Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:18 PM GMT

PDB ID	:	1JPN
Title	:	GMPPNP Complex of SRP GTPase NG Domain
Authors	:	Padmanabhan, S.; Freymann, D.M.
Deposited on	:	2001-08-02
Resolution	:	1.90 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
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:

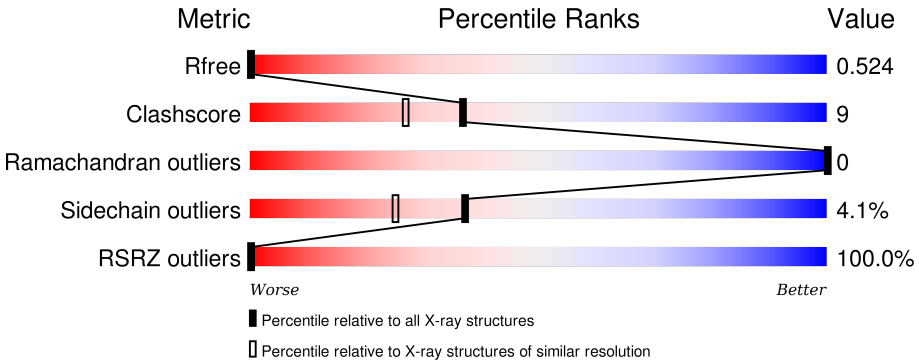
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 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	296	100% 81% 18%
1	B	296	100% 77% 21%

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	CA	A	901	-	-	-	X
3	GNP	A	911	-	-	-	X
3	GNP	B	910	-	-	-	X
4	ACY	A	952	-	-	X	X
4	ACY	A	953	-	-	-	X
4	ACY	B	950	-	-	-	X
4	ACY	B	951	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5117 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.

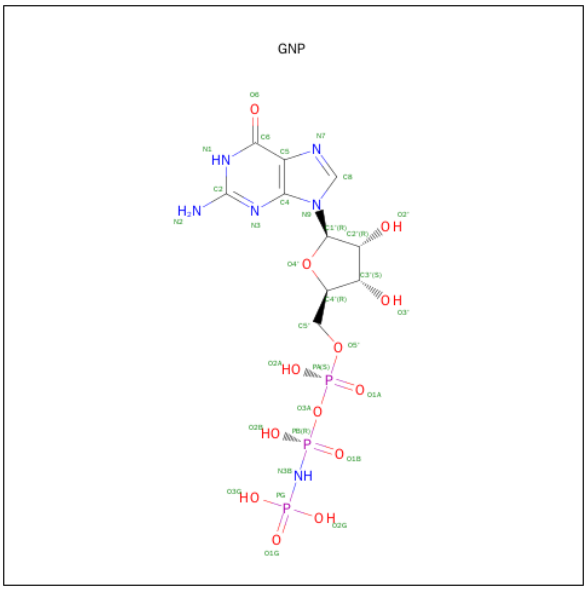
- Molecule 1 is a protein called SIGNAL RECOGNITION PARTICLE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	295	Total	C	N	O	S	0	6	0
			2318	1454	423	434	7			
1	A	296	Total	C	N	O	S	0	1	0
			2286	1435	416	428	7			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

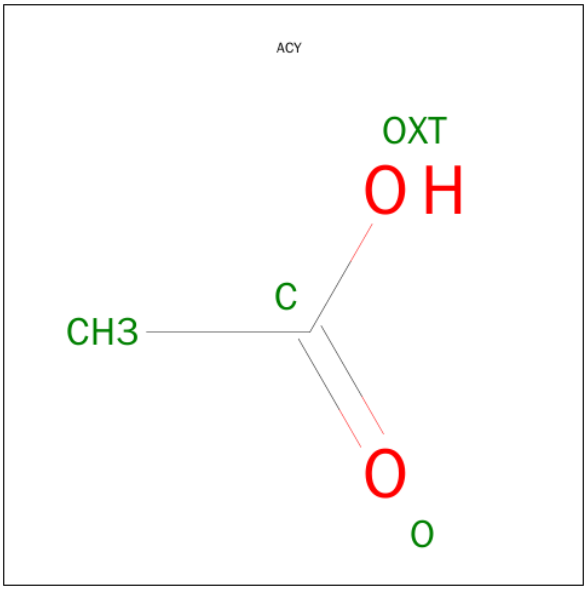
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

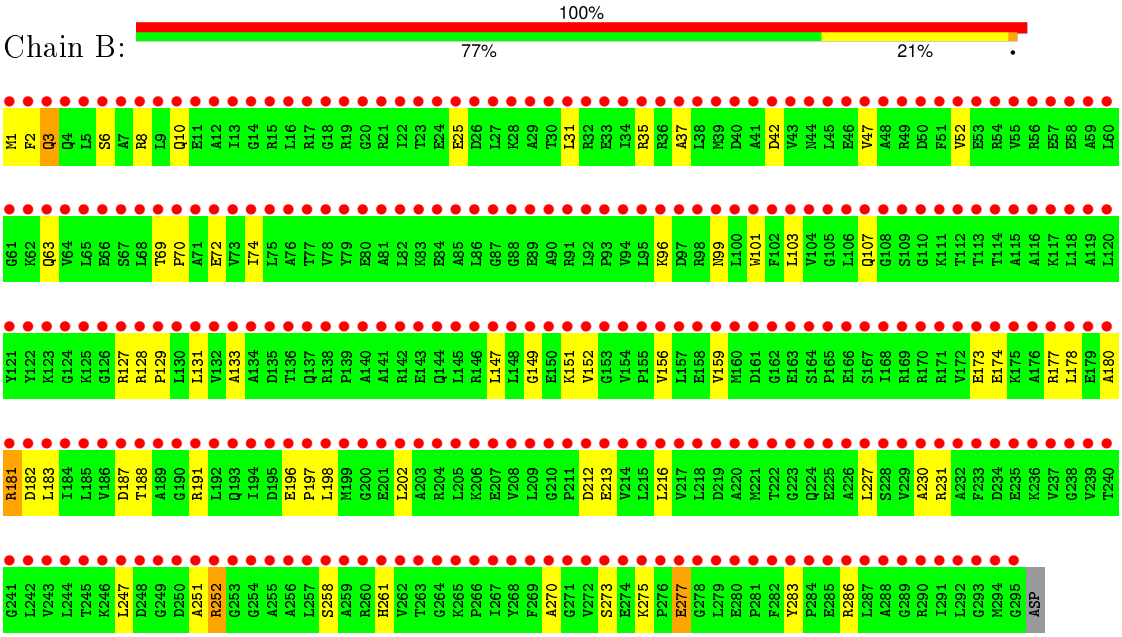
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	251	Total	O	0	0
			251	251		
5	B	180	Total	O	0	0
			180	180		

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.

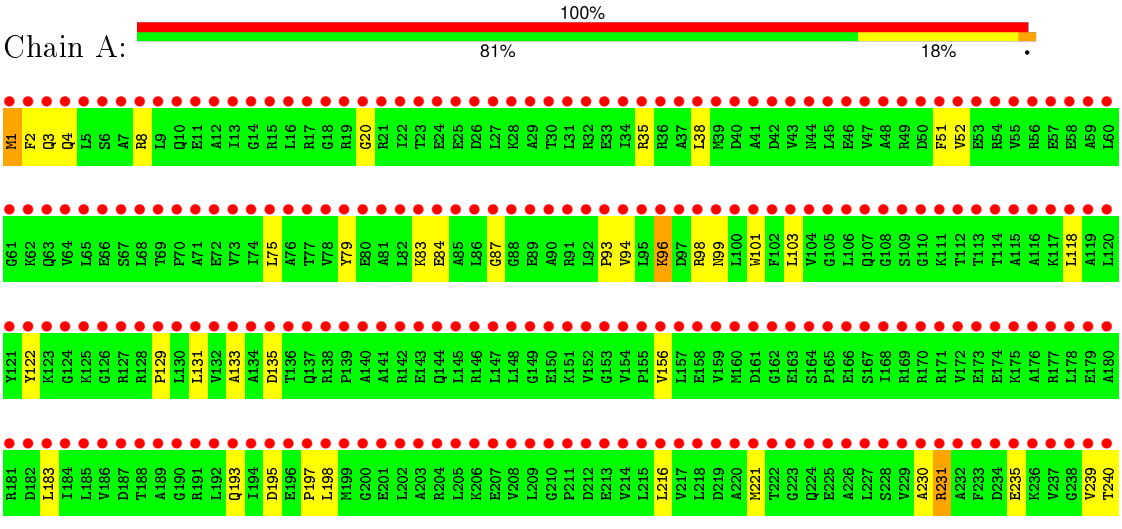
- Molecule 1: SIGNAL RECOGNITION PARTICLE PROTEIN

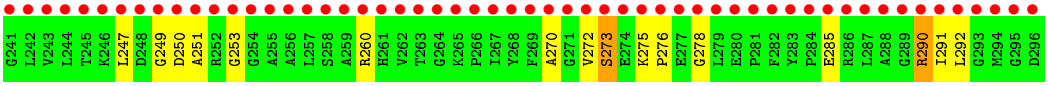
Chain B:



- Molecule 1: SIGNAL RECOGNITION PARTICLE PROTEIN

Chain A:




G241
L242
V243
L244
T245
K246
L247
D248
G249
D250
A251
R252
G253
G254
A255
A256
L257
S258
A259
R260
E261
V262
T263
G264
K265
P266
I267
Y268
F269
A270
G271
V272
S273
E274
K275
P276
E277
G278
L279
E280
P281
F282
Y283
P284
E285
R286
L287
A288
G289
R290
I291
L292
G293
M294
G295
D296

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	108.81Å 54.53Å 99.08Å 90.00° 97.42° 90.00°	Depositor
Resolution (Å)	15.00 – 1.90 17.84 – 0.78	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-1.90) 7.5 (17.84-0.78)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 0.78Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.190 , 0.241 0.517 , 0.524	Depositor DCC
R_{free} test set	469 reflections (4.53%)	DCC
Wilson B-factor (Å^2)	2.2	Xtriage
Anisotropy	2.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.01 , -1.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 48986 reflections	Xtriage
F_o,F_c correlation	0.43	EDS
Total number of atoms	5117	wwPDB-VP
Average B, all atoms (Å^2)	23.0	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 100.00 % 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 0.0000e+00.*

[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: ACY, CA, GNP

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	0.23	0/2311	0.46	0/3112
1	B	0.23	0/2343	0.45	0/3155
All	All	0.23	0/4654	0.45	0/6267

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2286	0	2385	37	0
1	B	2318	0	2416	53	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	32	0	13	0	0
3	B	32	0	13	1	0
4	A	8	0	6	3	0
4	B	8	0	6	1	0
5	A	251	0	0	4	3
5	B	180	0	0	2	3
All	All	5117	0	4839	90	4

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 9.

All (90) 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:96:LYS:H	1:B:99:ASN:HD21	1.06	0.93
1:A:96:LYS:H	1:A:99:ASN:HD21	1.13	0.92
1:B:35:ARG:HB2	1:B:52[A]:VAL:HG21	1.68	0.76
1:B:69:THR:HB	1:B:72:GLU:HG3	1.69	0.73
1:A:1:MET:HA	1:A:3:GLN:HE22	1.51	0.73
1:B:96:LYS:H	1:B:99:ASN:ND2	1.85	0.71
1:B:96:LYS:N	1:B:99:ASN:HD21	1.86	0.70
1:B:283:TYR:HB3	1:B:286:ARG:HG3	1.73	0.68
1:A:231:ARG:O	1:A:235:GLU:HG2	1.94	0.68
1:B:247:LEU:HD12	1:B:270:ALA:HB1	1.76	0.67
1:B:128:ARG:NH1	1:B:180:ALA:HB3	2.11	0.66
1:A:20:GLY:HA2	5:A:1476:HOH:O	1.96	0.64
1:A:247:LEU:HD12	1:A:270:ALA:HB1	1.80	0.63
1:B:275:LYS:HG3	1:B:277:GLU:HG2	1.83	0.60
1:B:283:TYR:CB	1:B:286:ARG:HG3	2.32	0.59
1:B:227:LEU:HD11	1:B:258:SER:HB2	1.85	0.58
1:B:273:SER:OG	1:B:275:LYS:HG2	2.04	0.58
1:A:195:ASP:HB3	1:A:198:LEU:HB3	1.84	0.58
1:B:128:ARG:HH12	1:B:180:ALA:HB3	1.69	0.58
1:A:272:VAL:HG22	1:A:278:GLY:O	2.05	0.57
1:A:1:MET:HG2	1:A:247:LEU:O	2.04	0.57
1:B:174:GLU:HG3	1:B:177:ARG:HH22	1.69	0.57
1:A:1:MET:SD	1:A:251:ALA:HB3	2.45	0.56
1:B:1:MET:N	1:B:3:GLN:HE22	2.04	0.55
1:A:1:MET:HA	1:A:3:GLN:NE2	2.19	0.55
1:A:35:ARG:HB2	1:A:52:VAL:HG21	1.88	0.54
1:B:42:ASP:HB2	1:B:252:ARG:HD3	1.88	0.54
1:B:196:GLU:HB3	1:B:197:PRO:HD3	1.89	0.54
1:A:290:ARG:HG3	1:A:291:ILE:N	2.23	0.53
1:B:8[A]:ARG:HG2	1:B:37:ALA:HB2	1.90	0.53
1:A:216:LEU:CD2	1:A:230:ALA:HA	2.39	0.53
1:B:25:GLU:HB2	5:B:1334:HOH:O	2.08	0.53
1:A:133:ALA:HB1	4:A:952:ACY:H2	1.90	0.52
1:A:87:GLY:HA2	1:A:260:ARG:HD2	1.91	0.52
1:B:191:ARG:HG2	1:B:198:LEU:HD13	1.91	0.51
1:B:47:VAL:HG22	1:B:261:HIS:CG	2.45	0.51
1:B:31:LEU:HD22	1:B:52[A]:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ASP:HB2	1:B:252:ARG:HH11	1.76	0.50
1:B:216:LEU:CD2	1:B:230:ALA:HA	2.42	0.49
1:B:273:SER:OG	1:B:275:LYS:HE3	2.13	0.48
1:B:31:LEU:HB3	1:B:52[B]:VAL:CG2	2.43	0.48
1:B:216:LEU:HD21	1:B:230:ALA:HA	1.97	0.47
1:A:216:LEU:HD21	1:A:230:ALA:HA	1.96	0.47
1:A:118:LEU:HD22	1:A:122:TYR:HE2	1.80	0.47
1:A:38:LEU:HD11	1:A:51:PHE:CD1	2.50	0.47
1:B:35:ARG:HG2	1:B:35:ARG:HH11	1.80	0.47
1:B:127:ARG:HH21	1:B:182:ASP:HB2	1.79	0.47
1:B:129:PRO:HA	1:B:183:LEU:O	2.16	0.46
1:B:1:MET:H1	1:B:3:GLN:HE22	1.63	0.46
1:B:131:LEU:HB2	1:B:156:VAL:HG22	1.97	0.46
1:A:129:PRO:HA	1:A:183:LEU:O	2.16	0.46
1:A:84:GLU:HG3	5:A:1452:HOH:O	2.15	0.45
1:B:133:ALA:O	1:B:159:VAL:HG22	2.17	0.45
1:B:1:MET:O	1:B:2:PHE:HB2	2.17	0.45
1:B:174:GLU:O	1:B:178:LEU:HG	2.17	0.45
1:A:193:GLN:HG2	5:A:1443:HOH:O	2.16	0.45
1:B:149:GLY:O	1:B:152:VAL:HG22	2.17	0.44
1:A:275:LYS:HB2	1:A:276:PRO:HD2	1.99	0.44
1:A:273:SER:OG	1:A:275:LYS:HG2	2.17	0.44
1:B:107:GLN:HA	3:B:910:GNP:O2G	2.17	0.44
1:B:128:ARG:NH2	1:B:181:ARG:HH21	2.15	0.44
1:A:93:PRO:HB2	1:A:101:TRP:CH2	2.53	0.44
1:B:188:THR:HB	1:B:202:LEU:HD21	2.00	0.44
1:A:135:ASP:HB2	4:A:952:ACY:H1	1.99	0.43
1:A:1:MET:HE3	1:A:253:GLY:HA2	1.99	0.43
1:A:1:MET:O	1:A:2:PHE:HB2	2.18	0.43
1:B:273:SER:HG	1:B:275:LYS:HE3	1.82	0.43
1:A:131:LEU:HB2	1:A:156:VAL:HG22	1.99	0.43
1:B:6[B]:SER:O	1:B:10:GLN:HG3	2.18	0.43
1:A:135:ASP:CB	4:A:952:ACY:H1	2.49	0.43
1:B:101:TRP:CD1	1:B:213:GLU:HB2	2.54	0.43
1:B:1:MET:N	1:B:3:GLN:NE2	2.66	0.42
1:A:195:ASP:CG	1:A:197:PRO:HD2	2.39	0.42
1:B:2:PHE:HE1	1:B:247:LEU:HD22	1.85	0.42
1:B:247:LEU:HD23	1:B:247:LEU:HA	1.91	0.42
1:B:6[A]:SER:O	1:B:10:GLN:HG3	2.19	0.42
1:A:94:VAL:HG23	5:A:1252:HOH:O	2.20	0.42
1:B:187:ASP:OD2	4:B:950:ACY:H2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HD12	1:A:292:LEU:HD13	2.01	0.42
1:A:8:ARG:HD3	1:A:8:ARG:HA	1.87	0.42
1:A:239:VAL:HG12	1:A:240:THR:N	2.35	0.42
1:B:1:MET:HG3	1:B:251:ALA:O	2.20	0.41
1:B:70:PRO:O	1:B:74:ILE:HG12	2.20	0.41
1:B:1:MET:HG2	1:B:2:PHE:CD1	2.55	0.41
1:A:221:MET:SD	1:A:249:GLY:HA3	2.61	0.41
1:B:31:LEU:HB3	1:B:52[A]:VAL:CG1	2.49	0.41
1:B:261:HIS:HB2	5:B:1266:HOH:O	2.20	0.41
1:A:79:TYR:OH	1:A:285:GLU:HG3	2.21	0.41
1:B:147:LEU:O	1:B:151:LYS:HB2	2.21	0.41
1:A:3:GLN:HB2	1:A:3:GLN:HE21	1.76	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1121:HOH:O	5:B:1407:HOH:O[2_656]	1.93	0.27
5:B:1299:HOH:O	5:A:1385:HOH:O[3_445]	2.02	0.18
5:A:1180:HOH:O	5:A:1321:HOH:O[2_655]	2.04	0.16
5:B:1158:HOH:O	5:A:1050:HOH:O[4_546]	2.11	0.09

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	295/296 (100%)	289 (98%)	6 (2%)	0	100	100
1	B	299/296 (101%)	295 (99%)	4 (1%)	0	100	100
All	All	594/592 (100%)	584 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	235/234 (100%)	225 (96%)	10 (4%)	35	23
1	B	239/234 (102%)	230 (96%)	9 (4%)	40	28
All	All	474/468 (101%)	455 (96%)	19 (4%)	37	26

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	GLN
1	B	63	GLN
1	B	103	LEU
1	B	173	GLU
1	B	181	ARG
1	B	212	ASP
1	B	231	ARG
1	B	252	ARG
1	B	277	GLU
1	A	1	MET
1	A	4	GLN
1	A	83	LYS
1	A	96	LYS
1	A	98	ARG
1	A	103	LEU
1	A	231	ARG
1	A	250	ASP
1	A	273	SER
1	A	290	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3	GLN
1	B	99	ASN
1	B	144	GLN

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Mol	Chain	Res	Type
1	B	193	GLN
1	B	261	HIS
1	A	44	ASN
1	A	99	ASN
1	A	224	GLN
1	A	261	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
3	GNP	A	911	-	28,34,34	2.03	11 (39%)	33,54,54	2.30	7 (21%)
4	ACY	A	952	-	1,3,3	3.85	1 (100%)	0,3,3	0.00	-
4	ACY	A	953	-	1,3,3	4.61	1 (100%)	0,3,3	0.00	-
3	GNP	B	910	-	28,34,34	2.00	12 (42%)	33,54,54	2.32	7 (21%)
4	ACY	B	950	-	1,3,3	4.59	1 (100%)	0,3,3	0.00	-
4	ACY	B	951	-	1,3,3	4.79	1 (100%)	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GNP	A	911	-	-	0/12/38/38	0/3/3/3
4	ACY	A	952	-	-	0/0/0/0	0/0/0/0
4	ACY	A	953	-	-	0/0/0/0	0/0/0/0
3	GNP	B	910	-	-	0/12/38/38	0/3/3/3
4	ACY	B	950	-	-	0/0/0/0	0/0/0/0
4	ACY	B	951	-	-	0/0/0/0	0/0/0/0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	910	GNP	C8-N7	-2.57	1.29	1.34
3	A	911	GNP	C8-N7	-2.56	1.29	1.34
3	B	910	GNP	PG-O2G	-2.37	1.50	1.56
3	A	911	GNP	PG-O3G	-2.36	1.50	1.56
3	B	910	GNP	PB-O2B	-2.25	1.50	1.56
3	A	911	GNP	PG-O2G	-2.25	1.50	1.56
3	A	911	GNP	PB-O2B	-2.22	1.50	1.56
3	B	910	GNP	PG-O3G	-2.18	1.50	1.56
3	B	910	GNP	C4-N3	2.06	1.38	1.35
3	B	910	GNP	C2-N1	2.60	1.40	1.35
3	A	911	GNP	C2-N1	2.63	1.40	1.35
3	B	910	GNP	C6-C5	2.78	1.46	1.41
3	A	911	GNP	C6-C5	2.86	1.47	1.41
3	B	910	GNP	PG-N3B	2.91	1.71	1.63
3	B	910	GNP	PB-N3B	2.93	1.71	1.63
3	A	911	GNP	PG-N3B	3.09	1.71	1.63
3	A	911	GNP	PB-N3B	3.16	1.71	1.63
3	B	910	GNP	PG-O1G	3.47	1.50	1.46
3	A	911	GNP	PG-O1G	3.54	1.50	1.46
4	A	952	ACY	CH3-C	3.85	1.54	1.48
3	A	911	GNP	PB-O1B	3.86	1.50	1.46
3	B	910	GNP	PB-O1B	3.87	1.50	1.46
3	B	910	GNP	C6-N1	4.12	1.40	1.33
3	A	911	GNP	C6-N1	4.17	1.40	1.33
4	B	950	ACY	CH3-C	4.59	1.55	1.48
4	A	953	ACY	CH3-C	4.61	1.55	1.48
4	B	951	ACY	CH3-C	4.79	1.55	1.48

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	911	GNP	C5-C6-N1	-8.06	112.57	123.59
3	B	910	GNP	C5-C6-N1	-8.02	112.62	123.59
3	B	910	GNP	N3-C2-N1	-3.52	122.08	127.44
3	A	911	GNP	N3-C2-N1	-3.49	122.12	127.44
3	B	910	GNP	O1G-PG-N3B	-2.24	108.46	111.90
3	A	911	GNP	O1B-PB-N3B	-2.14	108.62	111.90
3	B	910	GNP	O1B-PB-N3B	-2.11	108.66	111.90
3	A	911	GNP	O3A-PB-N3B	-2.11	100.64	106.44
3	A	911	GNP	C6-C5-C4	-2.07	118.43	120.90
3	B	910	GNP	C6-C5-C4	-2.03	118.47	120.90
3	B	910	GNP	O2B-PB-O1B	4.23	118.83	110.00
3	A	911	GNP	O2B-PB-O1B	4.24	118.85	110.00
3	A	911	GNP	C6-N1-C2	6.93	125.56	115.94
3	B	910	GNP	C6-N1-C2	6.96	125.61	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	952	ACY	3	0
3	B	910	GNP	1	0
4	B	950	ACY	1	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	296/296 (100%)	7.18	296 (100%)	0	0	8, 17, 37, 63	0
1	B	295/296 (99%)	7.43	295 (100%)	0	0	10, 20, 43, 65	0
All	All	591/592 (99%)	7.31	591 (100%)	0	0	8, 18, 42, 65	0

All (591) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	PRO	16.9
1	B	273	SER	16.9
1	A	251	ALA	16.6
1	B	194	ILE	16.5
1	B	295	GLY	16.1
1	B	272	VAL	15.3
1	B	192	LEU	14.1
1	B	23	THR	13.7
1	A	255	ALA	13.4
1	B	178	LEU	13.2
1	A	272	VAL	13.1
1	B	276	PRO	13.1
1	B	251	ALA	13.0
1	B	22	ILE	13.0
1	B	20	GLY	12.7
1	A	2	PHE	12.5
1	B	294	MET	12.4
1	B	94	VAL	12.4
1	B	195	ASP	12.4
1	A	194	ILE	12.2
1	B	274	GLU	12.2
1	B	193	GLN	12.2
1	B	1	MET	12.2
1	A	250	ASP	12.2

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Mol	Chain	Res	Type	RSRZ
1	A	273	SER	12.2
1	B	249	GLY	12.1
1	B	160	MET	12.1
1	A	254	GLY	11.9
1	B	2	PHE	11.9
1	A	252	ARG	11.7
1	A	249	GLY	11.7
1	A	278	GLY	11.7
1	A	192	LEU	11.7
1	B	197	PRO	11.2
1	B	26	ASP	11.2
1	A	98	ARG	11.1
1	A	193	GLN	11.1
1	B	95	LEU	11.0
1	B	65	LEU	11.0
1	B	196	GLU	11.0
1	A	275	LYS	10.9
1	A	94	VAL	10.9
1	A	195	ASP	10.9
1	A	274	GLU	10.9
1	B	252	ARG	10.8
1	B	198	LEU	10.7
1	B	19	ARG	10.7
1	A	95	LEU	10.6
1	A	18	GLY	10.6
1	A	253	GLY	10.6
1	A	133	ALA	10.5
1	A	132	VAL	10.5
1	A	131	LEU	10.4
1	A	243	VAL	10.2
1	B	275	LYS	10.1
1	A	198	LEU	10.1
1	A	101	TRP	10.1
1	B	126	GLY	10.1
1	A	283	TYR	10.1
1	B	177	ARG	10.1
1	B	293	GLY	10.1
1	B	283	TYR	10.0
1	B	214	VAL	10.0
1	A	97	ASP	10.0
1	A	217	VAL	9.9
1	B	123	LYS	9.9

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Mol	Chain	Res	Type	RSRZ
1	B	98	ARG	9.8
1	B	229	VAL	9.8
1	A	279	LEU	9.8
1	B	250	ASP	9.8
1	A	34	ILE	9.8
1	A	19	ARG	9.8
1	A	145	LEU	9.8
1	A	183	LEU	9.8
1	A	186	VAL	9.7
1	A	277	GLU	9.7
1	B	66	GLU	9.6
1	B	217	VAL	9.6
1	A	185	LEU	9.6
1	B	161	ASP	9.6
1	B	21	ARG	9.6
1	B	278	GLY	9.5
1	B	104	VAL	9.5
1	A	216	LEU	9.5
1	A	116	ALA	9.4
1	A	71	ALA	9.4
1	B	38	LEU	9.3
1	B	124	GLY	9.3
1	B	242	LEU	9.3
1	A	20	GLY	9.3
1	B	176	ALA	9.2
1	A	247	LEU	9.2
1	A	104	VAL	9.2
1	B	68	LEU	9.2
1	A	79	TYR	9.2
1	B	24	GLU	9.1
1	B	279	LEU	9.1
1	B	243	VAL	9.1
1	A	55	VAL	9.1
1	B	25	GLU	9.1
1	A	168	ILE	9.0
1	B	101	TRP	9.0
1	B	27	LEU	9.0
1	B	247	LEU	9.0
1	A	7	ALA	8.9
1	A	1	MET	8.9
1	B	152	VAL	8.9
1	A	154	VAL	8.9

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Mol	Chain	Res	Type	RSRZ
1	B	102	PHE	8.9
1	A	248	ASP	8.9
1	A	214	VAL	8.8
1	A	44	ASN	8.8
1	A	261	HIS	8.8
1	B	3	GLN	8.8
1	B	277	GLU	8.8
1	A	257	LEU	8.8
1	B	108	GLY	8.8
1	B	78	VAL	8.8
1	A	119	ALA	8.8
1	A	78	VAL	8.7
1	A	65	LEU	8.7
1	A	159	VAL	8.7
1	A	42	ASP	8.7
1	B	48	ALA	8.7
1	B	97	ASP	8.7
1	B	91	ARG	8.7
1	A	215	LEU	8.6
1	A	3	GLN	8.6
1	A	184	ILE	8.6
1	B	241	GLY	8.6
1	A	282	PHE	8.6
1	B	47	VAL	8.6
1	A	134	ALA	8.5
1	B	43	VAL	8.5
1	A	156	VAL	8.5
1	A	36	ARG	8.5
1	B	180	ALA	8.5
1	B	233	PHE	8.5
1	A	102	PHE	8.5
1	B	137	GLN	8.5
1	B	267	ILE	8.4
1	B	226	ALA	8.4
1	A	43	VAL	8.4
1	A	160[A]	MET	8.4
1	B	17	ARG	8.4
1	B	85	ALA	8.3
1	B	218	LEU	8.3
1	A	218	LEU	8.3
1	A	256	ALA	8.3
1	B	51	PHE	8.3

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Mol	Chain	Res	Type	RSRZ
1	B	186	VAL	8.3
1	A	73	VAL	8.3
1	B	45	LEU	8.2
1	A	286	ARG	8.2
1	A	130	LEU	8.2
1	A	120	LEU	8.2
1	A	242	LEU	8.2
1	B	184	ILE	8.2
1	A	157	LEU	8.1
1	B	230	ALA	8.1
1	B	208	VAL	8.1
1	B	174	GLU	8.1
1	A	118	LEU	8.1
1	A	233	PHE	8.1
1	B	96	LYS	8.1
1	B	89	GLU	8.1
1	B	52[A]	VAL	8.1
1	B	90	ALA	8.1
1	B	205	LEU	8.1
1	B	131	LEU	8.0
1	B	122	TYR	8.0
1	B	92	LEU	8.0
1	A	100	LEU	8.0
1	B	248	ASP	8.0
1	B	263	THR	8.0
1	A	75	LEU	8.0
1	A	121	TYR	7.9
1	B	60	LEU	7.9
1	A	59	ALA	7.9
1	A	51	PHE	7.9
1	B	120	LEU	7.9
1	B	216	LEU	7.9
1	B	39[A]	MET	7.9
1	B	290	ARG	7.9
1	A	92	LEU	7.9
1	A	172	VAL	7.9
1	B	255	ALA	7.8
1	A	81	ALA	7.8
1	A	74	ILE	7.8
1	A	9	LEU	7.8
1	A	292	LEU	7.8
1	B	172	VAL	7.8

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Mol	Chain	Res	Type	RSRZ
1	B	29	ALA	7.8
1	A	122	TYR	7.8
1	B	67	SER	7.7
1	A	197	PRO	7.7
1	B	79	TYR	7.7
1	B	32	ARG	7.7
1	A	60	LEU	7.7
1	B	153	GLY	7.7
1	B	256	ALA	7.7
1	B	125	LYS	7.7
1	A	113	THR	7.7
1	A	259	ALA	7.7
1	B	4	GLN	7.7
1	A	229	VAL	7.6
1	A	155	PRO	7.6
1	A	267	ILE	7.6
1	B	147	LEU	7.6
1	A	205	LEU	7.6
1	B	138	ARG	7.6
1	B	253	GLY	7.6
1	A	112	THR	7.6
1	A	126	GLY	7.6
1	B	237	VAL	7.6
1	A	196	GLU	7.6
1	A	244	LEU	7.6
1	B	159	VAL	7.6
1	B	170	ARG	7.6
1	A	280	GLU	7.6
1	B	182	ASP	7.6
1	A	91	ARG	7.6
1	A	38	LEU	7.5
1	A	224	GLN	7.5
1	A	239	VAL	7.5
1	B	151	LYS	7.5
1	B	154	VAL	7.5
1	A	76	ALA	7.5
1	A	27	LEU	7.5
1	A	64	VAL	7.5
1	A	115	ALA	7.5
1	A	203	ALA	7.5
1	B	75	LEU	7.5
1	A	68	LEU	7.5

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Mol	Chain	Res	Type	RSRZ
1	B	128	ARG	7.5
1	B	239	VAL	7.4
1	A	287	LEU	7.4
1	B	271	GLY	7.4
1	A	268	TYR	7.4
1	B	257	LEU	7.4
1	A	231	ARG	7.4
1	B	148	LEU	7.4
1	B	41	ALA	7.3
1	B	215	LEU	7.3
1	B	291	ILE	7.3
1	B	145	LEU	7.3
1	B	259	ALA	7.3
1	B	76	ALA	7.3
1	B	86	LEU	7.3
1	A	260	ARG	7.3
1	B	202	LEU	7.2
1	A	69	THR	7.2
1	A	180	ALA	7.2
1	B	63	GLN	7.2
1	A	5	LEU	7.2
1	B	7	ALA	7.2
1	B	258	SER	7.2
1	B	280	GLU	7.2
1	B	209	LEU	7.2
1	B	287	LEU	7.2
1	B	34	ILE	7.2
1	B	269	PHE	7.2
1	A	31	LEU	7.2
1	B	132	VAL	7.2
1	A	13	ILE	7.2
1	A	288	ALA	7.1
1	B	268	TYR	7.1
1	B	100	LEU	7.1
1	A	45	LEU	7.1
1	B	262	VAL	7.1
1	B	168	ILE	7.1
1	B	61	GLY	7.1
1	A	269	PHE	7.1
1	B	185	LEU	7.1
1	A	227	LEU	7.1
1	A	129	PRO	7.1

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Mol	Chain	Res	Type	RSRZ
1	B	13	ILE	7.1
1	A	285	GLU	7.1
1	B	88	GLY	7.1
1	B	264	GLY	7.1
1	B	93	PRO	7.1
1	B	82	LEU	7.1
1	B	55	VAL	7.1
1	A	291	ILE	7.1
1	A	178	LEU	7.0
1	A	48	ALA	7.0
1	A	141	ALA	7.0
1	B	231	ARG	7.0
1	B	227	LEU	7.0
1	A	148	LEU	7.0
1	B	183	LEU	7.0
1	B	156	VAL	7.0
1	A	103	LEU	7.0
1	A	90	ALA	7.0
1	A	237	VAL	7.0
1	A	202	LEU	7.0
1	A	85	ALA	6.9
1	A	177	ARG	6.9
1	B	121	TYR	6.9
1	A	52	VAL	6.9
1	A	262	VAL	6.9
1	A	88	GLY	6.9
1	B	103	LEU	6.9
1	A	151	LYS	6.9
1	A	208	VAL	6.9
1	B	59	ALA	6.9
1	A	24	GLU	6.9
1	B	181	ARG	6.9
1	B	16	LEU	6.9
1	B	64	VAL	6.9
1	A	290	ARG	6.9
1	B	28	LYS	6.8
1	B	130	LEU	6.8
1	B	240	THR	6.8
1	A	37	ALA	6.8
1	B	188	THR	6.8
1	A	226	ALA	6.8
1	B	8[A]	ARG	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	149	GLY	6.8
1	B	157	LEU	6.8
1	B	139	PRO	6.8
1	A	70	PRO	6.8
1	A	165	PRO	6.8
1	A	114	THR	6.8
1	A	106	LEU	6.7
1	A	209	LEU	6.7
1	A	124	GLY	6.7
1	B	173	GLU	6.7
1	A	245	THR	6.7
1	B	232	ALA	6.7
1	B	73	VAL	6.7
1	B	244	LEU	6.7
1	B	5	LEU	6.7
1	A	211	PRO	6.7
1	B	107	GLN	6.7
1	A	140	ALA	6.6
1	A	16	LEU	6.6
1	A	22	ILE	6.6
1	A	82	LEU	6.6
1	A	47	VAL	6.6
1	A	40	ASP	6.6
1	A	135	ASP	6.6
1	B	203	ALA	6.6
1	A	67	SER	6.6
1	B	18	GLY	6.6
1	B	69	THR	6.6
1	B	81	ALA	6.6
1	A	136	THR	6.6
1	A	96	LYS	6.6
1	B	105	GLY	6.5
1	A	29	ALA	6.5
1	B	36	ARG	6.5
1	B	62	LYS	6.5
1	A	86	LEU	6.5
1	B	222	THR	6.5
1	B	199	MET	6.5
1	B	54	ARG	6.5
1	A	176	ALA	6.5
1	A	189	ALA	6.5
1	B	245	THR	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	129	PRO	6.5
1	B	282	PHE	6.5
1	B	140	ALA	6.5
1	B	71	ALA	6.5
1	A	77	THR	6.5
1	B	155	PRO	6.4
1	B	115	ALA	6.4
1	B	113[A]	THR	6.4
1	B	220	ALA	6.4
1	A	41	ALA	6.4
1	B	292	LEU	6.4
1	A	220	ALA	6.4
1	A	152	VAL	6.4
1	B	37	ALA	6.4
1	B	133	ALA	6.4
1	A	235	GLU	6.4
1	A	199	MET	6.4
1	B	127	ARG	6.3
1	A	147	LEU	6.3
1	A	240	THR	6.3
1	B	112	THR	6.3
1	A	294	MET	6.3
1	B	70	PRO	6.3
1	A	170	ARG	6.3
1	A	187	ASP	6.3
1	A	164	SER	6.3
1	A	149	GLY	6.3
1	A	210	GLY	6.2
1	A	12	ALA	6.2
1	A	87	GLY	6.2
1	B	134	ALA	6.2
1	B	6[A]	SER	6.2
1	A	228	SER	6.2
1	A	63	GLN	6.2
1	A	225	GLU	6.2
1	B	266	PRO	6.2
1	A	137	GLN	6.2
1	B	162	GLY	6.2
1	B	74	ILE	6.2
1	A	107	GLN	6.2
1	A	266	PRO	6.1
1	A	212	ASP	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	212	ASP	6.1
1	A	17	ARG	6.1
1	A	105	GLY	6.1
1	B	189	ALA	6.1
1	A	4	GLN	6.1
1	A	30	THR	6.1
1	A	263	THR	6.1
1	B	109	SER	6.1
1	A	153	GLY	6.1
1	B	116	ALA	6.1
1	A	232	ALA	6.1
1	B	281	PRO	6.0
1	B	179	GLU	6.0
1	A	296	ASP	6.0
1	B	114	THR	6.0
1	A	142	ARG	6.0
1	A	62	LYS	6.0
1	A	139	PRO	6.0
1	B	99	ASN	6.0
1	A	167	SER	6.0
1	B	210	GLY	6.0
1	A	223	GLY	6.0
1	A	89	GLU	6.0
1	B	14	GLY	6.0
1	B	211	PRO	6.0
1	A	93	PRO	6.0
1	A	15	ARG	6.0
1	B	9	LEU	6.0
1	A	293	GLY	5.9
1	B	12	ALA	5.9
1	B	31	LEU	5.9
1	B	106	LEU	5.9
1	B	238	GLY	5.9
1	A	8	ARG	5.9
1	B	254	GLY	5.9
1	A	222	THR	5.9
1	B	265	LYS	5.9
1	A	39	MET	5.9
1	B	235	GLU	5.8
1	B	175	LYS	5.8
1	A	230	ALA	5.8
1	A	162	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	40	ASP	5.8
1	B	270	ALA	5.8
1	A	284	PRO	5.8
1	B	261	HIS	5.8
1	B	221	MET	5.8
1	B	44	ASN	5.8
1	B	30	THR	5.8
1	B	136	THR	5.8
1	B	223	GLY	5.8
1	A	238	GLY	5.7
1	A	171	ARG	5.7
1	B	141	ALA	5.7
1	B	284	PRO	5.7
1	A	108	GLY	5.7
1	A	188	THR	5.7
1	A	14	GLY	5.7
1	A	241	GLY	5.7
1	B	119	ALA	5.7
1	B	288	ALA	5.7
1	A	281	PRO	5.7
1	A	161	ASP	5.6
1	B	118	LEU	5.6
1	A	25	GLU	5.6
1	B	77	THR	5.5
1	B	190	GLY	5.5
1	A	270	ALA	5.5
1	B	260	ARG	5.5
1	A	23	THR	5.5
1	B	204	ARG	5.5
1	B	286	ARG	5.5
1	B	228	SER	5.5
1	B	35	ARG	5.5
1	A	146	ARG	5.5
1	A	264	GLY	5.5
1	B	15	ARG	5.4
1	A	295	GLY	5.4
1	B	224	GLN	5.4
1	A	181	ARG	5.4
1	B	169	ARG	5.4
1	B	164	SER	5.4
1	A	49	ARG	5.4
1	B	165	PRO	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	58	GLU	5.3
1	A	150	GLU	5.3
1	A	289	GLY	5.3
1	A	234	ASP	5.3
1	B	144	GLN	5.3
1	B	167	SER	5.3
1	A	271	GLY	5.3
1	A	35	ARG	5.3
1	A	61	GLY	5.3
1	A	125	LYS	5.3
1	B	200	GLY	5.2
1	A	128	ARG	5.2
1	B	289	GLY	5.2
1	A	54	ARG	5.2
1	B	150	GLU	5.2
1	B	49	ARG	5.1
1	A	221	MET	5.1
1	A	144	GLN	5.1
1	A	66	GLU	5.1
1	A	99	ASN	5.1
1	B	142	ARG	5.1
1	B	285	GLU	5.1
1	A	127	ARG	5.1
1	B	87	GLY	5.1
1	A	200	GLY	5.1
1	B	80[A]	GLU	5.1
1	A	110	GLY	5.1
1	B	11	GLU	5.0
1	A	46	GLU	5.0
1	B	191	ARG	5.0
1	A	32	ARG	5.0
1	B	219	ASP	5.0
1	A	258	SER	5.0
1	A	169	ARG	5.0
1	A	6	SER	5.0
1	A	109	SER	4.9
1	A	50	ASP	4.9
1	A	33	GLU	4.9
1	A	182	ASP	4.9
1	A	236	LYS	4.9
1	A	173	GLU	4.9
1	B	56	ARG	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	10	GLN	4.9
1	A	191	ARG	4.9
1	B	201	GLU	4.9
1	B	206	LYS	4.9
1	B	236	LYS	4.9
1	A	10	GLN	4.9
1	B	42	ASP	4.8
1	B	110	GLY	4.8
1	A	56	ARG	4.8
1	A	83	LYS	4.8
1	A	80	GLU	4.8
1	A	204	ARG	4.8
1	B	72	GLU	4.8
1	B	84	GLU	4.8
1	A	138	ARG	4.8
1	B	83	LYS	4.8
1	B	187	ASP	4.8
1	A	21	ARG	4.7
1	B	135	ASP	4.7
1	A	11	GLU	4.7
1	A	111	LYS	4.7
1	A	58	GLU	4.7
1	A	174	GLU	4.7
1	B	50	ASP	4.6
1	B	225	GLU	4.6
1	A	57	GLU	4.6
1	A	84	GLU	4.6
1	B	57	GLU	4.6
1	A	219	ASP	4.6
1	A	72	GLU	4.6
1	B	234	ASP	4.6
1	B	33	GLU	4.6
1	B	207	GLU	4.6
1	A	26	ASP	4.5
1	B	46	GLU	4.5
1	A	117	LYS	4.5
1	A	201	GLU	4.5
1	B	111	LYS	4.5
1	A	190	GLY	4.5
1	A	53	GLU	4.5
1	B	117	LYS	4.5
1	A	206	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	179	GLU	4.4
1	A	207	GLU	4.4
1	A	28	LYS	4.4
1	B	213	GLU	4.4
1	A	143	GLU	4.4
1	A	123	LYS	4.3
1	A	163	GLU	4.3
1	B	53	GLU	4.3
1	B	171	ARG	4.2
1	A	246	LYS	4.2
1	A	175	LYS	4.2
1	A	213	GLU	4.2
1	A	166	GLU	4.1
1	B	246	LYS	4.1
1	A	265	LYS	4.1
1	B	158	GLU	4.1
1	A	158	GLU	4.0
1	B	146	ARG	3.9
1	B	163	GLU	3.8
1	B	166	GLU	3.8
1	B	143	GLU	3.4

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	ACY	B	950	4/4	-0.06	0.70	12.11	41,42,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	ACY	A	953	4/4	-0.06	0.95	6.14	62,64,64,65	0
4	ACY	A	952	4/4	-0.04	0.91	6.01	90,90,91,92	0
4	ACY	B	951	4/4	-0.00	0.83	3.95	44,45,46,47	0
2	CA	A	901	1/1	0.71	0.57	1.51	37,37,37,37	0
3	GNP	B	910	32/32	0.16	0.72	1.04	23,51,71,71	0
3	GNP	A	911	32/32	0.28	0.63	0.90	20,31,48,50	0
2	CA	B	900	1/1	0.99	0.32	-4.56	16,16,16,16	0

6.5 Other polymers

There are no such residues in this entry.