



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:27 PM GMT

PDB ID : 4IDP  
Title : human atlastin-1 1-446, N440T, GppNHp  
Authors : Byrnes, L.J.; Singh, A.; Szeto, K.; Benveniste, N.M.; O'Donnell, J.P.; Zipfel, W.R.;  
Sondermann, H.  
Deposited on : 2012-12-12  
Resolution : 2.59 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](mailto: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.

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

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

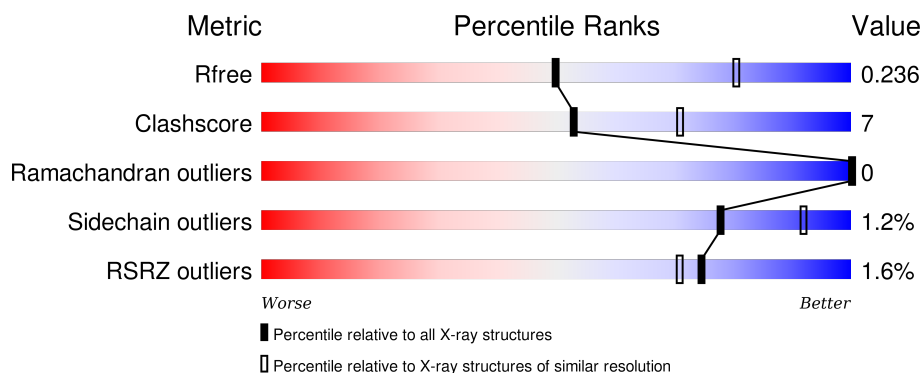
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	447	<div> <div>2%</div> <div>78% 14% 7%</div> </div>
1	B	447	<div> <div>2%</div> <div>78% 14% 7%</div> </div>
1	C	447	<div> <div>%</div> <div>79% 13% 7%</div> </div>
1	D	447	<div> <div>%</div> <div>79% 13% 7%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14015 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 Atlastin-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	Se	0	4	0
			3376	2159	565	639	4	9			
1	B	416	Total	C	N	O	S	Se	0	4	0
			3378	2160	569	636	4	9			
1	C	416	Total	C	N	O	S	Se	0	0	0
			3351	2143	562	633	4	9			
1	D	417	Total	C	N	O	S	Se	0	3	0
			3375	2158	566	638	4	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q8WXF7
A	440	THR	ASN	ENGINEERED MUTATION	UNP Q8WXF7
B	0	SER	-	EXPRESSION TAG	UNP Q8WXF7
B	440	THR	ASN	ENGINEERED MUTATION	UNP Q8WXF7
C	0	SER	-	EXPRESSION TAG	UNP Q8WXF7
C	440	THR	ASN	ENGINEERED MUTATION	UNP Q8WXF7
D	0	SER	-	EXPRESSION TAG	UNP Q8WXF7
D	440	THR	ASN	ENGINEERED MUTATION	UNP Q8WXF7

- Molecule 2 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
2	A	1	Total 32	C 10	N 6	O 13	P 3	0	0
2	B	1	Total 32	C 10	N 6	O 13	P 3	0	0
2	C	1	Total 32	C 10	N 6	O 13	P 3	0	0
2	D	1	Total 32	C 10	N 6	O 13	P 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	110	Total O 110 110	0	0

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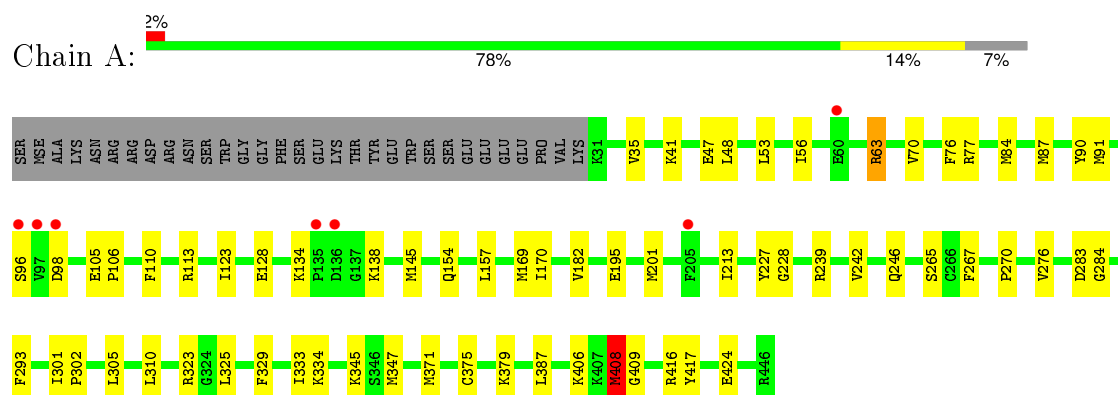
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	99	Total	O	0	0
			99	99		
4	C	99	Total	O	0	0
			99	99		
4	D	95	Total	O	0	0
			95	95		

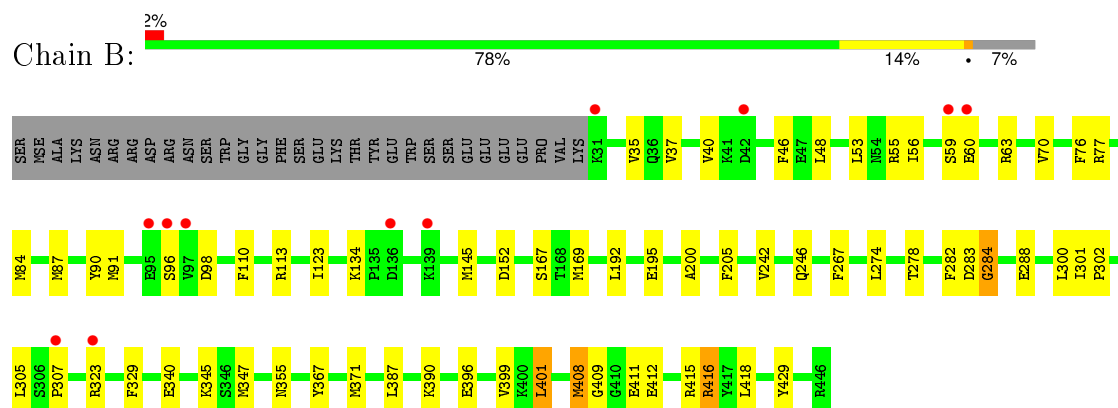
### 3 Residue-property plots

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.

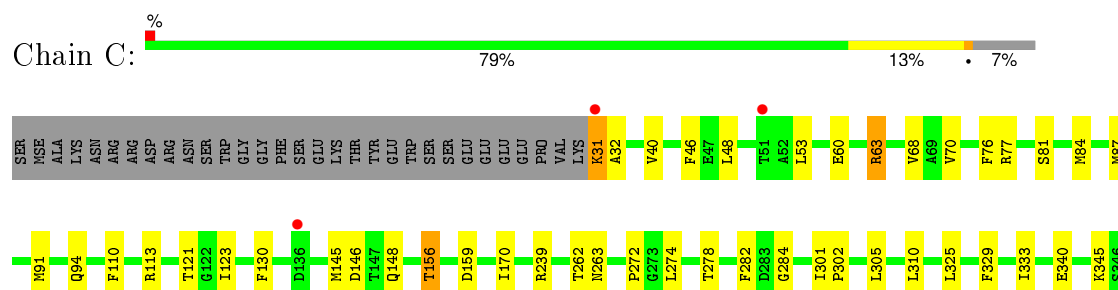
#### • Molecule 1: Atlastin-1

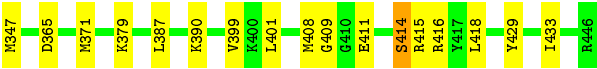


#### • Molecule 1: Atlastin-1

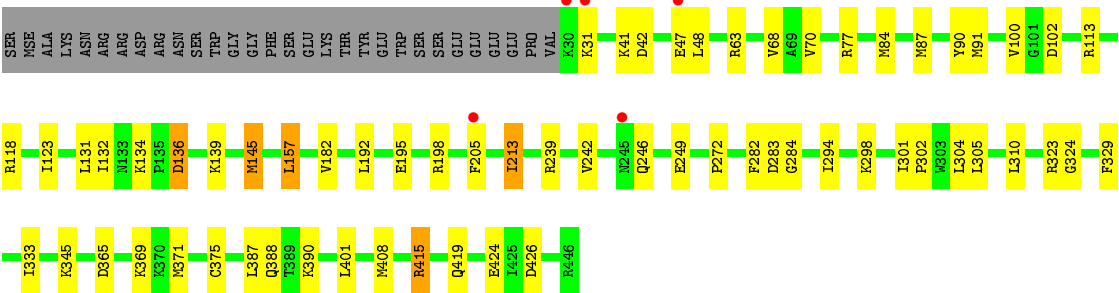
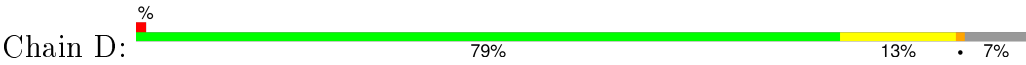


#### • Molecule 1: Atlastin-1





● Molecule 1: Atlastin-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.95Å 268.12Å 62.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 2.59 49.68 – 2.59	Depositor EDS
% Data completeness (in resolution range)	80.3 (49.68-2.59) 80.7 (49.68-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.201 , 0.236 0.198 , 0.236	Depositor DCC
$R_{free}$ test set	1985 reflections (3.52%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.56$ , $\langle L^2 \rangle = 0.41$	Xtriage
Outliers	17 of 56716 reflections (0.030%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14015	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	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 65.46 % 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 7.0629e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GNP, MG

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	0.69	2/3450 (0.1%)	0.84	8/4637 (0.2%)
1	B	0.65	1/3452 (0.0%)	0.81	8/4638 (0.2%)
1	C	0.65	0/3413	0.81	3/4587 (0.1%)
1	D	0.68	1/3446 (0.0%)	0.86	9/4631 (0.2%)
All	All	0.67	4/13761 (0.0%)	0.83	28/18493 (0.2%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	375	CYS	CB-SG	-8.12	1.68	1.82
1	A	375	CYS	CB-SG	-6.08	1.72	1.82
1	A	154	GLN	CG-CD	5.43	1.63	1.51
1	B	396	GLU	CG-CD	5.27	1.59	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	ILE	CG1-CB-CG2	-9.93	89.56	111.40
1	D	157	LEU	CB-CG-CD2	-9.04	95.63	111.00
1	D	283	ASP	CB-CG-OD2	-8.43	110.72	118.30
1	C	408	MSE	CA-CB-CG	7.72	126.42	113.30
1	D	415	ARG	NE-CZ-NH1	-6.72	116.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	145	MSE	CA-CB-CG	6.46	124.29	113.30
1	A	283	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	B	283	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	C	31	LYS	CG-CD-CE	-6.11	93.57	111.90
1	D	408	MSE	CA-CB-CG	6.00	123.49	113.30
1	D	401	LEU	CB-CG-CD1	-5.99	100.82	111.00
1	B	408	MSE	CA-CB-CG	5.94	123.39	113.30
1	A	323	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	A	138	LYS	CD-CE-NZ	-5.69	98.62	111.70
1	B	288	GLU	CA-CB-CG	-5.67	100.93	113.40
1	B	55	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	198	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	323	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	A	63	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	A	63	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	B	323	ARG	CG-CD-NE	5.24	122.80	111.80
1	A	284	GLY	N-CA-C	5.21	126.11	113.10
1	B	205	PHE	CB-CG-CD1	-5.19	117.17	120.80
1	C	365	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	401	LEU	CB-CG-CD1	-5.11	102.32	111.00
1	D	102	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	379	LYS	CD-CE-NZ	-5.05	100.09	111.70
1	B	284	GLY	N-CA-C	5.04	125.69	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	408	MSE	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3376	0	3356	48	0
1	B	3378	0	3367	51	0
1	C	3351	0	3328	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3375	0	3352	47	0
2	A	32	0	13	1	0
2	B	32	0	13	0	0
2	C	32	0	13	2	0
2	D	32	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	110	0	0	4	0
4	B	99	0	0	2	0
4	C	99	0	0	3	0
4	D	95	0	0	3	0
All	All	14015	0	13455	178	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 (178) 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:C:91:MSE:HE1	1:C:305:LEU:HD13	1.39	1.00
1:D:41:LYS:NZ	1:D:47:GLU:OE1	1.99	0.95
1:B:152:ASP:OD2	4:B:606:HOH:O	1.92	0.88
1:A:96:SER:OG	1:A:98:ASP:OD1	1.98	0.81
1:C:87:MSE:HE3	1:C:305:LEU:HD11	1.66	0.76
1:B:123:ILE:HG21	1:B:145:MSE:HE3	1.68	0.76
1:A:41:LYS:NZ	1:A:47:GLU:OE1	2.19	0.75
1:A:90:TYR:CD2	1:A:91:MSE:HE2	2.22	0.75
1:D:249:GLU:OE2	4:D:673:HOH:O	2.06	0.73
1:C:156:THR:HG22	1:C:159:ASP:H	1.55	0.71
1:A:276:VAL:O	4:A:608:HOH:O	2.09	0.70
1:B:87:MSE:HE3	1:B:305:LEU:HD11	1.72	0.70
1:D:87:MSE:HE3	1:D:305:LEU:HD11	1.73	0.69
1:B:145:MSE:HE1	1:B:167:SER:HA	1.76	0.68
1:D:131:LEU:HB3	1:D:139:LYS:HE3	1.76	0.68
1:A:91:MSE:HE3	1:A:305:LEU:HD13	1.76	0.67
1:A:77:ARG:NH2	1:A:113:ARG:O	2.28	0.67
1:A:406:LYS:HZ1	1:B:340[A]:GLU:CD	1.98	0.67
1:C:347:MSE:CE	1:D:157:LEU:HD21	2.26	0.66
1:C:340:GLU:N	1:C:340:GLU:OE1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:MSE:HE3	1:A:305:LEU:HD11	1.78	0.65
1:B:429:TYR:HE2	1:D:415:ARG:HH12	1.44	0.65
1:A:90:TYR:HD2	1:A:91:MSE:HE2	1.59	0.65
1:C:274:LEU:O	1:C:278:THR:HB	1.96	0.65
1:C:347:MSE:HE3	1:D:345:LYS:O	1.96	0.65
1:B:90:TYR:CD2	1:B:91:MSE:HE3	2.32	0.64
1:A:408:MSE:HE3	1:B:195:GLU:HG3	1.80	0.64
1:A:70:VAL:HG11	1:A:87:MSE:HE1	1.80	0.63
1:D:365:ASP:OD1	1:D:369:LYS:HE2	1.99	0.62
1:C:48:LEU:HD11	1:C:53:LEU:HD22	1.80	0.62
1:D:90:TYR:CD2	1:D:91:MSE:HE2	2.35	0.62
1:C:345:LYS:HE3	4:C:660:HOH:O	2.00	0.61
1:A:371:MSE:HE1	1:A:387:LEU:HD11	1.82	0.61
1:C:347:MSE:CE	1:D:192:LEU:HD22	2.30	0.61
1:B:355:ASN:HD22	1:B:408:MSE:H	1.48	0.61
1:C:416:ARG:NE	4:C:630:HOH:O	2.34	0.60
1:A:424:GLU:OE2	4:A:638:HOH:O	2.17	0.59
1:D:77:ARG:NH2	1:D:113:ARG:O	2.34	0.59
1:A:91:MSE:CE	1:A:305:LEU:HB3	2.31	0.59
1:A:91:MSE:HE3	1:A:305:LEU:HB3	1.85	0.59
1:C:123:ILE:HD13	1:C:145:MSE:HE2	1.83	0.59
1:B:274:LEU:O	1:B:278:THR:HB	2.03	0.59
1:B:416[A]:ARG:HH12	1:D:426:ASP:HB3	1.68	0.58
1:A:128:GLU:OE1	4:A:662:HOH:O	2.17	0.58
1:A:123:ILE:HG21	1:A:145:MSE:HE2	1.86	0.58
1:B:411:GLU:O	1:B:415:ARG:HG3	2.04	0.57
1:D:424:GLU:OE2	4:D:667:HOH:O	2.17	0.57
1:D:91:MSE:HE3	1:D:305:LEU:HB3	1.87	0.57
1:C:347:MSE:HE1	1:D:157:LEU:HD21	1.86	0.57
1:D:371:MSE:HE1	1:D:387:LEU:HD11	1.87	0.57
1:B:76:PHE:CD2	1:B:77:ARG:HG2	2.41	0.56
1:B:345:LYS:HE3	4:B:623:HOH:O	2.04	0.56
1:D:294:ILE:HG22	1:D:298:LYS:HD2	1.88	0.56
1:A:409:GLY:HA2	1:B:195:GLU:OE2	2.06	0.55
1:B:96:SER:OG	1:B:98:ASP:OD1	2.24	0.55
1:D:419:GLN:HG3	4:D:669:HOH:O	2.05	0.55
1:A:182:VAL:O	1:A:239:ARG:NH1	2.40	0.55
1:B:123:ILE:HD13	1:B:145:MSE:CE	2.37	0.54
1:B:77:ARG:NH2	1:B:113:ARG:O	2.40	0.54
1:A:301:ILE:HB	1:A:302:PRO:HD3	1.90	0.54
1:A:35:VAL:HG21	1:A:56:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ILE:HG21	1:B:145:MSE:CE	2.38	0.54
1:C:31:LYS:HG2	1:C:32:ALA:O	2.08	0.54
1:B:90:TYR:HD2	1:B:91:MSE:HE3	1.72	0.53
1:B:355:ASN:ND2	1:B:408:MSE:H	2.06	0.53
1:A:227:TYR:CZ	1:A:270:PRO:HB3	2.44	0.53
1:C:48:LEU:HB2	1:C:333:ILE:HD13	1.90	0.53
1:D:301:ILE:HB	1:D:302:PRO:HD3	1.91	0.52
1:D:90:TYR:HD2	1:D:91:MSE:HE2	1.74	0.52
1:A:87:MSE:CE	1:A:305:LEU:HD11	2.39	0.52
1:C:411:GLU:O	1:C:415:ARG:HG3	2.09	0.52
1:A:48:LEU:HB2	1:A:333:ILE:HD13	1.92	0.51
1:D:182:VAL:O	1:D:239:ARG:NH1	2.44	0.51
1:C:40:VAL:HG22	1:C:46:PHE:CD1	2.46	0.51
1:C:123:ILE:HG21	1:C:145:MSE:HE3	1.93	0.51
1:A:48:LEU:HD11	1:A:53:LEU:HD22	1.92	0.51
1:C:347:MSE:HE1	1:D:192:LEU:HD22	1.93	0.50
1:C:76:PHE:CD2	1:C:77:ARG:HG2	2.47	0.50
1:D:48:LEU:HB2	1:D:333:ILE:HD13	1.93	0.50
1:D:70:VAL:HG11	1:D:87:MSE:HE1	1.93	0.50
1:B:40:VAL:HG22	1:B:46:PHE:CD1	2.47	0.50
1:D:100:VAL:HG11	1:D:298:LYS:CG	2.41	0.50
1:A:90:TYR:HD2	1:A:91:MSE:CE	2.25	0.49
1:A:91:MSE:HE3	1:A:305:LEU:CD1	2.41	0.49
1:D:68:VAL:HG21	1:D:310:LEU:HB3	1.94	0.49
1:D:91:MSE:CE	1:D:305:LEU:HB3	2.42	0.49
1:D:63:ARG:HD3	1:D:323[A]:ARG:NH2	2.28	0.48
1:C:170:ILE:HG23	1:C:325:LEU:HD11	1.95	0.48
1:A:242:VAL:HA	1:A:246:GLN:OE1	2.14	0.48
1:A:90:TYR:CD2	1:A:91:MSE:CE	2.95	0.48
1:C:123:ILE:HD13	1:C:145:MSE:CE	2.43	0.48
1:D:90:TYR:HD2	1:D:91:MSE:CE	2.27	0.48
1:B:35:VAL:HG21	1:B:56:ILE:HD11	1.95	0.48
1:C:70:VAL:HG11	1:C:87:MSE:HE1	1.96	0.48
1:B:60:GLU:HA	1:B:63:ARG:HH21	1.79	0.48
1:C:409:GLY:HA2	1:D:195:GLU:OE2	2.12	0.47
1:C:94:GLN:O	4:C:607:HOH:O	2.19	0.47
1:B:416[A]:ARG:HG2	1:B:416[A]:ARG:H	1.45	0.47
1:C:68:VAL:HG21	1:C:310:LEU:HB3	1.97	0.47
1:B:371:MSE:HE1	1:B:387:LEU:HD11	1.97	0.47
1:D:90:TYR:CD2	1:D:91:MSE:CE	2.98	0.46
1:C:91:MSE:HB2	1:C:91:MSE:HE2	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLY:HA2	1:A:267:PHE:CZ	2.51	0.46
1:B:91:MSE:HA	1:B:91:MSE:HE2	1.97	0.46
1:D:323[B]:ARG:HG3	1:D:324:GLY:N	2.30	0.46
1:D:390:LYS:HD2	1:D:390:LYS:HA	1.77	0.46
1:D:242:VAL:HA	1:D:246:GLN:OE1	2.16	0.46
1:B:59:SER:O	1:B:63:ARG:HB3	2.15	0.46
1:B:48:LEU:HD11	1:B:53:LEU:HD22	1.97	0.46
1:C:81:SER:OG	1:C:146:ASP:OD2	2.34	0.46
1:B:301:ILE:HB	1:B:302:PRO:HD3	1.97	0.45
1:B:84:MSE:HB2	1:B:84:MSE:HE2	1.71	0.45
1:C:40:VAL:HG22	1:C:46:PHE:HD1	1.82	0.45
1:B:282:PHE:CZ	1:B:284:GLY:HA2	2.52	0.45
1:C:84:MSE:HB2	1:C:84:MSE:HE2	1.82	0.45
1:C:429:TYR:CZ	1:C:433:ILE:HD11	2.52	0.45
1:D:282:PHE:CZ	1:D:284:GLY:HA2	2.52	0.45
1:B:267:PHE:CG	1:B:300:LEU:HD13	2.52	0.45
1:B:134:LYS:HE2	1:B:307:PRO:O	2.16	0.45
1:C:371:MSE:HE1	1:C:387:LEU:HD11	1.99	0.44
1:A:345:LYS:HE3	4:A:622:HOH:O	2.17	0.44
1:C:91:MSE:HG2	1:C:130:PHE:CD2	2.52	0.44
1:B:70:VAL:HG11	1:B:87:MSE:HE1	1.99	0.44
1:B:412:GLU:HG2	1:D:388:GLN:OE1	2.17	0.44
1:A:76:PHE:CD2	1:A:77:ARG:HG2	2.53	0.44
1:B:60:GLU:CA	1:B:63:ARG:HH21	2.31	0.44
1:C:262:THR:HG22	1:C:263:ASN:OD1	2.17	0.44
1:C:282:PHE:CZ	1:C:284:GLY:HA2	2.53	0.44
1:D:134:LYS:C	1:D:136:ASP:N	2.71	0.44
1:B:84:MSE:HG2	1:B:110:PHE:CE2	2.53	0.43
1:A:77:ARG:NH1	2:A:501:GNP:HNB3	2.16	0.43
1:A:84:MSE:HE3	1:A:110:PHE:CE2	2.53	0.43
1:D:123:ILE:HG21	1:D:145:MSE:HE3	1.99	0.43
1:C:301:ILE:HB	1:C:302:PRO:HD3	2.01	0.43
1:B:40:VAL:HG22	1:B:46:PHE:HD1	1.82	0.43
1:C:390:LYS:HD3	1:C:390:LYS:HA	1.66	0.43
1:D:134:LYS:C	1:D:136:ASP:H	2.22	0.43
1:C:399:VAL:HG13	1:C:418:LEU:HD11	2.00	0.43
1:C:113:ARG:O	2:C:501:GNP:H5'1	2.19	0.43
1:A:134:LYS:HE2	1:A:310:LEU:O	2.18	0.42
1:A:91:MSE:HE3	1:A:305:LEU:CB	2.48	0.42
1:C:411:GLU:HA	1:C:414:SER:HB2	2.00	0.42
1:C:401:LEU:HA	1:C:401:LEU:HD12	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:MSE:HG2	1:C:110:PHE:CD2	2.54	0.42
1:C:347:MSE:HE3	1:D:157:LEU:HD21	1.99	0.42
1:C:60:GLU:CA	1:C:63:ARG:HH21	2.32	0.42
1:B:399:VAL:HG13	1:B:418:LEU:HD11	2.01	0.42
1:D:91:MSE:HE3	1:D:305:LEU:CB	2.49	0.42
1:A:347:MSE:SE	1:B:192:LEU:HD22	2.70	0.42
1:C:272:PRO:HG3	2:C:501:GNP:C6	2.50	0.42
1:D:272:PRO:HG3	2:D:501:GNP:C6	2.49	0.42
1:D:123:ILE:HD13	1:D:145:MSE:HE2	2.01	0.42
1:C:379:LYS:HD3	1:C:379:LYS:HA	1.89	0.42
1:A:213:ILE:HD13	1:A:265:SER:OG	2.20	0.41
1:D:70:VAL:CG1	1:D:87:MSE:HE1	2.50	0.41
1:A:195:GLU:OE2	1:B:409:GLY:HA2	2.20	0.41
1:A:170:ILE:HG23	1:A:325:LEU:HD11	2.02	0.41
1:A:70:VAL:CG1	1:A:87:MSE:HE1	2.47	0.41
1:A:157:LEU:HD21	1:B:347:MSE:SE	2.71	0.41
1:B:242:VAL:HA	1:B:246:GLN:OE1	2.21	0.41
1:C:84:MSE:HG2	1:C:110:PHE:CE2	2.56	0.41
1:A:270:PRO:HG2	1:A:293:PHE:HA	2.03	0.41
1:C:347:MSE:HE2	1:C:347:MSE:HB3	1.91	0.41
1:B:169:MSE:HE1	1:B:200:ALA:HB3	2.03	0.41
1:B:367:TYR:CZ	1:B:371:MSE:HG3	2.56	0.40
1:A:416:ARG:NE	1:A:417:TYR:CE2	2.88	0.40
1:B:37:VAL:O	1:B:48:LEU:HD12	2.21	0.40
1:C:121:THR:HA	1:C:148:GLN:HB2	2.02	0.40
1:A:169:MSE:HE3	1:A:201:MSE:HG3	2.04	0.40
1:B:401:LEU:HD12	1:B:401:LEU:HA	1.83	0.40
1:D:205:PHE:HD1	1:D:205:PHE:HA	1.73	0.40
1:D:84:MSE:HB2	1:D:84:MSE:HE2	1.81	0.40
1:A:91:MSE:HE1	1:A:305:LEU:HB3	2.00	0.40
1:B:90:TYR:CE2	1:B:91:MSE:HE3	2.57	0.40
1:A:105[A]:GLU:HA	1:A:106:PRO:HD3	1.95	0.40
1:A:195:GLU:HG2	1:B:408:MSE:HG3	2.03	0.40
1:B:390:LYS:HA	1:B:390:LYS:HD3	1.84	0.40
1:D:213:ILE:HD12	1:D:304:LEU:CD2	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	418/447 (94%)	411 (98%)	7 (2%)	0	100	100
1	B	418/447 (94%)	412 (99%)	6 (1%)	0	100	100
1	C	414/447 (93%)	407 (98%)	7 (2%)	0	100	100
1	D	418/447 (94%)	412 (99%)	6 (1%)	0	100	100
All	All	1668/1788 (93%)	1642 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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	371/385 (96%)	367 (99%)	4 (1%)	80	93
1	B	371/385 (96%)	368 (99%)	3 (1%)	86	95
1	C	367/385 (95%)	362 (99%)	5 (1%)	74	90
1	D	370/385 (96%)	364 (98%)	6 (2%)	70	88
All	All	1479/1540 (96%)	1461 (99%)	18 (1%)	78	92

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	329	PHE

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Mol	Chain	Res	Type
1	A	334	LYS
1	A	408	MSE
1	B	329	PHE
1	B	416[A]	ARG
1	B	416[B]	ARG
1	C	63	ARG
1	C	156	THR
1	C	239	ARG
1	C	329	PHE
1	C	414	SER
1	D	31	LYS
1	D	42	ASP
1	D	118	ARG
1	D	136	ASP
1	D	213	ILE
1	D	329	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	355	ASN
1	C	133	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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	GNP	A	501	3	28,34,34	1.83	5 (17%)	33,54,54	2.50	4 (12%)
2	GNP	B	501	3	28,34,34	1.97	7 (25%)	33,54,54	2.39	6 (18%)
2	GNP	C	501	3	28,34,34	1.84	7 (25%)	33,54,54	2.37	6 (18%)
2	GNP	D	501	3	28,34,34	1.70	6 (21%)	33,54,54	2.69	10 (30%)

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	GNP	A	501	3	-	0/12/38/38	0/3/3/3
2	GNP	B	501	3	-	1/12/38/38	0/3/3/3
2	GNP	C	501	3	-	0/12/38/38	0/3/3/3
2	GNP	D	501	3	-	0/12/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	GNP	PB-O3A	-3.66	1.54	1.59
2	C	501	GNP	PB-O3A	-3.62	1.54	1.59
2	B	501	GNP	PB-O3A	-3.48	1.54	1.59
2	D	501	GNP	PB-O3A	-3.28	1.55	1.59
2	A	501	GNP	PB-O2B	-3.05	1.48	1.56
2	D	501	GNP	PB-O2B	-3.00	1.48	1.56
2	A	501	GNP	PG-O2G	-2.88	1.48	1.56
2	C	501	GNP	PB-O2B	-2.86	1.48	1.56
2	B	501	GNP	PB-O2B	-2.75	1.49	1.56
2	D	501	GNP	C8-N7	-2.73	1.29	1.34
2	D	501	GNP	PG-O2G	-2.43	1.49	1.56
2	C	501	GNP	C8-N7	-2.31	1.30	1.34
2	B	501	GNP	PG-O2G	-2.31	1.50	1.56
2	B	501	GNP	C8-N7	-2.28	1.30	1.34
2	C	501	GNP	PG-O2G	-2.09	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	GNP	PB-O1B	2.38	1.48	1.46
2	B	501	GNP	PB-O1B	2.80	1.49	1.46
2	B	501	GNP	C6-N1	2.96	1.38	1.33
2	A	501	GNP	C6-N1	3.02	1.38	1.33
2	D	501	GNP	C6-N1	3.02	1.38	1.33
2	C	501	GNP	C6-N1	3.33	1.39	1.33
2	D	501	GNP	PG-O1G	4.34	1.51	1.46
2	C	501	GNP	PG-O1G	4.73	1.51	1.46
2	A	501	GNP	PG-O1G	5.82	1.52	1.46
2	B	501	GNP	PG-O1G	6.74	1.53	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	GNP	C5-C6-N1	-9.76	110.25	123.59
2	D	501	GNP	C5-C6-N1	-9.70	110.33	123.59
2	C	501	GNP	C5-C6-N1	-9.62	110.44	123.59
2	B	501	GNP	C5-C6-N1	-9.16	111.06	123.59
2	D	501	GNP	O1G-PG-N3B	-5.08	104.11	111.90
2	A	501	GNP	O1G-PG-N3B	-3.88	105.94	111.90
2	D	501	GNP	O4'-C1'-N9	-3.70	100.35	108.10
2	B	501	GNP	O3G-PG-O1G	-3.52	104.14	113.49
2	C	501	GNP	O3G-PG-O1G	-3.25	104.85	113.49
2	C	501	GNP	O4'-C1'-N9	-2.74	102.35	108.10
2	A	501	GNP	N3-C2-N1	-2.67	123.37	127.44
2	B	501	GNP	N3-C2-N1	-2.56	123.55	127.44
2	D	501	GNP	N2-C2-N1	-2.19	113.58	117.20
2	B	501	GNP	O1G-PG-N3B	-2.15	108.60	111.90
2	C	501	GNP	N3-C2-N1	-2.05	124.32	127.44
2	D	501	GNP	N2-C2-N3	2.04	121.72	117.80
2	D	501	GNP	C4-C5-N7	2.08	111.39	109.48
2	D	501	GNP	C2'-C1'-N9	2.47	118.07	114.29
2	C	501	GNP	O3G-PG-O2G	2.61	115.33	107.58
2	B	501	GNP	O3G-PG-O2G	2.64	115.42	107.58
2	D	501	GNP	O2B-PB-O1B	2.67	115.58	110.00
2	D	501	GNP	O3G-PG-O2G	2.94	116.29	107.58
2	C	501	GNP	C6-N1-C2	6.28	124.65	115.94
2	B	501	GNP	C6-N1-C2	6.99	125.64	115.94
2	D	501	GNP	C6-N1-C2	7.09	125.78	115.94
2	A	501	GNP	C6-N1-C2	7.79	126.76	115.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	GNP	O1B-PB-N3B-PG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GNP	1	0
2	C	501	GNP	2	0
2	D	501	GNP	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	407/447 (91%)	0.00	7 (1%) 73 69	11, 24, 54, 95	0
1	B	407/447 (91%)	0.03	11 (2%) 58 54	11, 25, 54, 92	0
1	C	407/447 (91%)	-0.04	3 (0%) 89 87	10, 25, 51, 90	0
1	D	408/447 (91%)	-0.09	5 (1%) 81 78	11, 24, 50, 85	0
All	All	1629/1788 (91%)	-0.02	26 (1%) 74 71	10, 25, 53, 95	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	30	LYS	4.8
1	A	60	GLU	4.1
1	B	59	SER	2.9
1	C	31	LYS	2.8
1	A	98	ASP	2.7
1	C	136	ASP	2.6
1	A	96	SER	2.6
1	B	60	GLU	2.6
1	B	323	ARG	2.5
1	B	136	ASP	2.5
1	A	205	PHE	2.5
1	B	95	GLU	2.5
1	D	31	LYS	2.5
1	D	245	ASN	2.4
1	B	307	PRO	2.3
1	B	31	LYS	2.3
1	B	96	SER	2.3
1	A	97	VAL	2.2
1	C	51	THR	2.1
1	A	135	PRO	2.1
1	B	139	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	205	PHE	2.1
1	D	47	GLU	2.1
1	B	97	VAL	2.0
1	A	136	ASP	2.0
1	B	42	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.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	MG	B	502	1/1	0.92	0.18	1.02	44,44,44,44	0
3	MG	C	502	1/1	0.96	0.16	0.66	35,35,35,35	0
2	GNP	D	501	32/32	0.99	0.12	-0.82	8,18,23,24	0
2	GNP	C	501	32/32	0.98	0.12	-1.00	6,18,21,22	0
3	MG	A	502	1/1	0.97	0.12	-1.36	35,35,35,35	0
2	GNP	A	501	32/32	0.99	0.11	-1.51	8,17,22,23	0
2	GNP	B	501	32/32	0.99	0.11	-1.79	7,15,20,22	0
3	MG	D	502	1/1	0.97	0.09	-2.47	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.