WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 11:11 PM EDT

PDB ID	:	2NVA
Title	:	The X-ray crystal structure of the Paramecium bursaria Chlorella virus arginine decarboxylase bound to agmatine
Authors	:	Shah, R.H.; Akella, R.; Goldsmith, E.; Phillips, M.A.
Deposited on	:	unknown
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 ⓘ symbol.

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

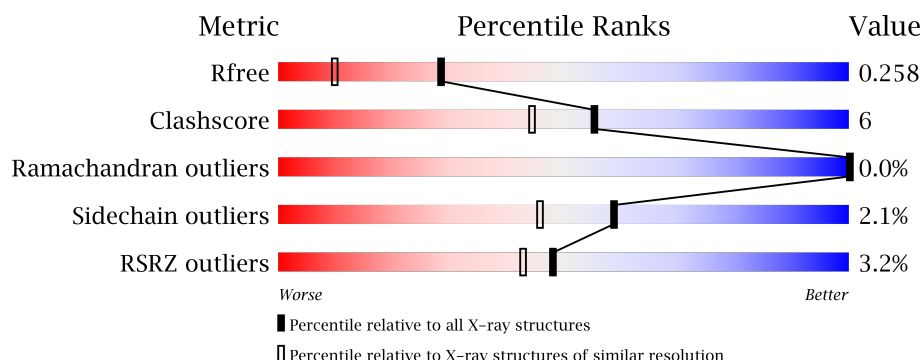|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 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.
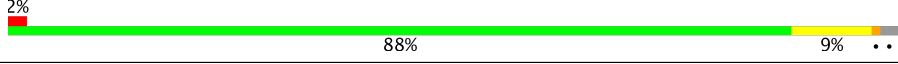
Metric	Percentile Ranks	Value
Rfree		0.258
Clashscore		6
Ramachandran outliers		0.0%
Sidechain outliers		2.1%
RSRZ outliers		3.2%

Worse ... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (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	372	3% / 92% / 6% ··
1	B	372	2% / 91% / 8% ·
1	C	372	5% / 87% / 12% ··
1	D	372	4% / 88% / 10% ··
1	E	372	88% / 11% ··

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Mol	Chain	Length	Quality of chain
1	F	372	2% / 88% / 10%
1	G	372	6% / 89% / 9%
1	H	372	2% / 88% / 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PL2	H	2008	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25034 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 arginine decarboxylase, A207R protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total 2939	C 1884	N 480	O 562	S 13	0	1	0
1	B	369	Total 2933	C 1880	N 478	O 562	S 13	0	1	0
1	C	367	Total 2916	C 1867	N 475	O 561	S 13	0	1	0
1	D	371	Total 2941	C 1884	N 480	O 564	S 13	0	1	0
1	E	370	Total 2945	C 1886	N 479	O 567	S 13	0	1	0
1	F	368	Total 2917	C 1869	N 476	O 559	S 13	0	1	0
1	G	368	Total 2902	C 1858	N 475	O 556	S 13	0	1	0
1	H	364	Total 2882	C 1845	N 469	O 555	S 13	0	1	0

- Molecule 2 is (4-{[(4-{[AMINO(IMINO)METHYL]AMINO}BUTYL)AMINO]METHYL}-5-HYDROXY-6-METHYLPYRIDIN-3-YL)METHYL DIHYDROGEN PHOSPHATE (three-letter code: PL2) (formula: $C_{13}H_{24}N_5O_5P$).

PL2
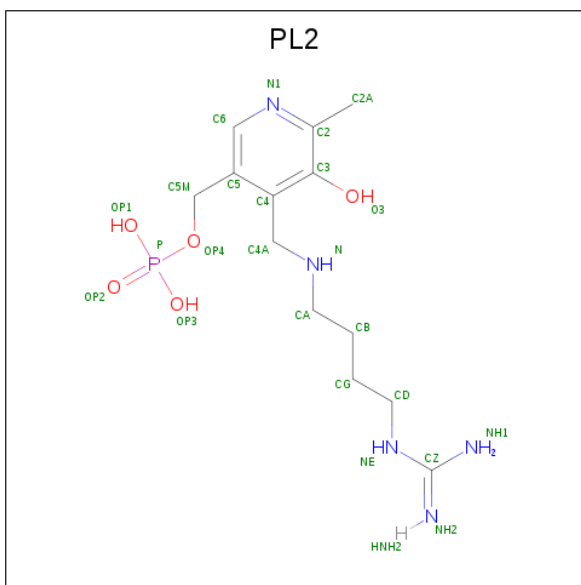
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	13	5	5	1		
2	B	1	Total	C	N	O	P	0	0
			24	13	5	5	1		
2	C	1	Total	C	N	O	P	0	0
			24	13	5	5	1		
2	D	1	Total	C	N	O	P	0	0
			24	13	5	5	1		
2	E	1	Total	C	N	O	P	0	0
			24	13	5	5	1		
2	F	1	Total	C	N	O	P	0	0
			24	13	5	5	1		
2	G	1	Total	C	N	O	P	0	0
			24	13	5	5	1		
2	H	1	Total	C	N	O	P	0	0
			24	13	5	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	219	Total	O	0	0
			219	219		
3	B	193	Total	O	0	0
			193	193		
3	C	163	Total	O	0	0
			163	163		
3	D	173	Total	O	0	0
			173	173		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	211	Total 211	O 211	0	0
3	F	174	Total 174	O 174	0	0
3	G	149	Total 149	O 149	0	0
3	H	185	Total 185	O 185	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 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 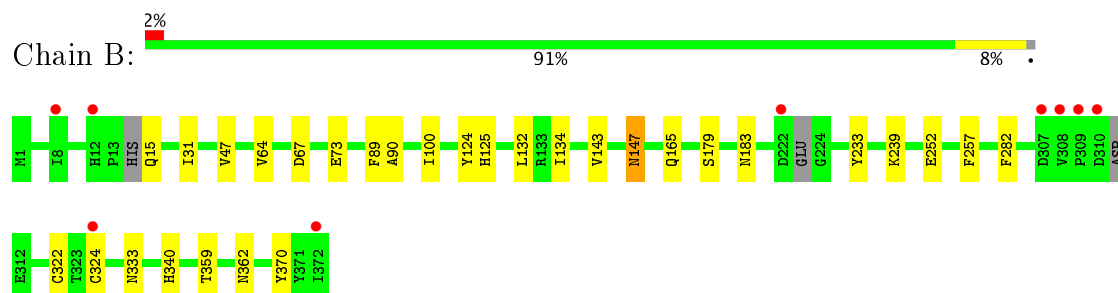one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: arginine decarboxylase, A207R protein
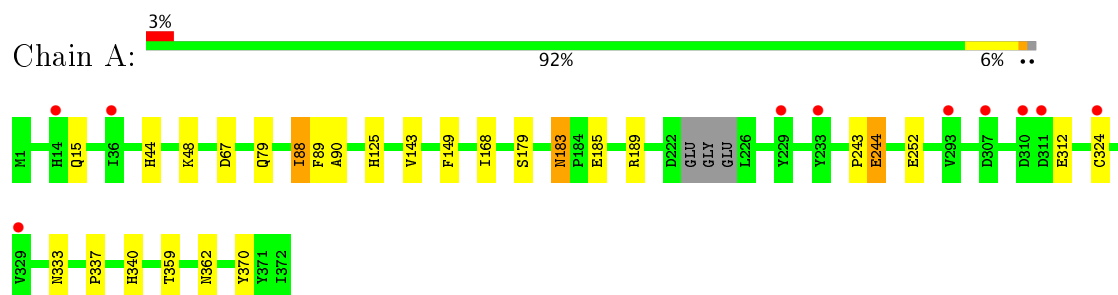
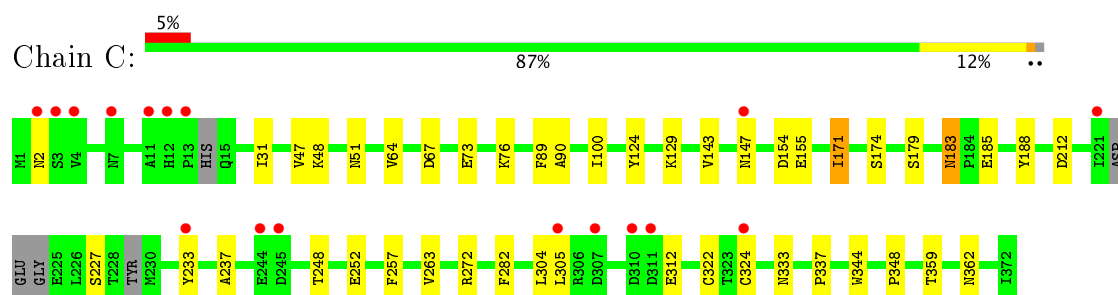- Molecule 1: arginine decarboxylase, A207R protein
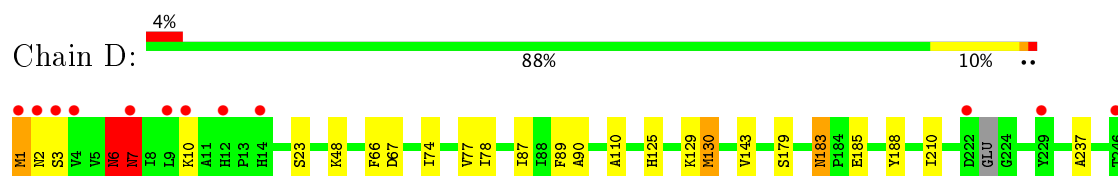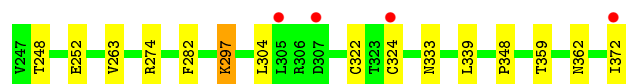

- Molecule 1: arginine decarboxylase, A207R protein

- Molecule 1: arginine decarboxylase, A207R protein

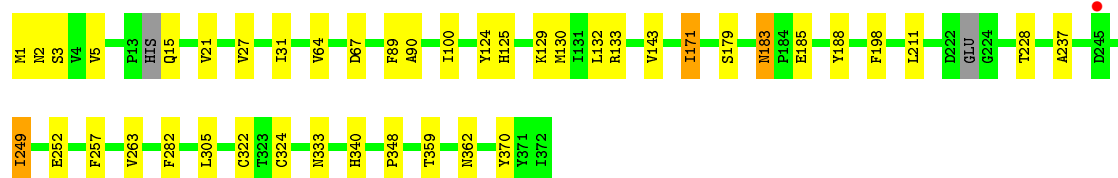• Molecule 1: arginine decarboxylase, A207R protein
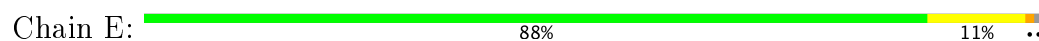
Chain E:

• Molecule 1: arginine decarboxylase, A207R protein

Chain F:

• Molecule 1: arginine decarboxylase, A207R protein

Chain G:

• Molecule 1: arginine decarboxylase, A207R protein

Chain H:
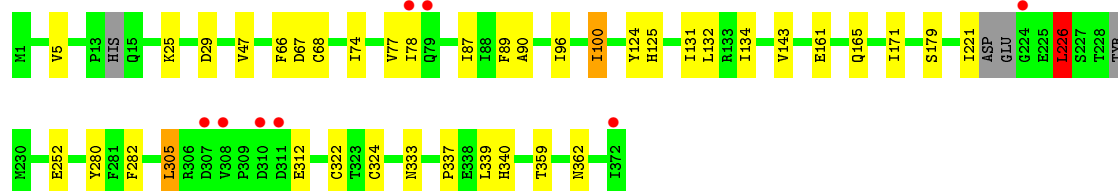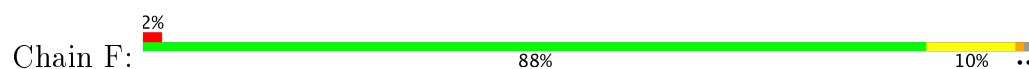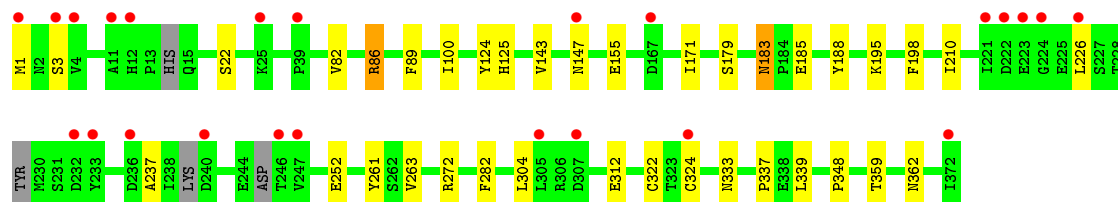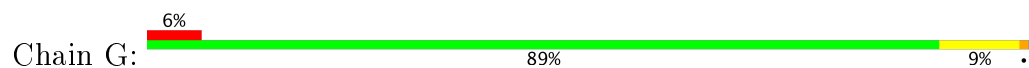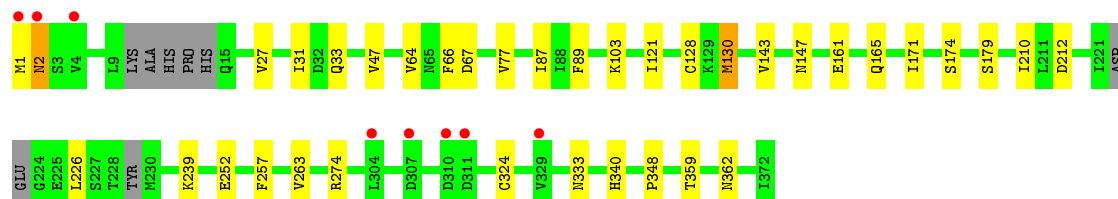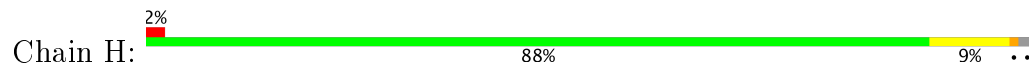
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.21Å 117.28Å 268.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.74 – 1.80 44.77 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.74-1.80) 99.7 (44.77-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.238 0.233 , 0.258	Depositor DCC
R_{free} test set	2052 reflections (0.61%)	DCC
Wilson B-factor (Å^2)	15.6	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 43.3	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25034	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.93 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.2439e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: PL2

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	0.53	0/3014	0.58	0/4095
1	B	0.51	0/3005	0.55	0/4079
1	C	0.51	0/2987	0.59	2/4056 (0.0%)
1	D	0.53	0/3015	0.59	2/4095 (0.0%)
1	E	0.50	0/3018	0.55	0/4099
1	F	0.51	0/2988	0.58	2/4055 (0.0%)
1	G	0.52	0/2972	0.59	2/4033 (0.0%)
1	H	0.52	0/2951	0.57	0/4004
All	All	0.52	0/23950	0.57	8/32516 (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	D	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	86	ARG	CB-CA-C	-6.88	96.63	110.40
1	D	7	ASN	N-CA-C	5.95	127.06	111.00
1	F	226	LEU	CA-CB-CG	5.49	127.92	115.30
1	C	272	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	G	272	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	D	6	ASN	N-CA-C	5.38	125.52	111.00
1	F	305	LEU	CA-CB-CG	-5.29	103.15	115.30
1	C	272	ARG	NE-CZ-NH1	5.22	122.91	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	6	ASN	Peptide

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	2939	0	2834	27	0
1	B	2933	0	2828	33	0
1	C	2916	0	2807	39	0
1	D	2941	0	2832	39	0
1	E	2945	0	2836	37	0
1	F	2917	0	2814	47	0
1	G	2902	0	2786	25	0
1	H	2882	0	2772	38	0
2	A	24	0	21	2	0
2	B	24	0	21	3	0
2	C	24	0	21	3	0
2	D	24	0	21	4	0
2	E	24	0	21	3	0
2	F	24	0	21	4	0
2	G	24	0	21	3	0
2	H	24	0	21	5	0
3	A	219	0	0	3	0
3	B	193	0	0	1	0
3	C	163	0	0	0	0
3	D	173	0	0	0	0
3	E	211	0	0	1	0
3	F	174	0	0	2	0
3	G	149	0	0	0	0
3	H	185	0	0	3	0
All	All	25034	0	22677	271	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 6.

All (271) 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:G:324[B]:CYS:SG	2:H:2008:PL2:HA2	1.65	1.33
2:G:2007:PL2:HA2	1:H:324[B]:CYS:SG	1.83	1.18
1:H:121:ILE:HG13	1:H:130:MET:HE3	1.22	1.16
1:G:324[B]:CYS:SG	2:H:2008:PL2:CA	2.36	1.13
1:D:130:MET:HA	1:D:130:MET:HE2	1.28	1.13
2:E:2005:PL2:HA2	1:F:324[B]:CYS:SG	1.96	1.06
1:C:324[B]:CYS:SG	2:D:2004:PL2:HA2	2.00	1.01
1:H:121:ILE:HG13	1:H:130:MET:CE	1.91	1.00
1:B:31:ILE:HD12	1:B:64:VAL:HG21	1.43	0.98
1:A:244:GLU:N	1:A:244:GLU:OE1	1.97	0.96
1:A:185:GLU:CG	1:A:189:ARG:NH1	2.33	0.92
1:C:51:ASN:HB2	1:C:76:LYS:HE2	1.51	0.90
1:A:185:GLU:HG3	1:A:189:ARG:HH11	1.38	0.88
2:A:2001:PL2:HA2	1:B:324[B]:CYS:SG	2.15	0.86
2:C:2003:PL2:HA2	1:D:324[B]:CYS:SG	2.17	0.84
1:F:100:ILE:CD1	1:F:124:TYR:HB3	2.08	0.83
1:D:130:MET:CE	1:D:130:MET:HA	2.09	0.83
1:A:185:GLU:HG2	1:A:189:ARG:NH1	1.92	0.83
1:A:185:GLU:CG	1:A:189:ARG:HH11	1.91	0.82
1:E:5:VAL:HG21	1:E:305:LEU:HD21	1.62	0.81
1:H:31:ILE:HD12	1:H:64:VAL:HG21	1.62	0.81
1:H:239:LYS:HE2	3:H:2103:HOH:O	1.80	0.81
2:G:2007:PL2:CA	1:H:324[B]:CYS:SG	2.68	0.80
1:F:5:VAL:HG21	1:F:305:LEU:HD21	1.62	0.80
1:E:324[B]:CYS:SG	2:F:2006:PL2:HA2	2.21	0.79
1:C:129:LYS:HB3	1:C:171:ILE:HD12	1.64	0.79
1:B:333:ASN:HD21	1:C:333:ASN:HD21	1.29	0.79
1:A:324[A]:CYS:SG	2:B:2002:PL2:HA2	2.23	0.78
1:E:31:ILE:HD13	1:E:257:PHE:CE1	2.20	0.77
1:B:31:ILE:HD12	1:B:64:VAL:CG2	2.16	0.76
1:C:31:ILE:HD12	1:C:64:VAL:HG21	1.68	0.75
1:F:77:VAL:HG11	1:F:87:ILE:HD11	1.70	0.74
1:F:5:VAL:CG2	1:F:305:LEU:CD2	2.65	0.74
2:E:2005:PL2:CA	1:F:324[B]:CYS:SG	2.75	0.74
1:E:5:VAL:CG2	1:E:305:LEU:HD21	2.18	0.73
1:D:110:ALA:HB3	1:D:130:MET:HE1	1.71	0.72
1:F:252:GLU:O	2:F:2006:PL2:H6	1.89	0.72
1:G:82:VAL:HG13	1:G:86:ARG:HD3	1.69	0.72
1:E:252:GLU:O	2:E:2005:PL2:H6	1.88	0.72
1:D:252:GLU:O	2:D:2004:PL2:H6	1.88	0.71
1:E:1:MET:O	1:E:5:VAL:HG22	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:ASN:ND2	1:D:7:ASN:H	1.88	0.71
1:A:252:GLU:O	2:A:2001:PL2:H6	1.89	0.71
1:F:5:VAL:CG2	1:F:305:LEU:HD21	2.21	0.71
1:F:100:ILE:HD11	1:F:124:TYR:HB3	1.73	0.70
1:D:7:ASN:HD22	1:D:7:ASN:H	1.39	0.70
1:D:210:ILE:HD13	1:D:248:THR:HB	1.74	0.70
1:B:147:ASN:HD22	1:B:147:ASN:H	1.38	0.69
1:H:2:ASN:N	1:H:2:ASN:HD22	1.90	0.69
1:B:252:GLU:O	2:B:2002:PL2:H6	1.93	0.69
1:B:31:ILE:CD1	1:B:64:VAL:HG21	2.21	0.68
1:C:305:LEU:HD12	1:C:344:TRP:CB	2.22	0.68
1:A:185:GLU:HG2	1:A:189:ARG:HH12	1.58	0.68
1:D:77:VAL:HG11	1:D:87:ILE:HD11	1.76	0.67
1:E:5:VAL:HG23	1:E:305:LEU:HD22	1.77	0.67
1:E:5:VAL:HG23	1:E:305:LEU:CD2	2.25	0.67
1:F:333:ASN:HD21	1:H:333:ASN:HD21	1.41	0.67
1:C:324[B]:CYS:SG	2:D:2004:PL2:CA	2.82	0.66
1:C:31:ILE:HD12	1:C:64:VAL:CG2	2.26	0.66
1:G:252:GLU:O	2:G:2007:PL2:H6	1.95	0.66
1:D:130:MET:CA	1:D:130:MET:HE2	2.17	0.66
1:C:100:ILE:HD11	1:C:124:TYR:CD1	2.31	0.65
1:D:23:SER:HB3	1:D:372:ILE:HG13	1.79	0.65
1:H:66:PHE:HB2	1:H:87:ILE:HD12	1.79	0.65
1:B:147:ASN:HD22	1:B:147:ASN:N	1.94	0.65
1:F:5:VAL:CG2	1:F:305:LEU:HD22	2.27	0.65
1:H:31:ILE:HD13	1:H:257:PHE:CE1	2.33	0.64
1:H:252:GLU:O	2:H:2008:PL2:H6	1.99	0.63
1:H:121:ILE:CG1	1:H:130:MET:HE3	2.15	0.62
1:C:31:ILE:CD1	1:C:64:VAL:HG21	2.30	0.62
1:E:5:VAL:CG2	1:E:305:LEU:CD2	2.77	0.62
1:F:100:ILE:HD11	1:F:124:TYR:CD1	2.35	0.62
1:C:305:LEU:HD12	1:C:344:TRP:HB3	1.80	0.62
1:H:121:ILE:CG1	1:H:130:MET:CE	2.75	0.62
1:C:31:ILE:HD13	1:C:257:PHE:CE1	2.35	0.62
1:C:100:ILE:HD11	1:C:124:TYR:HD1	1.65	0.61
1:F:5:VAL:HG23	1:F:305:LEU:HD22	1.81	0.61
1:E:324[B]:CYS:H	1:E:362:ASN:ND2	1.98	0.61
1:E:333:ASN:HD21	1:G:333:ASN:HD21	1.47	0.60
1:A:333:ASN:HD21	1:D:333:ASN:HD21	1.47	0.60
1:G:155:GLU:OE1	1:H:274:ARG:HD3	2.01	0.60
1:B:239:LYS:HE2	1:E:228:THR:OG1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:CYS:CB	1:F:74:ILE:HD13	2.33	0.58
1:C:155:GLU:OE1	1:D:274:ARG:HD3	2.03	0.58
1:C:252:GLU:O	2:C:2003:PL2:H6	2.03	0.58
1:E:129:LYS:HB3	1:E:171:ILE:HD12	1.84	0.58
1:B:132:LEU:CD2	1:B:134:ILE:HG23	2.34	0.58
1:H:47:VAL:HG12	1:H:67:ASP:O	2.04	0.57
1:F:340:HIS:HE1	3:F:2102:HOH:O	1.85	0.57
1:F:66:PHE:HB2	1:F:87:ILE:HD12	1.85	0.57
1:C:324[A]:CYS:H	1:C:362:ASN:HD21	1.53	0.57
1:D:297:LYS:HD2	1:D:297:LYS:N	2.19	0.56
1:C:359:THR:HG22	1:D:359:THR:HG22	1.87	0.56
1:H:27:VAL:O	1:H:31:ILE:HG12	2.06	0.56
1:G:324[A]:CYS:H	1:G:362:ASN:HD21	1.54	0.56
1:E:67:ASP:OD2	1:E:90:ALA:HB3	2.06	0.55
1:H:143:VAL:HG11	2:H:2008:PL2:HG1	1.86	0.55
1:H:143:VAL:HB	1:H:179:SER:HB3	1.88	0.55
1:B:132:LEU:HD23	1:B:132:LEU:C	2.26	0.55
1:B:31:ILE:HD13	1:B:257:PHE:CE1	2.42	0.55
1:E:324[B]:CYS:H	1:E:362:ASN:HD21	1.54	0.55
1:D:7:ASN:HD22	1:D:7:ASN:N	1.99	0.55
1:C:324[A]:CYS:H	1:C:362:ASN:ND2	2.04	0.55
1:E:31:ILE:HD12	1:E:64:VAL:HG21	1.87	0.55
1:F:5:VAL:HG21	1:F:305:LEU:CD2	2.31	0.54
1:C:324[B]:CYS:SG	1:D:48:LYS:HD2	2.48	0.54
1:B:15:GLN:NE2	1:B:370:TYR:OH	2.41	0.54
1:F:74:ILE:HD12	1:F:87:ILE:HG21	1.90	0.54
1:D:66:PHE:HB2	1:D:87:ILE:HD12	1.88	0.54
1:E:324[A]:CYS:H	1:E:362:ASN:ND2	2.05	0.54
1:E:324[A]:CYS:H	1:E:362:ASN:HD21	1.55	0.53
1:H:31:ILE:HD12	1:H:64:VAL:CG2	2.37	0.53
1:F:47:VAL:HG12	1:F:67:ASP:O	2.09	0.53
1:C:48:LYS:HD3	1:D:324[B]:CYS:SG	2.49	0.53
1:A:143:VAL:HB	1:A:179:SER:HB3	1.90	0.53
1:D:282:PHE:O	1:D:322:CYS:HB3	2.08	0.53
1:E:359:THR:HG22	1:F:359:THR:HG22	1.90	0.53
1:B:324[A]:CYS:H	1:B:362:ASN:HD21	1.56	0.52
1:G:324[B]:CYS:SG	2:H:2008:PL2:N	2.83	0.52
1:F:312:GLU:HG2	1:F:337:PRO:HB3	1.91	0.52
1:D:74:ILE:HG22	1:D:78:ILE:HD12	1.92	0.52
1:H:77:VAL:HG11	1:H:87:ILE:HD11	1.91	0.52
1:A:324[A]:CYS:H	1:A:362:ASN:ND2	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:VAL:HG11	1:B:73:GLU:HB3	1.92	0.51
1:C:324[B]:CYS:H	1:C:362:ASN:HD21	1.57	0.51
1:E:100:ILE:HD11	1:E:124:TYR:CD1	2.46	0.51
1:H:171:ILE:HD12	1:H:210:ILE:HD12	1.91	0.51
1:H:324[B]:CYS:H	1:H:362:ASN:ND2	2.08	0.51
2:B:2002:PL2:H4A2	2:B:2002:PL2:OP4	2.10	0.51
1:E:171:ILE:HD13	1:E:171:ILE:H	1.76	0.51
1:G:100:ILE:HD11	1:G:124:TYR:HD1	1.76	0.51
1:F:74:ILE:CD1	1:F:87:ILE:HG21	2.40	0.51
1:E:100:ILE:HD11	1:E:124:TYR:HD1	1.74	0.51
1:F:324[B]:CYS:H	1:F:362:ASN:ND2	2.08	0.50
1:H:263:VAL:HG12	1:H:348:PRO:HA	1.93	0.50
1:H:324[A]:CYS:H	1:H:362:ASN:ND2	2.09	0.50
1:F:161:GLU:O	1:F:165:GLN:HG3	2.10	0.50
1:F:77:VAL:HG11	1:F:87:ILE:CD1	2.40	0.50
1:G:324[B]:CYS:H	1:G:362:ASN:HD21	1.57	0.50
1:D:324[A]:CYS:H	1:D:362:ASN:ND2	2.09	0.50
1:B:324[B]:CYS:H	1:B:362:ASN:HD21	1.58	0.50
1:F:132:LEU:HD23	1:F:132:LEU:C	2.32	0.50
1:H:324[A]:CYS:H	1:H:362:ASN:HD21	1.59	0.50
1:B:324[A]:CYS:H	1:B:362:ASN:ND2	2.09	0.50
1:E:143:VAL:HB	1:E:179:SER:HB3	1.93	0.50
2:C:2003:PL2:CA	1:D:324[B]:CYS:SG	2.97	0.50
1:D:324[A]:CYS:H	1:D:362:ASN:HD21	1.60	0.50
1:B:147:ASN:ND2	1:B:147:ASN:N	2.61	0.49
2:D:2004:PL2:OP4	2:D:2004:PL2:H4A2	2.12	0.49
1:G:263:VAL:HG12	1:G:348:PRO:HA	1.93	0.49
1:H:161:GLU:O	1:H:165:GLN:HG3	2.12	0.49
1:C:305:LEU:HD12	1:C:344:TRP:HB2	1.93	0.49
1:A:168:ILE:HD13	3:A:2079:HOH:O	2.11	0.49
1:C:324[B]:CYS:H	1:C:362:ASN:ND2	2.10	0.49
1:G:359:THR:HG22	1:H:359:THR:HG22	1.95	0.49
1:E:324[B]:CYS:SG	2:F:2006:PL2:CA	2.98	0.49
1:D:130:MET:CA	1:D:130:MET:CE	2.83	0.49
1:H:324[B]:CYS:H	1:H:362:ASN:HD21	1.61	0.49
1:B:239:LYS:HE2	1:E:228:THR:HG1	1.77	0.49
1:A:67:ASP:OD2	1:A:90:ALA:HB3	2.14	0.48
1:A:183:ASN:HD22	1:A:183:ASN:C	2.17	0.48
1:E:340:HIS:HD2	3:E:2018:HOH:O	1.97	0.48
1:F:132:LEU:HD22	1:F:134:ILE:HG23	1.95	0.48
1:B:324[B]:CYS:H	1:B:362:ASN:ND2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:LEU:CD2	1:F:134:ILE:HG23	2.44	0.48
1:G:324[A]:CYS:H	1:G:362:ASN:ND2	2.10	0.48
1:C:143:VAL:HB	1:C:179:SER:HB3	1.94	0.48
1:F:74:ILE:O	1:F:78:ILE:HG22	2.14	0.48
1:H:174:SER:HB3	1:H:212:ASP:HB3	1.96	0.48
1:F:100:ILE:HD12	1:F:124:TYR:HB3	1.92	0.48
1:F:324[A]:CYS:H	1:F:362:ASN:HD21	1.62	0.47
1:F:324[B]:CYS:H	1:F:362:ASN:HD21	1.62	0.47
1:F:324[A]:CYS:H	1:F:362:ASN:ND2	2.11	0.47
1:D:324[B]:CYS:H	1:D:362:ASN:ND2	2.11	0.47
1:D:324[B]:CYS:H	1:D:362:ASN:HD21	1.62	0.47
1:F:143:VAL:HB	1:F:179:SER:HB3	1.96	0.47
1:H:340:HIS:HD2	3:H:2058:HOH:O	1.97	0.47
1:F:131:ILE:CD1	1:F:171:ILE:HG13	2.45	0.47
1:G:188:TYR:CD1	1:G:237:ALA:HB2	2.50	0.47
1:G:171:ILE:HD12	1:G:210:ILE:HD12	1.97	0.47
2:F:2006:PL2:OP4	2:F:2006:PL2:H4A2	2.15	0.47
1:D:1:MET:HG3	1:D:2:ASN:N	2.28	0.46
1:E:27:VAL:O	1:E:31:ILE:HG12	2.15	0.46
1:A:324[A]:CYS:H	1:A:362:ASN:HD21	1.63	0.46
1:D:1:MET:HG3	1:D:3:SER:H	1.80	0.46
1:F:67:ASP:OD2	1:F:90:ALA:HB3	2.15	0.46
1:G:195:LYS:HA	1:G:195:LYS:HD2	1.78	0.46
1:G:183:ASN:HD21	1:G:185:GLU:HB3	1.80	0.46
1:C:312:GLU:HG2	1:C:337:PRO:HB3	1.97	0.46
1:B:47:VAL:HG12	1:B:67:ASP:O	2.16	0.46
1:H:33:GLN:HB3	1:H:226:LEU:HD12	1.98	0.46
1:E:132:LEU:HD23	1:E:133:ARG:N	2.31	0.46
1:F:131:ILE:HD11	1:F:171:ILE:HG13	1.97	0.46
1:D:7:ASN:ND2	1:D:7:ASN:N	2.56	0.46
1:A:359:THR:HG22	1:B:359:THR:HG22	1.97	0.45
1:H:128:CYS:HB3	1:H:130:MET:HE2	1.98	0.45
1:H:31:ILE:CD1	1:H:64:VAL:HG21	2.42	0.45
1:C:183:ASN:HD22	1:C:183:ASN:C	2.19	0.45
1:F:25:LYS:HE2	1:F:29:ASP:OD2	2.17	0.45
1:B:67:ASP:OD2	1:B:90:ALA:HB3	2.17	0.45
1:A:324[B]:CYS:H	1:A:362:ASN:ND2	2.14	0.45
1:E:130:MET:O	1:E:171:ILE:HD13	2.17	0.45
1:E:211:LEU:HD23	1:E:249:ILE:HD13	1.98	0.45
1:A:312:GLU:HG2	1:A:337:PRO:HB3	1.98	0.45
1:A:185:GLU:HG3	1:A:189:ARG:NH1	2.07	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:HD11	1:B:124:TYR:HD1	1.81	0.44
1:D:143:VAL:HB	1:D:179:SER:HB3	1.98	0.44
1:F:221:ILE:HG12	1:F:226:LEU:HD13	1.99	0.44
1:B:143:VAL:HB	1:B:179:SER:HB3	1.99	0.44
1:E:183:ASN:HD22	1:E:183:ASN:C	2.21	0.44
1:C:47:VAL:HG21	1:C:73:GLU:HB3	1.99	0.44
1:A:48:LYS:HD3	1:B:324[B]:CYS:SG	2.57	0.44
1:G:324[B]:CYS:H	1:G:362:ASN:ND2	2.14	0.44
1:D:183:ASN:HD21	1:D:185:GLU:HB3	1.83	0.44
1:F:96:ILE:O	1:F:100:ILE:HD13	2.17	0.44
1:E:282:PHE:O	1:E:322:CYS:HB3	2.17	0.44
1:A:15:GLN:NE2	1:A:370:TYR:OH	2.51	0.43
1:D:304:LEU:HD11	1:D:339:LEU:HD21	2.00	0.43
1:F:100:ILE:N	1:F:100:ILE:CD1	2.81	0.43
1:A:324[B]:CYS:H	1:A:362:ASN:HD21	1.65	0.43
1:D:77:VAL:HG11	1:D:87:ILE:CD1	2.45	0.43
1:G:1:MET:HG3	1:G:3:SER:H	1.83	0.43
1:A:168:ILE:CD1	3:A:2079:HOH:O	2.66	0.43
1:C:48:LYS:CD	1:D:324[B]:CYS:SG	3.06	0.43
1:F:340:HIS:HD2	3:F:2053:HOH:O	2.00	0.43
1:C:100:ILE:CD1	1:C:124:TYR:HB3	2.49	0.43
1:C:263:VAL:HG12	1:C:348:PRO:HA	2.01	0.43
1:C:47:VAL:HG23	1:C:73:GLU:CD	2.39	0.43
1:H:66:PHE:HB2	1:H:87:ILE:CD1	2.47	0.42
1:D:129:LYS:C	1:D:130:MET:HE3	2.39	0.42
1:H:174:SER:CB	1:H:212:ASP:HB3	2.49	0.42
1:B:132:LEU:HD22	1:B:134:ILE:HG23	2.01	0.42
1:B:282:PHE:O	1:B:322:CYS:HB3	2.19	0.42
1:B:340:HIS:HD2	3:B:2020:HOH:O	2.01	0.42
1:G:143:VAL:HB	1:G:179:SER:HB3	2.02	0.42
1:H:2:ASN:H	1:H:2:ASN:HD22	1.66	0.42
1:E:5:VAL:HG12	1:E:21:VAL:HG21	2.01	0.42
1:B:132:LEU:CD2	1:B:134:ILE:CG2	2.98	0.42
1:B:47:VAL:HG13	1:B:73:GLU:CD	2.39	0.42
1:C:100:ILE:HD13	1:C:124:TYR:HB3	2.00	0.42
1:E:188:TYR:CD1	1:E:237:ALA:HB2	2.55	0.42
1:E:183:ASN:HD21	1:E:185:GLU:HB2	1.83	0.42
1:F:66:PHE:HB2	1:F:87:ILE:CD1	2.49	0.42
1:F:280:TYR:CE1	1:F:339:LEU:HB2	2.55	0.42
1:E:15:GLN:NE2	1:E:370:TYR:OH	2.53	0.41
1:H:239:LYS:HB3	3:H:2103:HOH:O	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:HD11	1:B:124:TYR:CD1	2.56	0.41
1:G:304:LEU:HD13	1:G:339:LEU:HD22	2.02	0.41
1:C:76:LYS:HB3	1:C:76:LYS:HE3	1.59	0.41
1:D:263:VAL:HG12	1:D:348:PRO:HA	2.00	0.41
1:A:149:PHE:HE2	1:B:324[B]:CYS:O	2.02	0.41
1:C:183:ASN:HD21	1:C:185:GLU:HB2	1.85	0.41
1:C:188:TYR:CD1	1:C:237:ALA:HB2	2.56	0.41
1:G:22:SER:HB3	1:G:261:TYR:CZ	2.56	0.41
1:C:174:SER:HB3	1:C:212:ASP:HB3	2.03	0.41
1:F:100:ILE:HD11	1:F:124:TYR:CB	2.46	0.41
1:G:100:ILE:HD11	1:G:124:TYR:CD1	2.56	0.41
1:A:340:HIS:HD2	3:A:2010:HOH:O	2.04	0.41
1:D:188:TYR:CD1	1:D:237:ALA:HB2	2.56	0.41
1:E:263:VAL:HG12	1:E:348:PRO:HA	2.02	0.41
1:F:282:PHE:O	1:F:322:CYS:HB3	2.21	0.41
1:A:243:PRO:N	1:A:244:GLU:OE1	2.54	0.41
1:C:147:ASN:HD22	1:C:147:ASN:HA	1.69	0.41
1:F:100:ILE:HD13	1:F:100:ILE:N	2.36	0.40
1:G:312:GLU:HG2	1:G:337:PRO:HB3	2.03	0.40
1:C:67:ASP:OD2	1:C:90:ALA:HB3	2.21	0.40
1:D:67:ASP:OD2	1:D:90:ALA:HB3	2.22	0.40
1:A:44:HIS:CE1	1:A:88:ILE:HD13	2.57	0.40
1:C:282:PHE:O	1:C:322:CYS:HB3	2.22	0.40
1:G:282:PHE:O	1:G:322:CYS:HB3	2.21	0.40
1:H:77:VAL:HG11	1:H:87:ILE:CD1	2.51	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	366/372 (98%)	357 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	362/372 (97%)	354 (98%)	8 (2%)	0	100	100
1	C	360/372 (97%)	350 (97%)	10 (3%)	0	100	100
1	D	368/372 (99%)	358 (97%)	9 (2%)	1 (0%)	44	29
1	E	365/372 (98%)	355 (97%)	10 (3%)	0	100	100
1	F	361/372 (97%)	352 (98%)	9 (2%)	0	100	100
1	G	359/372 (96%)	350 (98%)	9 (2%)	0	100	100
1	H	357/372 (96%)	348 (98%)	9 (2%)	0	100	100
All	All	2898/2976 (97%)	2824 (97%)	73 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	7	ASN

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	326/329 (99%)	320 (98%)	6 (2%)	64	53
1	B	325/329 (99%)	319 (98%)	6 (2%)	64	53
1	C	324/329 (98%)	315 (97%)	9 (3%)	49	34
1	D	325/329 (99%)	316 (97%)	9 (3%)	49	34
1	E	327/329 (99%)	319 (98%)	8 (2%)	54	40
1	F	323/329 (98%)	319 (99%)	4 (1%)	75	69
1	G	320/329 (97%)	314 (98%)	6 (2%)	62	50
1	H	319/329 (97%)	313 (98%)	6 (2%)	62	50
All	All	2589/2632 (98%)	2535 (98%)	54 (2%)	59	46

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	88	ILE
1	A	89	PHE
1	A	125	HIS
1	A	183	ASN
1	A	244	GLU
1	B	89	PHE
1	B	125	HIS
1	B	147	ASN
1	B	165	GLN
1	B	183	ASN
1	B	233	TYR
1	C	2	ASN
1	C	89	PHE
1	C	154	ASP
1	C	171	ILE
1	C	183	ASN
1	C	227	SER
1	C	233	TYR
1	C	248	THR
1	C	304	LEU
1	D	1	MET
1	D	6	ASN
1	D	7	ASN
1	D	10	LYS
1	D	89	PHE
1	D	125	HIS
1	D	130	MET
1	D	183	ASN
1	D	297	LYS
1	E	2	ASN
1	E	3	SER
1	E	89	PHE
1	E	125	HIS
1	E	171	ILE
1	E	183	ASN
1	E	198	PHE
1	E	249	ILE
1	F	89	PHE
1	F	100	ILE
1	F	125	HIS
1	F	226	LEU
1	G	89	PHE

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Mol	Chain	Res	Type
1	G	125	HIS
1	G	147	ASN
1	G	183	ASN
1	G	198	PHE
1	G	226	LEU
1	H	1	MET
1	H	2	ASN
1	H	89	PHE
1	H	103	LYS
1	H	130	MET
1	H	147	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	15	GLN
1	A	79	GLN
1	A	144	GLN
1	A	165	GLN
1	A	183	ASN
1	A	218	HIS
1	A	340	HIS
1	A	362	ASN
1	B	6	ASN
1	B	7	ASN
1	B	15	GLN
1	B	63	ASN
1	B	147	ASN
1	B	165	GLN
1	B	183	ASN
1	B	218	HIS
1	B	340	HIS
1	B	362	ASN
1	C	6	ASN
1	C	147	ASN
1	C	183	ASN
1	C	199	ASN
1	C	218	HIS
1	C	333	ASN
1	C	340	HIS
1	C	362	ASN

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Mol	Chain	Res	Type
1	D	2	ASN
1	D	6	ASN
1	D	7	ASN
1	D	79	GLN
1	D	165	GLN
1	D	183	ASN
1	D	218	HIS
1	D	333	ASN
1	D	340	HIS
1	D	362	ASN
1	E	2	ASN
1	E	6	ASN
1	E	7	ASN
1	E	15	GLN
1	E	147	ASN
1	E	183	ASN
1	E	340	HIS
1	E	362	ASN
1	F	6	ASN
1	F	7	ASN
1	F	15	GLN
1	F	127	ASN
1	F	218	HIS
1	F	332	HIS
1	F	333	ASN
1	F	340	HIS
1	F	362	ASN
1	G	6	ASN
1	G	7	ASN
1	G	127	ASN
1	G	183	ASN
1	G	333	ASN
1	G	340	HIS
1	G	362	ASN
1	H	2	ASN
1	H	63	ASN
1	H	218	HIS
1	H	340	HIS
1	H	362	ASN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6   Ligand geometry (i)

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	$\#|Z| > 2$
2	PL2	A	2001	-	24,24,24	1.34	4 (16%)	29,32,32	1.65	6 (20%)
2	PL2	B	2002	-	24,24,24	1.20	3 (12%)	29,32,32	1.55	6 (20%)
2	PL2	C	2003	-	24,24,24	1.20	4 (16%)	29,32,32	1.71	6 (20%)
2	PL2	D	2004	-	24,24,24	1.16	2 (8%)	29,32,32	1.54	4 (13%)
2	PL2	E	2005	-	24,24,24	1.34	3 (12%)	29,32,32	1.71	6 (20%)
2	PL2	F	2006	-	24,24,24	1.22	3 (12%)	29,32,32	1.62	6 (20%)
2	PL2	G	2007	-	24,24,24	1.19	3 (12%)	29,32,32	1.77	5 (17%)
2	PL2	H	2008	-	24,24,24	1.23	3 (12%)	29,32,32	1.59	5 (17%)

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	PL2	A	2001	-	-	0/16/16/16	0/1/1/1
2	PL2	B	2002	-	-	0/16/16/16	0/1/1/1
2	PL2	C	2003	-	-	0/16/16/16	0/1/1/1
2	PL2	D	2004	-	-	0/16/16/16	0/1/1/1
2	PL2	E	2005	-	-	0/16/16/16	0/1/1/1
2	PL2	F	2006	-	-	0/16/16/16	0/1/1/1
2	PL2	G	2007	-	-	0/16/16/16	0/1/1/1
2	PL2	H	2008	-	-	0/16/16/16	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	PL2	P-OP3	2.04	1.63	1.54
2	C	2003	PL2	C2A-C2	2.14	1.54	1.50
2	G	2007	PL2	C4A-C4	2.14	1.54	1.51
2	H	2008	PL2	P-OP2	2.15	1.58	1.50
2	B	2002	PL2	C2A-C2	2.20	1.54	1.50
2	C	2003	PL2	P-OP3	2.22	1.63	1.54
2	B	2002	PL2	P-OP2	2.24	1.58	1.50
2	C	2003	PL2	P-OP2	2.31	1.58	1.50
2	A	2001	PL2	C2A-C2	2.32	1.54	1.50
2	D	2004	PL2	C2A-C2	2.35	1.54	1.50
2	F	2006	PL2	C2A-C2	2.41	1.54	1.50
2	G	2007	PL2	P-OP2	2.46	1.59	1.50
2	C	2003	PL2	C4A-C4	2.56	1.55	1.51
2	F	2006	PL2	C4A-C4	2.63	1.55	1.51
2	B	2002	PL2	C4A-C4	2.66	1.55	1.51
2	E	2005	PL2	C2A-C2	2.70	1.55	1.50
2	E	2005	PL2	C4A-C4	2.72	1.55	1.51
2	G	2007	PL2	C2A-C2	2.85	1.55	1.50
2	F	2006	PL2	P-OP2	2.85	1.60	1.50
2	H	2008	PL2	C4A-C4	2.90	1.55	1.51
2	H	2008	PL2	C2A-C2	2.92	1.55	1.50
2	D	2004	PL2	C4A-C4	2.96	1.55	1.51
2	A	2001	PL2	P-OP2	3.00	1.60	1.50
2	E	2005	PL2	P-OP2	3.44	1.62	1.50
2	A	2001	PL2	C4A-C4	3.61	1.56	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2007	PL2	C3-C4-C5	-3.30	115.46	118.71
2	F	2006	PL2	C3-C4-C5	-2.92	115.82	118.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2005	PL2	C3-C4-C5	-2.72	116.03	118.71
2	D	2004	PL2	C3-C4-C5	-2.65	116.09	118.71
2	H	2008	PL2	C3-C4-C5	-2.58	116.16	118.71
2	A	2001	PL2	C3-C4-C5	-2.48	116.27	118.71
2	F	2006	PL2	CG-CD-NE	-2.41	105.24	112.18
2	C	2003	PL2	CG-CD-NE	-2.39	105.31	112.18
2	E	2005	PL2	CG-CD-NE	-2.32	105.50	112.18
2	A	2001	PL2	CG-CD-NE	-2.06	106.25	112.18
2	B	2002	PL2	C3-C4-C5	-2.06	116.68	118.71
2	C	2003	PL2	C4A-C4-C5	-2.02	117.91	119.75
2	C	2003	PL2	C3-C2-N1	-2.01	118.11	120.75
2	B	2002	PL2	C5-C6-N1	-2.00	120.48	123.87
2	H	2008	PL2	C6-C5-C4	2.04	119.65	118.13
2	H	2008	PL2	OP1-P-OP4	2.14	112.42	106.73
2	G	2007	PL2	OP1-P-OP4	2.35	112.98	106.73
2	C	2003	PL2	OP1-P-OP4	2.41	113.16	106.73
2	E	2005	PL2	OP1-P-OP4	2.55	113.53	106.73
2	B	2002	PL2	OP1-P-OP4	2.62	113.70	106.73
2	A	2001	PL2	C6-C5-C4	2.71	120.15	118.13
2	A	2001	PL2	OP1-P-OP4	2.76	114.07	106.73
2	F	2006	PL2	OP1-P-OP4	2.79	114.16	106.73
2	B	2002	PL2	C6-C5-C4	2.97	120.34	118.13
2	D	2004	PL2	C6-C5-C4	3.12	120.45	118.13
2	A	2001	PL2	C4A-C4-C3	3.26	123.25	119.65
2	F	2006	PL2	C6-C5-C4	3.34	120.61	118.13
2	E	2005	PL2	C6-C5-C4	3.35	120.62	118.13
2	F	2006	PL2	OP4-C5M-C5	3.54	116.44	109.32
2	B	2002	PL2	OP4-C5M-C5	3.71	116.78	109.32
2	D	2004	PL2	OP4-C5M-C5	3.72	116.79	109.32
2	C	2003	PL2	OP4-C5M-C5	3.79	116.94	109.32
2	F	2006	PL2	C4A-C4-C3	3.93	123.99	119.65
2	D	2004	PL2	C4A-C4-C3	4.03	124.10	119.65
2	G	2007	PL2	OP4-C5M-C5	4.12	117.61	109.32
2	E	2005	PL2	OP4-C5M-C5	4.13	117.62	109.32
2	B	2002	PL2	C4A-C4-C3	4.22	124.31	119.65
2	G	2007	PL2	C6-C5-C4	4.29	121.32	118.13
2	G	2007	PL2	C4A-C4-C3	4.29	124.38	119.65
2	E	2005	PL2	C4A-C4-C3	4.29	124.38	119.65
2	H	2008	PL2	C4A-C4-C3	4.31	124.41	119.65
2	H	2008	PL2	OP4-C5M-C5	4.50	118.36	109.32
2	A	2001	PL2	OP4-C5M-C5	5.03	119.44	109.32
2	C	2003	PL2	C4A-C4-C3	5.13	125.31	119.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	PL2	2	0
2	B	2002	PL2	3	0
2	C	2003	PL2	3	0
2	D	2004	PL2	4	0
2	E	2005	PL2	3	0
2	F	2006	PL2	4	0
2	G	2007	PL2	3	0
2	H	2008	PL2	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 (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	369/372 (99%)	0.29	10 (2%)	55	50	12, 13, 16, 17	0
1	B	369/372 (99%)	0.23	9 (2%)	59	55	11, 13, 16, 18	0
1	C	367/372 (98%)	0.29	17 (4%)	33	28	12, 14, 17, 19	0
1	D	371/372 (99%)	0.20	16 (4%)	36	30	13, 14, 17, 19	0
1	E	370/372 (99%)	0.16	1 (0%)	93	92	12, 13, 16, 18	0
1	F	368/372 (98%)	0.27	8 (2%)	62	58	12, 14, 16, 19	0
1	G	368/372 (98%)	0.33	24 (6%)	20	16	12, 14, 17, 20	0
1	H	364/372 (97%)	0.13	8 (2%)	62	58	13, 14, 16, 19	0
All	All	2946/2976 (98%)	0.24	93 (3%)	48	43	11, 14, 16, 20	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	TYR	4.6
1	F	224	GLY	4.3
1	H	310	ASP	3.7
1	G	372	ILE	3.7
1	F	311	ASP	3.5
1	G	247	VAL	3.5
1	G	226	LEU	3.5
1	G	223	GLU	3.4
1	G	4	VAL	3.4
1	C	310	ASP	3.4
1	H	2	ASN	3.2
1	D	10	LYS	3.2
1	D	372	ILE	3.1
1	B	310	ASP	3.1
1	E	245	ASP	3.1
1	H	307	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	307	ASP	3.1
1	H	311	ASP	3.0
1	C	245	ASP	3.0
1	C	305	LEU	3.0
1	H	1	MET	3.0
1	C	11	ALA	3.0
1	G	11	ALA	3.0
1	D	305	LEU	2.9
1	G	246	THR	2.9
1	G	307	ASP	2.9
1	C	12	HIS	2.9
1	G	222	ASP	2.9
1	C	13	PRO	2.8
1	G	3	SER	2.8
1	D	324[A]	CYS	2.8
1	D	14	HIS	2.8
1	D	3	SER	2.8
1	D	222	ASP	2.8
1	C	311	ASP	2.7
1	A	324[A]	CYS	2.7
1	D	7	ASN	2.7
1	G	224	GLY	2.7
1	G	233	TYR	2.7
1	G	305	LEU	2.7
1	G	1	MET	2.6
1	G	39	PRO	2.6
1	F	79	GLN	2.6
1	G	167	ASP	2.6
1	A	14	HIS	2.6
1	B	372	ILE	2.6
1	C	324[A]	CYS	2.6
1	G	324[A]	CYS	2.6
1	D	4	VAL	2.5
1	C	7	ASN	2.5
1	G	232	ASP	2.5
1	G	221	ILE	2.5
1	F	310	ASP	2.5
1	C	307	ASP	2.5
1	D	2	ASN	2.5
1	D	9	LEU	2.5
1	A	36	ILE	2.5
1	D	12	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	307	ASP	2.5
1	G	25	LYS	2.5
1	C	3	SER	2.5
1	B	222	ASP	2.4
1	F	308	VAL	2.4
1	F	78	ILE	2.4
1	C	147	ASN	2.4
1	D	1	MET	2.4
1	G	236	ASP	2.4
1	A	310	ASP	2.3
1	A	233	TYR	2.3
1	H	4	VAL	2.3
1	B	309	PRO	2.3
1	B	324[A]	CYS	2.3
1	C	221	ILE	2.3
1	G	147	ASN	2.3
1	A	307	ASP	2.2
1	B	8	ILE	2.2
1	F	372	ILE	2.2
1	C	244	GLU	2.2
1	C	4	VAL	2.2
1	A	311	ASP	2.1
1	G	12	HIS	2.1
1	D	246	THR	2.1
1	H	304	LEU	2.1
1	C	233	TYR	2.1
1	A	293	VAL	2.1
1	B	308	VAL	2.1
1	H	329	VAL	2.1
1	D	307	ASP	2.1
1	D	229	TYR	2.0
1	A	329	VAL	2.0
1	B	12	HIS	2.0
1	C	2	ASN	2.0
1	G	240	ASP	2.0

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

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

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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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	PL2	H	2008	24/24	0.90	0.18	2.23	14,16,17,17	0
2	PL2	G	2007	24/24	0.91	0.16	1.89	14,17,18,18	0
2	PL2	F	2006	24/24	0.91	0.15	1.09	13,16,17,18	0
2	PL2	B	2002	24/24	0.91	0.16	0.71	13,16,17,17	0
2	PL2	C	2003	24/24	0.91	0.15	0.70	14,16,18,18	0
2	PL2	D	2004	24/24	0.92	0.14	0.69	15,16,17,18	0
2	PL2	E	2005	24/24	0.92	0.13	0.06	12,16,17,17	0
2	PL2	A	2001	24/24	0.92	0.13	-0.10	13,16,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.