/2
3	ADP	C	2100	-	-	2/12/32/32	0/3/3/3
3	ADP	A	2100	-	-	2/12/32/32	0/3/3/3
2	BTI	C	1183	-	-	4/5/27/27	0/2/2/2
2	BTI	C	2000	1	-	4/5/27/27	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	BTI	O3-C3	4.83	1.33	1.23
2	B	2000	BTI	O3-C3	4.79	1.33	1.23
2	C	1183	BTI	O3-C3	4.73	1.33	1.23
2	C	2000	BTI	O3-C3	4.58	1.33	1.23
2	B	2000	BTI	C2-S1	-3.73	1.76	1.82
2	C	2000	BTI	C2-S1	-3.57	1.76	1.82
2	A	2000	BTI	C2-S1	-3.55	1.76	1.82
2	C	1183	BTI	C2-S1	-3.39	1.77	1.82
3	A	2100	ADP	C5-C4	2.60	1.47	1.40
3	C	2100	ADP	C5-C4	2.60	1.47	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2000	BTI	C2-C4-N2	-6.91	106.94	113.13
2	C	2000	BTI	C6-C5-N3	-6.29	105.04	113.03
2	C	1183	BTI	C2-C4-N2	-6.06	107.69	113.13
2	B	2000	BTI	C6-C5-N3	-5.91	105.52	113.03
2	C	2000	BTI	C2-C4-N2	-5.72	108.00	113.13
2	C	1183	BTI	C6-C5-N3	-5.45	106.10	113.03
2	A	2000	BTI	C6-C5-N3	-5.43	106.13	113.03
2	B	2000	BTI	C2-C4-N2	-4.08	109.47	113.13
2	C	1183	BTI	C4-C2-S1	3.47	108.51	105.20
3	A	2100	ADP	N3-C2-N1	-3.32	123.48	128.68
3	C	2100	ADP	N3-C2-N1	-3.31	123.50	128.68
3	C	2100	ADP	PA-O3A-PB	-3.30	121.51	132.83
3	A	2100	ADP	PA-O3A-PB	-3.25	121.67	132.83
2	B	2000	BTI	C5-C6-S1	3.07	108.94	106.31
2	C	1183	BTI	N2-C3-N3	2.89	111.47	108.76
2	B	2000	BTI	N2-C3-N3	2.82	111.41	108.76
3	A	2100	ADP	C4-C5-N7	-2.75	106.54	109.40
3	C	2100	ADP	C4-C5-N7	-2.71	106.57	109.40
3	A	2100	ADP	C3'-C2'-C1'	2.65	104.96	100.98
2	C	2000	BTI	N2-C3-N3	2.50	111.11	108.76
2	A	2000	BTI	N2-C3-N3	2.41	111.03	108.76
2	C	1183	BTI	C8-C7-C2	-2.37	109.06	113.86
2	A	2000	BTI	C4-C2-S1	2.33	107.42	105.20
3	C	2100	ADP	C3'-C2'-C1'	2.02	104.02	100.98

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2000	BTI	C11-C10-C9-C8
2	A	2000	BTI	S1-C2-C7-C8
2	A	2000	BTI	C4-C2-C7-C8
2	B	2000	BTI	S1-C2-C7-C8
2	B	2000	BTI	C4-C2-C7-C8
2	C	2000	BTI	C11-C10-C9-C8
2	C	2000	BTI	S1-C2-C7-C8
2	C	2000	BTI	C4-C2-C7-C8
2	C	1183	BTI	C11-C10-C9-C8
2	C	1183	BTI	S1-C2-C7-C8
2	C	1183	BTI	C4-C2-C7-C8
2	C	1183	BTI	C7-C8-C9-C10
3	A	2100	ADP	O4'-C4'-C5'-O5'
3	A	2100	ADP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	2000	BTI	C7-C8-C9-C10
2	C	2000	BTI	C7-C8-C9-C10
3	C	2100	ADP	O4'-C4'-C5'-O5'
3	C	2100	ADP	C3'-C4'-C5'-O5'

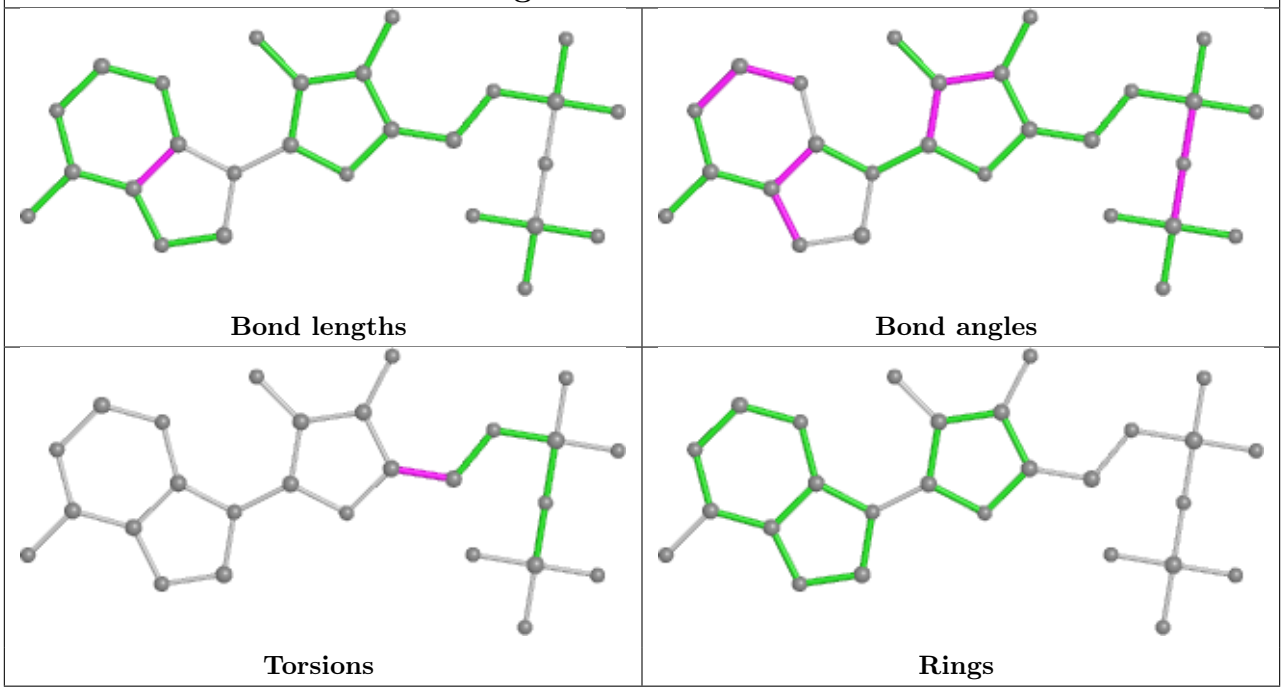
There are no ring outliers.

3 monomers are involved in 3 short contacts:

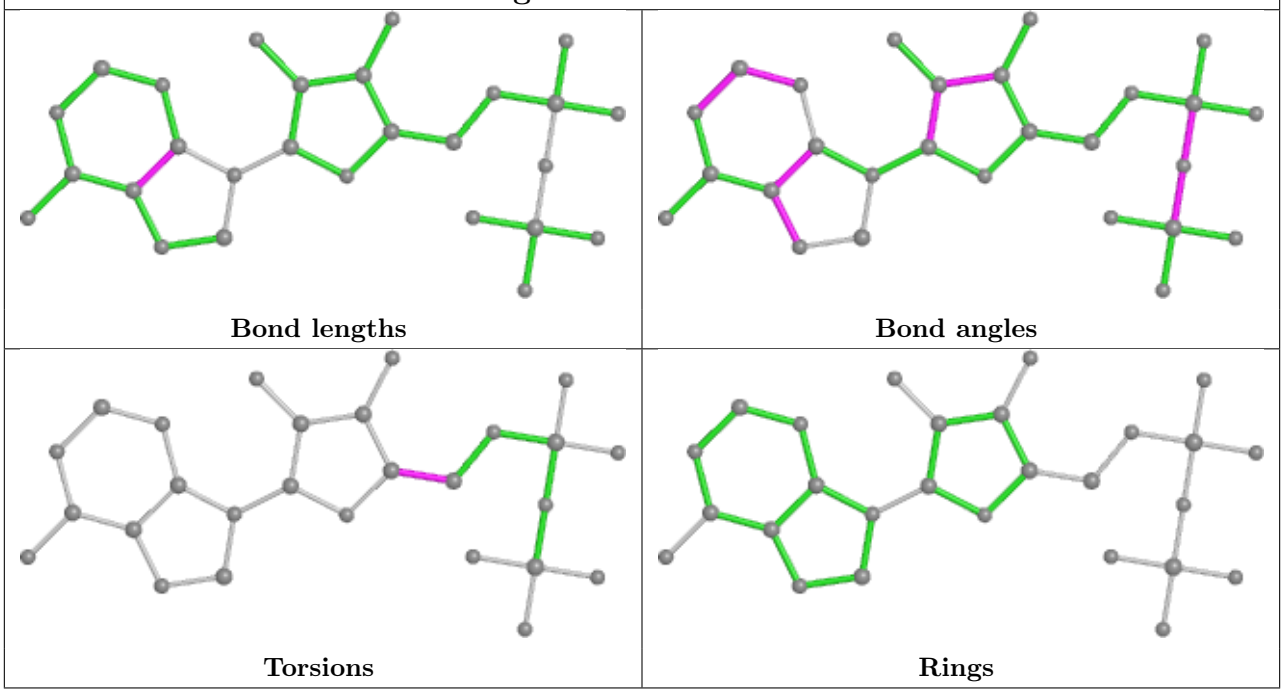
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2000	BTI	1	0
2	B	2000	BTI	1	0
2	C	2000	BTI	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP C 2100



Ligand ADP A 2100



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1133/1150 (98%)	-0.10	51 (4%)	33	29	19, 45, 109, 169	0
1	B	1074/1150 (93%)	0.08	46 (4%)	35	31	29, 60, 127, 178	0
1	C	1067/1150 (92%)	-0.02	37 (3%)	44	38	29, 61, 102, 147	0
1	D	993/1150 (86%)	-0.10	31 (3%)	49	44	17, 44, 138, 192	0
All	All	4267/4600 (92%)	-0.04	165 (3%)	39	35	17, 55, 121, 192	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	492	PRO	8.9
1	B	240	ASP	6.6
1	D	490	ILE	6.5
1	D	494	LEU	5.8
1	C	421	TYR	5.4
1	A	177	TYR	5.3
1	B	490	ILE	5.2
1	D	1142	ALA	5.2
1	A	185	GLU	5.0
1	A	181	LYS	5.0
1	D	168	PRO	5.0
1	D	239	ILE	5.0
1	B	493	SER	4.8
1	B	491	GLN	4.8
1	D	88	SER	4.7
1	A	421	TYR	4.7
1	B	88	SER	4.7
1	A	195	ALA	4.7
1	B	1095	HIS	4.6
1	A	206	ILE	4.5
1	A	226	LYS	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	233	VAL	4.3
1	C	491	GLN	4.1
1	A	999	GLN	4.1
1	A	215	ASP	4.1
1	B	89	ASP	4.0
1	A	232	GLU	4.0
1	B	421	TYR	3.9
1	C	1140	THR	3.9
1	B	452	ILE	3.8
1	A	224	ALA	3.8
1	B	494	LEU	3.8
1	A	1001	PRO	3.7
1	A	227	SER	3.7
1	A	282	GLY	3.6
1	A	196	THR	3.6
1	D	282	GLY	3.6
1	B	524	TYR	3.5
1	A	220	ALA	3.5
1	D	417	GLU	3.5
1	C	218	HIS	3.5
1	D	87	GLY	3.4
1	B	271	HIS	3.4
1	B	459	ILE	3.4
1	C	229	GLY	3.4
1	B	239	ILE	3.4
1	B	713	PRO	3.4
1	D	412	GLY	3.4
1	C	222	SER	3.4
1	B	397	TYR	3.4
1	D	421	TYR	3.4
1	D	89	ASP	3.3
1	B	38	LYS	3.3
1	B	527	ALA	3.3
1	C	412	GLY	3.3
1	C	492	PRO	3.3
1	B	160	ILE	3.3
1	A	189	PHE	3.2
1	B	168	PRO	3.2
1	A	219	ARG	3.2
1	C	880	SER	3.2
1	C	197	SER	3.1
1	B	87	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	208	ARG	3.1
1	C	209	GLU	3.1
1	C	213	LEU	3.1
1	A	384	LEU	3.1
1	A	222	SER	3.1
1	D	386	ASP	3.1
1	D	241	ASN	3.1
1	D	271	HIS	3.0
1	C	416	ALA	3.0
1	B	1054	LYS	3.0
1	A	180	ALA	3.0
1	A	494	LEU	3.0
1	B	282	GLY	3.0
1	C	188	GLY	3.0
1	A	218	HIS	3.0
1	A	420	PRO	3.0
1	C	420	PRO	3.0
1	B	412	GLY	3.0
1	D	357(A)	PHE	3.0
1	D	153	VAL	3.0
1	C	1093	ASN	2.9
1	A	176	SER	2.9
1	B	270	ARG	2.9
1	A	174	ILE	2.9
1	A	1095	HIS	2.8
1	D	156	ARG	2.8
1	A	386	ASP	2.8
1	D	388	MET	2.7
1	A	213	LEU	2.7
1	A	493	SER	2.7
1	B	384	LEU	2.7
1	A	526	LEU	2.7
1	A	234	TYR	2.7
1	A	393	THR	2.7
1	A	175	LYS	2.7
1	C	183	PHE	2.7
1	C	189	PHE	2.7
1	C	496	ARG	2.7
1	D	358	GLU	2.7
1	B	1001	PRO	2.7
1	C	885	GLU	2.6
1	D	240	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	418	ILE	2.6
1	B	981	TYR	2.5
1	C	397	TYR	2.5
1	B	391	THR	2.5
1	A	1128	GLY	2.5
1	B	454	GLY	2.5
1	D	91	GLY	2.5
1	A	207	VAL	2.5
1	C	1001	PRO	2.4
1	C	411	ASP	2.4
1	A	452	ILE	2.4
1	B	1093	ASN	2.4
1	C	453	ARG	2.4
1	C	936	TYR	2.4
1	A	89	ASP	2.4
1	D	359	GLU	2.4
1	A	225	GLU	2.4
1	B	320	PHE	2.4
1	A	91	GLY	2.3
1	C	88	SER	2.3
1	D	286	THR	2.3
1	D	93	ALA	2.3
1	B	1097	ASN	2.3
1	B	1098	ALA	2.3
1	B	457	THR	2.3
1	C	269	ARG	2.3
1	C	881	LEU	2.3
1	C	387	PHE	2.3
1	B	386	ASP	2.2
1	A	394	ILE	2.2
1	C	418	ILE	2.2
1	D	999	GLN	2.2
1	D	151	ASP	2.2
1	A	412	GLY	2.2
1	C	924	ASN	2.2
1	A	1127	VAL	2.2
1	B	409	ALA	2.2
1	C	282	GLY	2.2
1	B	153	VAL	2.2
1	B	427	VAL	2.1
1	C	970	GLY	2.1
1	B	167	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	285	PRO	2.1
1	A	94	GLU	2.1
1	A	217	PHE	2.1
1	C	89	ASP	2.1
1	A	192	MET	2.1
1	B	73	SER	2.1
1	C	876	GLN	2.1
1	D	242	PRO	2.1
1	B	472	THR	2.1
1	C	285	PRO	2.1
1	D	1054	LYS	2.1
1	A	523	ASP	2.0
1	B	393	THR	2.0
1	A	223	GLU	2.0
1	A	92	PRO	2.0
1	B	385	ASN	2.0
1	D	475	ASP	2.0
1	B	383	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	A	2100	27/27	0.88	0.20	99,100,103,103	0
4	MN	A	2002	1/1	0.91	0.13	63,63,63,63	0
3	ADP	C	2100	27/27	0.93	0.17	78,78,78,79	0
4	MN	B	2002	1/1	0.94	0.13	77,77,77,77	0
2	BTI	C	2000	15/15	0.95	0.17	45,45,57,57	0

Continued on next page...

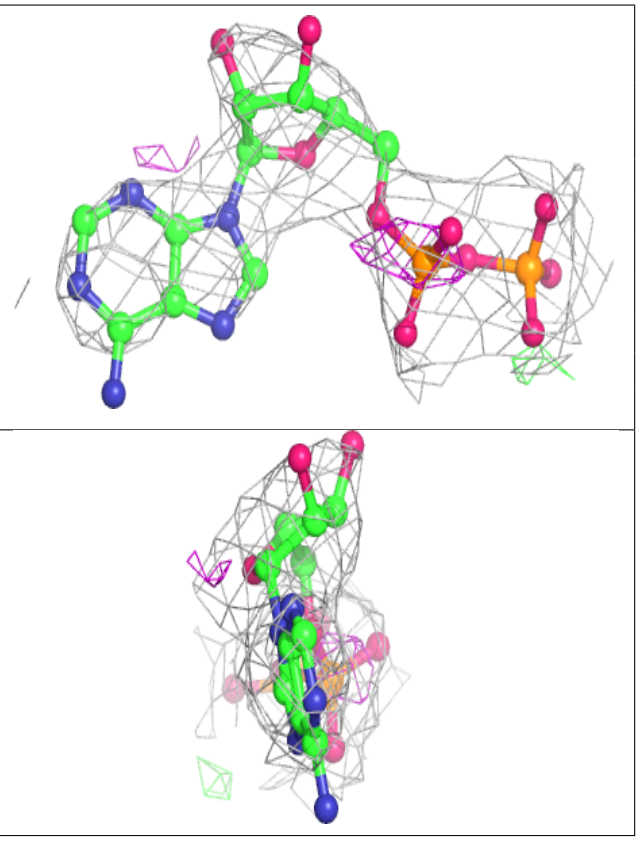
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BTI	C	1183	15/15	0.95	0.16	48,48,49,49	0
2	BTI	B	2000	15/15	0.95	0.15	48,48,51,51	0
4	MN	C	2002	1/1	0.95	0.11	75,75,75,75	0
2	BTI	A	2000	15/15	0.96	0.15	50,51,53,53	0
4	MN	D	2002	1/1	0.97	0.20	57,57,57,57	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

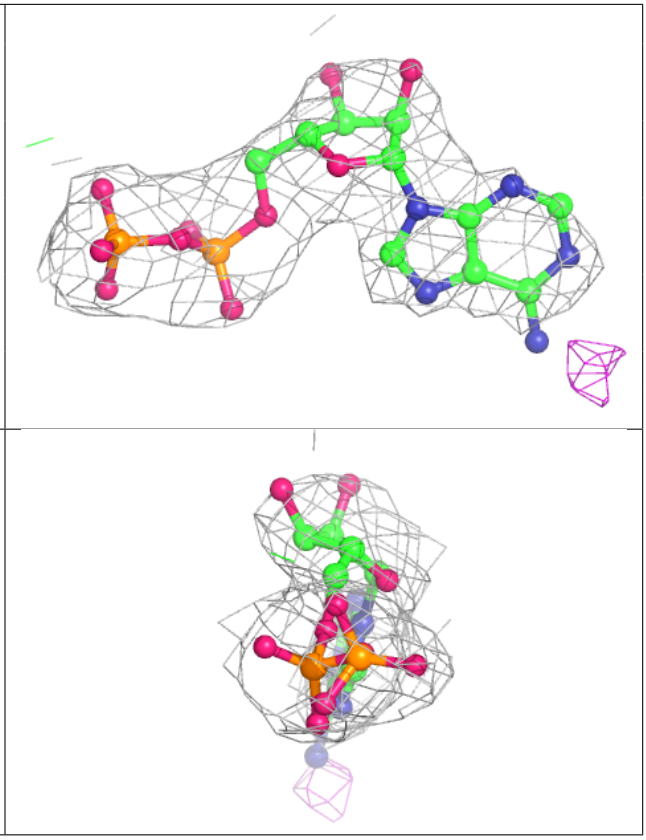
Electron density around ADP A 2100:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP C 2100:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.