



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 02:29 pm GMT

PDB ID : 2QTV  
Title : Structure of Sec23-Sar1 complexed with the active fragment of Sec31  
Authors : Goldberg, J.; Bi, X.; Mancias, J.D.  
Deposited on : 2007-08-02  
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

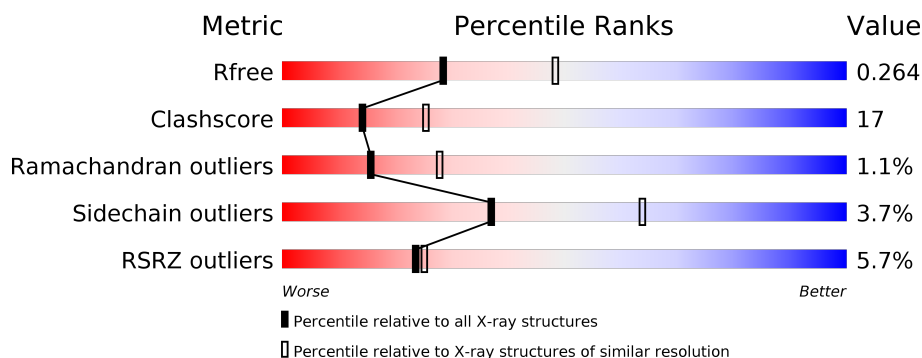
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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	772	<div> <div>4%</div> <div>68%</div> <div>25%</div> <div>5%</div> </div>
2	B	167	<div> <div>6%</div> <div>59%</div> <div>35%</div> <div>•</div> </div>
3	D	49	<div> <div>18%</div> <div>55%</div> <div>18%</div> <div>27%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7619 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 Protein transport protein SEC23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	733	Total	C	N	O	S	0	0	0
			5780	3679	969	1109	23			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P15303
A	-2	ALA	-	EXPRESSION TAG	UNP P15303
A	-1	MET	-	EXPRESSION TAG	UNP P15303
A	0	GLY	-	EXPRESSION TAG	UNP P15303
A	1	SER	-	EXPRESSION TAG	UNP P15303

- Molecule 2 is a protein called Small COPII coat GTPase SAR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total	C	N	O	S	0	0	0
			1299	836	220	239	4			

- Molecule 3 is a protein called Protein transport protein SEC31.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	36	Total	C	N	O	0	0	0
			275	171	54	50			

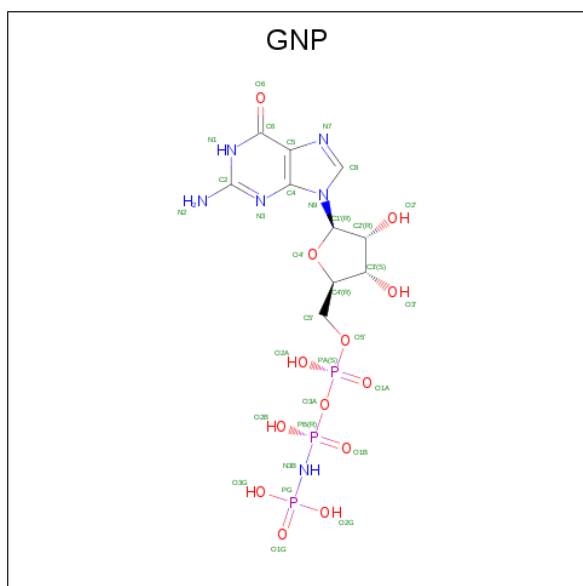
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).



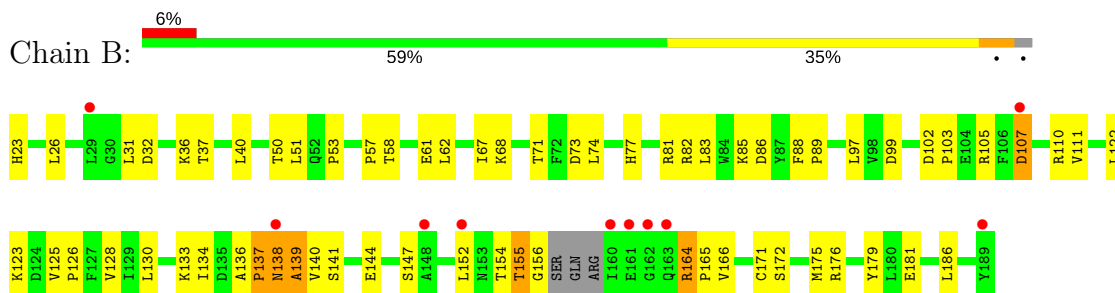
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

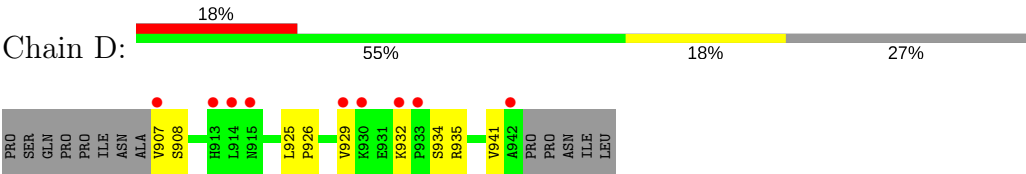
#### • Molecule 1: Protein transport protein SEC23



#### • Molecule 2: Small COPII coat GTPase SAR1



#### • Molecule 3: Protein transport protein SEC31



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.75Å 133.21Å 82.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.4 (30.00-2.50) 91.3 (29.47-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.79 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.205 , 0.262 0.210 , 0.264	Depositor DCC
$R_{free}$ test set	1693 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7619	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN, MG, 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	0.38	0/5915	0.62	0/8052
2	B	0.34	0/1327	0.61	0/1800
3	D	0.35	0/280	0.61	0/378
All	All	0.37	0/7522	0.62	0/10230

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	5780	0	5663	180	0
2	B	1299	0	1288	61	0
3	D	275	0	285	14	0
4	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	32	0	13	5	0
7	A	193	0	0	7	0
7	B	31	0	0	2	0
7	D	7	0	0	1	0
All	All	7619	0	7249	244	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 17.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:ASN:H	1:A:651:ASN:HD22	1.05	1.00
1:A:121:PRO:HG3	3:D:941:VAL:HG21	1.47	0.96
1:A:153:PRO:HG3	3:D:935:ARG:HD3	1.52	0.91
1:A:722:ARG:HD3	6:B:200:GNP:H5'1	1.57	0.85
1:A:96:LEU:HG	1:A:97:SER:H	1.43	0.83
1:A:164:ASN:N	1:A:164:ASN:HD22	1.82	0.78
2:B:140:VAL:HG12	2:B:141:SER:N	1.99	0.77
1:A:616:GLU:HG3	1:A:620:ASN:HB2	1.63	0.77
2:B:140:VAL:HG12	2:B:141:SER:H	1.52	0.75
1:A:114:THR:HG22	1:A:115:ASN:H	1.50	0.75
1:A:512:LEU:HD13	1:A:516:THR:HG21	1.70	0.74
1:A:708:LEU:HD21	3:D:929:VAL:HG11	1.69	0.74
1:A:382:GLN:HB3	3:D:929:VAL:HG21	1.69	0.74
1:A:164:ASN:HD22	1:A:164:ASN:H	1.33	0.73
1:A:651:ASN:H	1:A:651:ASN:ND2	1.85	0.72
1:A:674:ARG:HA	1:A:679:GLN:NE2	2.04	0.71
1:A:347:ALA:HB2	1:A:353:ILE:HD13	1.73	0.70
1:A:430:ASN:HD22	1:A:430:ASN:H	1.39	0.70
1:A:616:GLU:CG	1:A:620:ASN:HB2	2.21	0.70
1:A:615:ARG:NH1	7:A:815:HOH:O	2.23	0.69
1:A:399:ALA:HB3	1:A:450:LEU:HD13	1.74	0.69
1:A:114:THR:HG22	1:A:115:ASN:N	2.07	0.69
2:B:36:LYS:HG2	2:B:97:LEU:HD13	1.75	0.68
1:A:96:LEU:CG	1:A:97:SER:H	2.07	0.68
1:A:634:MET:HE1	1:A:686:ASP:O	1.95	0.67
2:B:130:LEU:HD22	2:B:171:CYS:SG	2.35	0.67
2:B:61:GLU:OE2	2:B:68:LYS:HE2	1.95	0.66
1:A:745:VAL:CG1	2:B:50:THR:HG21	2.25	0.66
1:A:177:ASP:OD1	1:A:237:LYS:HE3	1.96	0.65
1:A:757:THR:O	1:A:761:GLN:HG3	1.97	0.65
1:A:164:ASN:H	1:A:164:ASN:ND2	1.94	0.65
1:A:651:ASN:N	1:A:651:ASN:HD22	1.81	0.64
1:A:323:LYS:O	1:A:327:LYS:HG2	1.97	0.64
1:A:432:ILE:HD13	1:A:442:THR:HA	1.78	0.64
1:A:19:PHE:HB2	1:A:511:LEU:HD23	1.80	0.64
1:A:722:ARG:HH12	6:B:200:GNP:HNB3	1.46	0.64
3:D:907:VAL:HG12	3:D:908:SER:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:ARG:HG2	2:B:166:VAL:HG23	1.80	0.63
1:A:170:ASP:C	1:A:171:LEU:HD12	2.19	0.62
2:B:140:VAL:CG1	2:B:141:SER:H	2.12	0.62
1:A:96:LEU:HD21	1:A:101:MET:SD	2.39	0.62
1:A:136:ASN:HD21	1:A:374:ALA:HB1	1.65	0.62
1:A:219:VAL:HG22	1:A:225:ASN:ND2	2.14	0.62
2:B:154:THR:HB	2:B:166:VAL:O	2.00	0.62
1:A:411:ASP:OD2	1:A:411:ASP:N	2.33	0.62
1:A:750:VAL:HA	7:A:949:HOH:O	2.00	0.60
2:B:23:HIS:CD2	2:B:67:ILE:HA	2.36	0.60
1:A:618:THR:O	1:A:622:LEU:HG	2.01	0.59
1:A:410:LYS:HD3	7:A:944:HOH:O	2.03	0.59
1:A:10:ASN:O	1:A:12:VAL:HG23	2.03	0.58
1:A:511:LEU:O	1:A:512:LEU:HD23	2.03	0.58
1:A:681:ASP:HB2	1:A:682:PRO:HD2	1.84	0.58
2:B:141:SER:OG	2:B:144:GLU:HG3	2.03	0.58
2:B:140:VAL:CG1	2:B:141:SER:N	2.65	0.58
1:A:450:LEU:N	1:A:450:LEU:HD12	2.19	0.57
1:A:44:ASP:O	1:A:45:GLU:HG3	2.04	0.57
2:B:83:LEU:O	2:B:86:ASP:HB2	2.04	0.57
1:A:708:LEU:CD2	3:D:929:VAL:HG11	2.34	0.57
1:A:722:ARG:NH1	6:B:200:GNP:HNB3	2.01	0.57
1:A:102:PRO:HD2	1:A:105:LEU:HD12	1.87	0.57
2:B:140:VAL:CG1	2:B:144:GLU:HB2	2.34	0.57
2:B:122:LEU:O	2:B:164:ARG:NH2	2.38	0.57
3:D:929:VAL:HG23	3:D:929:VAL:O	2.05	0.56
1:A:634:MET:HE3	1:A:634:MET:HA	1.87	0.56
1:A:77:SER:HA	1:A:89:LEU:HB2	1.88	0.56
1:A:96:LEU:HG	1:A:97:SER:N	2.18	0.56
1:A:234:VAL:HG12	1:A:234:VAL:O	2.04	0.56
1:A:65:LEU:HD11	1:A:105:LEU:HD21	1.88	0.56
1:A:635:GLU:CD	1:A:635:GLU:H	2.08	0.55
2:B:23:HIS:HD2	2:B:67:ILE:HA	1.70	0.55
2:B:57:PRO:HB3	2:B:74:LEU:HD13	1.89	0.55
1:A:219:VAL:HG22	1:A:225:ASN:HD22	1.71	0.55
1:A:46:LEU:HD12	1:A:47:ASN:H	1.71	0.55
1:A:634:MET:HA	1:A:634:MET:CE	2.36	0.55
1:A:145:ILE:HA	1:A:148:LEU:HD12	1.88	0.55
2:B:137:PRO:HG2	2:B:138:ASN:H	1.71	0.55
1:A:679:GLN:HG3	1:A:687:PHE:CE2	2.41	0.55
1:A:96:LEU:HD11	1:A:102:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:SER:O	1:A:534:ARG:NH2	2.40	0.54
1:A:583:TYR:HB3	1:A:584:PRO:HD3	1.88	0.54
1:A:564:ALA:HB2	1:A:576:LEU:HD13	1.89	0.54
1:A:68:TYR:O	1:A:81:PRO:HG3	2.07	0.54
2:B:102:ASP:N	2:B:103:PRO:HD3	2.22	0.54
1:A:566:TYR:CG	1:A:764:VAL:HG12	2.42	0.54
1:A:710:ARG:HD2	7:D:214:HOH:O	2.08	0.54
1:A:114:THR:HG22	1:A:116:LYS:H	1.72	0.54
1:A:679:GLN:HG2	1:A:691:LEU:CD1	2.38	0.54
1:A:644:ASP:OD1	1:A:645:SER:N	2.41	0.53
1:A:761:GLN:O	1:A:765:SER:HB2	2.07	0.53
2:B:155:THR:CG2	2:B:166:VAL:H	2.21	0.53
1:A:430:ASN:ND2	1:A:430:ASN:H	2.06	0.53
2:B:50:THR:HG23	2:B:50:THR:O	2.07	0.53
2:B:128:VAL:HG23	2:B:186:LEU:HD13	1.91	0.53
2:B:58:THR:HG22	7:B:224:HOH:O	2.09	0.53
1:A:723:PHE:O	1:A:727:LYS:HG2	2.09	0.52
2:B:32:ASP:OD1	2:B:77:HIS:HA	2.10	0.52
2:B:155:THR:HG22	2:B:166:VAL:H	1.75	0.52
2:B:82:ARG:O	2:B:85:LYS:HE2	2.09	0.52
3:D:925:LEU:HD12	3:D:926:PRO:HD2	1.92	0.52
7:A:908:HOH:O	3:D:935:ARG:NE	2.42	0.52
1:A:171:LEU:HD22	1:A:234:VAL:HG11	1.91	0.52
1:A:682:PRO:O	1:A:683:GLN:HB3	2.10	0.52
2:B:136:ALA:HB1	2:B:137:PRO:HD2	1.92	0.51
1:A:745:VAL:HG13	2:B:50:THR:HG21	1.92	0.51
2:B:107:ASP:O	2:B:111:VAL:HG23	2.11	0.51
2:B:155:THR:HG23	2:B:156:GLY:N	2.26	0.51
1:A:682:PRO:C	1:A:684:TYR:H	2.13	0.51
1:A:114:THR:CG2	1:A:115:ASN:H	2.23	0.50
1:A:307:PRO:HB3	7:B:220:HOH:O	2.10	0.50
1:A:144:ILE:O	1:A:148:LEU:HG	2.11	0.50
1:A:171:LEU:HD12	1:A:171:LEU:N	2.25	0.50
1:A:365:THR:HB	1:A:448:ALA:HB3	1.92	0.50
1:A:739:ARG:HH11	1:A:739:ARG:HG3	1.76	0.50
2:B:172:SER:OG	2:B:175:MET:HG2	2.11	0.50
1:A:66:ASN:HD22	1:A:68:TYR:H	1.60	0.49
2:B:176:ARG:HA	2:B:179:TYR:HE2	1.77	0.49
1:A:171:LEU:CD2	1:A:234:VAL:HG11	2.43	0.49
1:A:147:SER:HB3	1:A:384:TYR:CE2	2.48	0.49
1:A:644:ASP:OD2	1:A:731:SER:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:VAL:HG13	2:B:144:GLU:CD	2.33	0.49
1:A:645:SER:HA	1:A:728:LEU:HD13	1.94	0.49
2:B:88:PHE:N	2:B:89:PRO:CD	2.76	0.49
1:A:390:LYS:N	1:A:390:LYS:HD2	2.28	0.49
1:A:395:TYR:CD2	1:A:497:SER:HA	2.48	0.48
1:A:390:LYS:HE3	3:D:934:SER:O	2.13	0.48
2:B:32:ASP:HB3	2:B:77:HIS:N	2.29	0.48
2:B:85:LYS:HA	2:B:88:PHE:CD2	2.48	0.48
2:B:176:ARG:HA	2:B:179:TYR:CE2	2.48	0.48
1:A:739:ARG:HG2	1:A:744:ILE:HD11	1.96	0.48
1:A:17:ASN:HB2	1:A:522:SER:HB2	1.96	0.48
2:B:99:ASP:OD1	2:B:133:LYS:HD2	2.14	0.48
1:A:430:ASN:HD22	1:A:430:ASN:N	2.03	0.48
1:A:451:SER:C	1:A:453:TYR:H	2.17	0.47
1:A:615:ARG:NH2	7:A:976:HOH:O	2.44	0.47
1:A:42:GLU:OE2	1:A:397:LYS:HE2	2.14	0.47
2:B:137:PRO:C	2:B:139:ALA:H	2.18	0.47
1:A:432:ILE:CD1	1:A:442:THR:HA	2.43	0.47
1:A:96:LEU:CG	1:A:97:SER:N	2.76	0.47
1:A:674:ARG:HB3	7:A:992:HOH:O	2.15	0.47
1:A:164:ASN:HD22	1:A:165:VAL:H	1.63	0.47
2:B:134:ILE:HG12	2:B:172:SER:HB2	1.96	0.47
1:A:66:ASN:HD21	1:A:68:TYR:HB2	1.80	0.47
2:B:103:PRO:HG3	2:B:140:VAL:HG21	1.96	0.47
1:A:485:ALA:HB2	1:A:511:LEU:HD11	1.97	0.46
1:A:594:GLN:HE21	1:A:601:ASN:HD21	1.63	0.46
1:A:661:PHE:HA	1:A:709:PRO:HB2	1.97	0.46
2:B:23:HIS:HD2	2:B:68:LYS:H	1.62	0.46
1:A:561:GLN:HG2	1:A:763:ALA:HA	1.97	0.46
1:A:96:LEU:HD11	1:A:101:MET:HA	1.97	0.46
3:D:907:VAL:CG1	3:D:908:SER:N	2.78	0.46
1:A:616:GLU:CG	1:A:620:ASN:CB	2.91	0.46
1:A:687:PHE:CE2	1:A:691:LEU:HD11	2.51	0.46
2:B:62:LEU:HD12	2:B:71:THR:HG21	1.96	0.46
2:B:31:LEU:HD22	2:B:81:ARG:NH2	2.31	0.46
1:A:551:TRP:CE3	1:A:552:LEU:HD13	2.50	0.46
1:A:722:ARG:NH1	6:B:200:GNP:N3B	2.57	0.46
1:A:19:PHE:HB2	1:A:511:LEU:CD2	2.44	0.46
1:A:343:VAL:O	1:A:362:THR:HG22	2.16	0.46
1:A:114:THR:CG2	1:A:115:ASN:N	2.76	0.45
1:A:556:LEU:HD22	1:A:587:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:LEU:O	1:A:644:ASP:N	2.48	0.45
2:B:32:ASP:O	2:B:105:ARG:NH2	2.49	0.45
2:B:110:ARG:HG3	2:B:110:ARG:HH11	1.82	0.45
1:A:734:TYR:HA	1:A:744:ILE:HG21	1.98	0.45
3:D:907:VAL:HG12	3:D:908:SER:H	1.81	0.45
2:B:97:LEU:N	2:B:97:LEU:HD12	2.31	0.45
2:B:40:LEU:HD22	2:B:73:ASP:HB2	1.99	0.45
1:A:679:GLN:HG3	1:A:687:PHE:HE2	1.79	0.45
1:A:464:ASN:ND2	1:A:465:THR:H	2.15	0.45
1:A:111:GLU:HB2	1:A:503:ARG:HD3	1.99	0.45
2:B:134:ILE:CG1	2:B:172:SER:HB2	2.47	0.45
2:B:155:THR:OG1	2:B:156:GLY:N	2.50	0.44
1:A:46:LEU:HG	1:A:47:ASN:N	2.32	0.44
1:A:69:CYS:SG	1:A:81:PRO:HD3	2.58	0.44
1:A:588:TYR:O	1:A:591:ARG:HG2	2.18	0.44
2:B:155:THR:HG21	2:B:165:PRO:HA	2.00	0.44
1:A:44:ASP:C	1:A:45:GLU:HG3	2.37	0.44
1:A:15:THR:HG22	1:A:528:ALA:HA	1.99	0.44
1:A:561:GLN:CG	1:A:763:ALA:HA	2.48	0.44
1:A:599:PHE:HD2	2:B:51:LEU:HD22	1.82	0.44
2:B:85:LYS:HA	2:B:88:PHE:CE2	2.52	0.44
1:A:550:ARG:O	1:A:554:ARG:HG3	2.18	0.43
1:A:653:ILE:HG13	1:A:670:ILE:HD13	2.00	0.43
2:B:125:VAL:HA	2:B:126:PRO:HD3	1.86	0.43
1:A:138:ASP:HA	1:A:141:LYS:HD2	1.99	0.43
1:A:283:ARG:NE	1:A:344:ASP:OD2	2.51	0.43
1:A:187:GLU:HB2	1:A:296:PRO:HG3	1.99	0.43
2:B:37:THR:HG22	2:B:51:LEU:HD13	1.99	0.43
1:A:281:PRO:HB3	1:A:400:PHE:HB3	2.00	0.43
1:A:512:LEU:HA	1:A:513:PRO:HD3	1.79	0.43
1:A:417:LEU:C	1:A:417:LEU:HD23	2.39	0.43
1:A:80:CYS:HA	1:A:81:PRO:HD3	1.86	0.43
1:A:66:ASN:ND2	1:A:68:TYR:H	2.16	0.42
2:B:181:GLU:H	2:B:181:GLU:CD	2.22	0.42
1:A:677:GLY:O	1:A:679:GLN:N	2.52	0.42
1:A:15:THR:HG23	1:A:531:LEU:HD12	2.00	0.42
1:A:360:GLN:HG2	1:A:364:SER:OG	2.19	0.42
1:A:574:PHE:CD2	1:A:760:GLN:HG2	2.55	0.42
2:B:147:SER:OG	2:B:152:LEU:HD21	2.19	0.42
1:A:661:PHE:C	1:A:661:PHE:CD1	2.93	0.42
1:A:66:ASN:HB2	1:A:67:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:ASP:HA	6:B:200:GNP:O3G	2.18	0.42
1:A:151:LEU:O	3:D:935:ARG:HG3	2.20	0.42
1:A:243:GLU:HA	1:A:243:GLU:OE1	2.20	0.42
1:A:411:ASP:HA	1:A:463:ALA:HB3	2.02	0.42
1:A:632:PHE:N	1:A:632:PHE:CD1	2.88	0.42
1:A:63:SER:OG	1:A:82:ILE:HG13	2.20	0.42
1:A:53:PRO:HG3	1:A:112:TYR:CG	2.55	0.42
1:A:632:PHE:CE2	1:A:693:GLU:HG3	2.55	0.42
1:A:561:GLN:HG2	1:A:763:ALA:O	2.20	0.42
1:A:90:PRO:HA	1:A:91:PRO:HD3	1.86	0.42
1:A:576:LEU:HG	1:A:580:PHE:HB3	2.02	0.42
1:A:420:HIS:CE1	1:A:615:ARG:HB2	2.55	0.42
3:D:932:LYS:C	3:D:934:SER:H	2.22	0.42
1:A:42:GLU:HG3	1:A:452:PRO:HB3	2.02	0.41
1:A:83:CYS:O	1:A:84:ASN:HB2	2.20	0.41
2:B:26:LEU:HB2	2:B:71:THR:HG22	2.02	0.41
1:A:332:ILE:HG22	1:A:361:LEU:HD21	2.02	0.41
1:A:66:ASN:ND2	1:A:68:TYR:HB2	2.35	0.41
1:A:569:ASP:C	1:A:571:PRO:HD3	2.41	0.41
1:A:651:ASN:ND2	1:A:651:ASN:N	2.53	0.41
1:A:658:THR:O	1:A:659:PHE:HB3	2.20	0.41
1:A:722:ARG:CZ	2:B:53:PRO:HG3	2.51	0.41
1:A:120:VAL:HA	1:A:121:PRO:HD3	1.94	0.41
1:A:140:LEU:O	1:A:144:ILE:HG13	2.21	0.41
1:A:20:PRO:HB3	1:A:25:ASP:HB2	2.02	0.41
2:B:164:ARG:HG2	2:B:164:ARG:O	2.21	0.41
1:A:451:SER:C	1:A:453:TYR:N	2.75	0.41
1:A:70:VAL:HB	1:A:79:SER:OG	2.21	0.41
1:A:171:LEU:HB3	1:A:237:LYS:HD3	2.03	0.41
1:A:461:GLU:HA	7:A:934:HOH:O	2.20	0.41
1:A:464:ASN:ND2	1:A:465:THR:N	2.69	0.41
1:A:164:ASN:HD22	1:A:165:VAL:N	2.19	0.40
1:A:643:LEU:HD12	1:A:728:LEU:HD23	2.03	0.40
1:A:702:LEU:O	1:A:703:VAL:C	2.59	0.40
1:A:41:LYS:O	1:A:503:ARG:NH2	2.54	0.40
1:A:52:ASN:HA	1:A:53:PRO:HD3	1.87	0.40
1:A:602:SER:OG	1:A:605:GLU:HB2	2.22	0.40
1:A:67:PRO:HD3	1:A:104:GLU:O	2.21	0.40
1:A:96:LEU:O	1:A:97:SER:HB3	2.21	0.40
1:A:239:ASN:O	1:A:243:GLU:HB2	2.20	0.40
1:A:234:VAL:O	1:A:235:GLU:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:ASP:O	1:A:571:PRO:HD3	2.20	0.40
1:A:653:ILE:HD11	1:A:691:LEU:HD23	2.04	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	727/772 (94%)	687 (94%)	35 (5%)	5 (1%)	24	42
2	B	160/167 (96%)	142 (89%)	13 (8%)	5 (3%)	4	6
3	D	34/49 (69%)	30 (88%)	4 (12%)	0	100	100
All	All	921/988 (93%)	859 (93%)	52 (6%)	10 (1%)	16	28

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	703	VAL
2	B	139	ALA
2	B	155	THR
1	A	678	TYR
1	A	73	PRO
1	A	97	SER
2	B	123	LYS
2	B	137	PRO
1	A	94	THR
2	B	138	ASN

### 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	644/669 (96%)	616 (96%)	28 (4%)	32	56
2	B	138/141 (98%)	136 (99%)	2 (1%)	69	88
3	D	30/42 (71%)	30 (100%)	0	100	100
All	All	812/852 (95%)	782 (96%)	30 (4%)	37	64

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	125	PHE
1	A	132	SER
1	A	136	ASN
1	A	164	ASN
1	A	166	VAL
1	A	243	GLU
1	A	245	LEU
1	A	250	TRP
1	A	252	VAL
1	A	309	ARG
1	A	411	ASP
1	A	430	ASN
1	A	450	LEU
1	A	503	ARG
1	A	534	ARG
1	A	544	ASP
1	A	552	LEU
1	A	592	ARG
1	A	601	ASN
1	A	635	GLU
1	A	651	ASN
1	A	679	GLN
1	A	697	GLU
1	A	700	GLU
1	A	708	LEU

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Mol	Chain	Res	Type
1	A	749	ASP
1	A	765	SER
2	B	107	ASP
2	B	164	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	66	ASN
1	A	136	ASN
1	A	164	ASN
1	A	189	GLN
1	A	233	GLN
1	A	279	ASN
1	A	430	ASN
1	A	464	ASN
1	A	601	ASN
1	A	651	ASN
1	A	679	GLN
1	A	735	GLN
1	A	760	GLN
2	B	23	HIS
2	B	66	ASN

### 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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
6	GNP	B	200	5	27,34,34	2.36	8 (29%)	30,54,54	1.92	4 (13%)

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
6	GNP	B	200	5	-	0/16/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	200	GNP	C4-N9	-7.13	1.38	1.47
6	B	200	GNP	PG-O2G	-4.35	1.44	1.56
6	B	200	GNP	PB-O2B	-4.04	1.45	1.56
6	B	200	GNP	C5-C6	-3.32	1.47	1.52
6	B	200	GNP	C8-N9	-2.60	1.39	1.46
6	B	200	GNP	C5-C4	-2.01	1.40	1.52
6	B	200	GNP	PB-O3A	2.23	1.61	1.59
6	B	200	GNP	C6-N1	4.68	1.41	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	200	GNP	C5-C6-N1	-5.26	112.00	118.27
6	B	200	GNP	O6-C6-N1	-2.88	118.88	122.71
6	B	200	GNP	O6-C6-C5	4.50	129.11	119.82
6	B	200	GNP	C4-C5-N7	5.57	109.85	102.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	200	GNP	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	733/772 (94%)	0.07	34 (4%) 32 35	14, 28, 61, 92	0
2	B	164/167 (98%)	0.50	10 (6%) 21 22	20, 48, 70, 86	0
3	D	36/49 (73%)	1.01	9 (25%) 0 0	23, 51, 71, 75	0
All	All	933/988 (94%)	0.18	53 (5%) 24 25	14, 31, 67, 92	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	740	GLY	5.3
1	A	250	TRP	4.3
2	B	161	GLU	4.2
2	B	163	GLN	4.1
2	B	162	GLY	4.1
2	B	160	ILE	3.8
1	A	684	TYR	3.8
1	A	99	GLU	3.6
1	A	768	ALA	3.6
1	A	678	TYR	3.5
3	D	930	LYS	3.5
3	D	933	PRO	3.4
1	A	74	ARG	3.3
1	A	676	ALA	3.3
1	A	95	ASN	3.2
1	A	739	ARG	3.1
1	A	683	GLN	2.9
1	A	44	ASP	2.9
3	D	932	LYS	2.8
1	A	100	ASN	2.8
2	B	152	LEU	2.7
1	A	93	TYR	2.7
3	D	907	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	86	ARG	2.6
3	D	929	VAL	2.6
3	D	913	HIS	2.6
1	A	96	LEU	2.6
1	A	94	THR	2.6
1	A	426	LYS	2.5
1	A	681	ASP	2.5
1	A	89	LEU	2.5
2	B	148	ALA	2.5
1	A	60	HIS	2.4
1	A	98	GLN	2.4
1	A	767	GLN	2.4
2	B	138	ASN	2.3
1	A	252	VAL	2.3
3	D	942	ALA	2.3
1	A	686	ASP	2.2
2	B	107	ASP	2.2
1	A	251	SER	2.2
1	A	200	GLN	2.1
1	A	737	MET	2.1
1	A	514	PHE	2.1
1	A	483	HIS	2.1
1	A	687	PHE	2.1
1	A	677	GLY	2.1
2	B	29	LEU	2.0
3	D	915	ASN	2.0
1	A	35	CYS	2.0
3	D	914	LEU	2.0
1	A	45	GLU	2.0
2	B	189	TYR	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	B	210	1/1	0.90	0.19	28,28,28,28	0
6	GNP	B	200	32/32	0.97	0.14	25,33,39,40	0
4	ZN	A	800	1/1	0.99	0.09	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.