



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:50 pm GMT

PDB ID : 5CA8  
Title : Structures of the yeast dynamin-like GTPase Sey1p in complex with GDP  
Authors : Yan, L.  
Deposited on : 2015-06-29  
Resolution : 2.30 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
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) : recalc28949

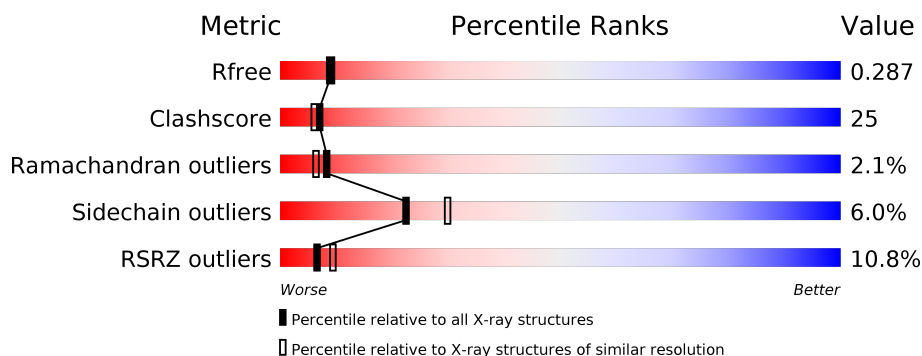
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	692	<div> <div>10%</div> <div>60%</div> <div>26%</div> <div>5%</div> <div>8%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5300 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 SEY1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	636	Total	C	N	O	S	0	0	0
			5136	3297	843	985	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	LEU	SER	see sequence details	UNP Q9C0L9
A	221	LEU	SER	see sequence details	UNP Q9C0L9
A	270	GLY	ASP	see sequence details	UNP Q9C0L9
A	337	THR	ALA	see sequence details	UNP Q9C0L9
A	479	VAL	ILE	see sequence details	UNP Q9C0L9
A	665	LEU	SER	see sequence details	UNP Q9C0L9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 10	N 5	O 11	P 2	0	0

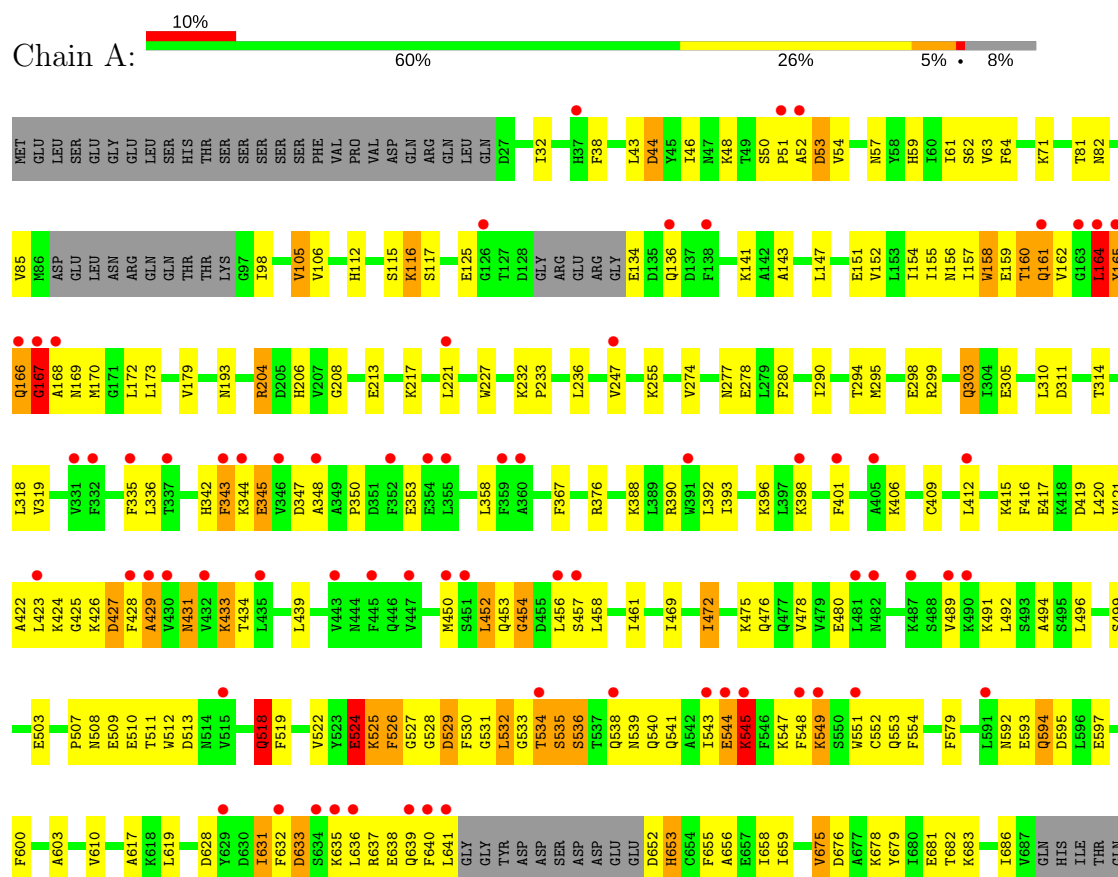
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	135	Total O 135 135	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: Protein SEY1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	228.12Å 43.62Å 97.56Å 90.00° 108.12° 90.00°	Depositor
Resolution (Å)	46.36 – 2.30 46.36 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.36-2.30) 98.9 (46.36-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.230 , 0.285 0.238 , 0.287	Depositor DCC
$R_{free}$ test set	2047 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.5	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 62.5	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	0.94	EDS
Total number of atoms	5300	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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: GDP, 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	0.56	0/5235	0.75	10/7073 (0.1%)

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	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	ALA	CB-CA-C	8.34	122.60	110.10
1	A	158	TRP	CB-CA-C	8.09	126.58	110.40
1	A	160	THR	N-CA-C	-7.40	91.02	111.00
1	A	518	GLN	CA-CB-CG	7.04	128.88	113.40
1	A	204	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	524	GLU	CB-CA-C	-6.03	98.34	110.40
1	A	545	LYS	N-CA-CB	-5.94	99.91	110.60
1	A	533	GLY	N-CA-C	-5.42	99.56	113.10
1	A	454	GLY	N-CA-C	5.18	126.05	113.10
1	A	633	ASP	CB-CA-C	5.18	120.76	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	GLY	Peptide
1	A	343	PHE	Peptide
1	A	344	LYS	Peptide
1	A	545	LYS	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	5136	0	5096	261	3
2	A	1	0	0	0	0
3	A	28	0	12	2	0
4	A	135	0	0	6	0
All	All	5300	0	5108	261	3

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 25.

All (261) 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:531:GLY:C	1:A:532:LEU:HD23	1.09	1.47
1:A:164:LEU:HD12	1:A:166:GLN:NE2	1.37	1.35
1:A:161:GLN:HE22	1:A:167:GLY:N	1.27	1.31
1:A:526:PHE:CE2	1:A:543:ILE:HA	1.63	1.30
1:A:161:GLN:NE2	1:A:167:GLY:CA	1.99	1.24
1:A:531:GLY:C	1:A:532:LEU:CD2	2.05	1.23
1:A:536:SER:OG	4:A:801:HOH:O	1.56	1.20
1:A:161:GLN:OE1	1:A:168:ALA:N	1.76	1.18
1:A:164:LEU:CD1	1:A:166:GLN:NE2	2.05	1.18
1:A:165:TYR:O	1:A:168:ALA:O	1.62	1.18
1:A:531:GLY:O	1:A:532:LEU:HD23	1.44	1.16
1:A:534:THR:HB	1:A:539:ASN:ND2	1.63	1.12
1:A:57:ASN:OD1	1:A:117:SER:OG	1.68	1.11
1:A:532:LEU:N	1:A:532:LEU:HD23	1.52	1.11
1:A:525:LYS:HG2	1:A:525:LYS:O	1.50	1.09
1:A:496:LEU:HA	1:A:518:GLN:HE22	1.21	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:PHE:HE2	1:A:543:ILE:CA	1.70	1.04
1:A:161:GLN:NE2	1:A:167:GLY:HA3	1.70	1.04
1:A:159:GLU:O	1:A:162:VAL:CG1	2.05	1.03
1:A:534:THR:CG2	1:A:539:ASN:HD21	1.71	1.02
1:A:161:GLN:NE2	1:A:167:GLY:N	2.04	1.01
1:A:531:GLY:O	1:A:532:LEU:CD2	2.06	1.00
1:A:526:PHE:HE2	1:A:543:ILE:HA	1.02	0.97
1:A:164:LEU:HB2	1:A:166:GLN:HG2	1.46	0.96
1:A:159:GLU:O	1:A:162:VAL:HG13	1.63	0.95
1:A:161:GLN:HE22	1:A:167:GLY:H	1.13	0.95
1:A:429:ALA:N	1:A:531:GLY:O	2.00	0.95
1:A:496:LEU:HA	1:A:518:GLN:NE2	1.81	0.95
1:A:161:GLN:HE22	1:A:167:GLY:CA	1.71	0.94
1:A:164:LEU:HD12	1:A:166:GLN:HE21	1.21	0.94
1:A:534:THR:CB	1:A:539:ASN:ND2	2.31	0.92
1:A:165:TYR:O	1:A:167:GLY:N	2.03	0.91
1:A:526:PHE:CZ	1:A:543:ILE:HA	2.06	0.90
1:A:526:PHE:CE2	1:A:543:ILE:CA	2.49	0.90
1:A:545:LYS:HE3	1:A:548:PHE:CG	2.07	0.89
1:A:534:THR:HG22	1:A:539:ASN:HD21	1.35	0.89
1:A:159:GLU:O	1:A:161:GLN:N	2.05	0.88
1:A:159:GLU:C	1:A:161:GLN:N	2.24	0.88
1:A:159:GLU:C	1:A:161:GLN:H	1.73	0.87
1:A:161:GLN:CD	1:A:167:GLY:C	2.33	0.87
1:A:159:GLU:O	1:A:162:VAL:HG12	1.75	0.86
1:A:165:TYR:HA	1:A:168:ALA:O	1.76	0.85
1:A:631:ILE:HG22	1:A:632:PHE:H	1.41	0.85
1:A:227:TRP:O	1:A:232:LYS:NZ	2.08	0.85
1:A:526:PHE:O	1:A:526:PHE:CD2	2.30	0.84
1:A:545:LYS:HG2	1:A:548:PHE:HB2	1.60	0.83
1:A:165:TYR:CE2	1:A:170:MET:HB2	2.13	0.83
1:A:429:ALA:HB2	1:A:531:GLY:HA2	1.61	0.82
1:A:545:LYS:HE2	1:A:640:PHE:CG	2.14	0.82
1:A:303:GLN:NE2	4:A:802:HOH:O	2.13	0.82
1:A:524:GLU:O	1:A:524:GLU:HG3	1.78	0.81
1:A:429:ALA:HB2	1:A:531:GLY:CA	2.10	0.81
1:A:162:VAL:CG2	1:A:162:VAL:O	2.30	0.79
1:A:162:VAL:HG22	1:A:162:VAL:O	1.83	0.79
1:A:165:TYR:H	1:A:165:TYR:HD2	1.31	0.79
1:A:193:ASN:ND2	4:A:803:HOH:O	2.15	0.78
1:A:165:TYR:C	1:A:168:ALA:O	2.20	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:THR:CG2	1:A:539:ASN:ND2	2.43	0.78
1:A:161:GLN:OE1	1:A:167:GLY:C	2.21	0.77
1:A:161:GLN:CG	1:A:161:GLN:O	2.30	0.77
1:A:159:GLU:O	1:A:162:VAL:N	2.16	0.77
1:A:161:GLN:NE2	1:A:167:GLY:C	2.37	0.77
1:A:342:HIS:O	1:A:345:GLU:HB3	1.84	0.76
1:A:525:LYS:CG	1:A:525:LYS:O	2.29	0.76
1:A:165:TYR:CA	1:A:168:ALA:O	2.33	0.75
1:A:508:ASN:OD1	1:A:509:GLU:N	2.19	0.75
1:A:165:TYR:N	1:A:165:TYR:HD2	1.85	0.74
1:A:452:LEU:O	1:A:453:GLN:C	2.24	0.74
1:A:545:LYS:HE3	1:A:548:PHE:HB2	1.70	0.71
1:A:169:ASN:HB3	1:A:172:LEU:HB2	1.73	0.71
1:A:545:LYS:HE3	1:A:548:PHE:CB	2.21	0.70
1:A:545:LYS:CG	1:A:548:PHE:HB2	2.21	0.70
1:A:472:ILE:HA	1:A:475:LYS:HB2	1.74	0.70
1:A:161:GLN:CD	1:A:168:ALA:N	2.44	0.70
1:A:161:GLN:CD	1:A:161:GLN:O	2.30	0.69
1:A:164:LEU:CD1	1:A:166:GLN:HE22	2.05	0.69
1:A:106:VAL:HG21	1:A:274:VAL:HG21	1.75	0.69
1:A:431:ASN:HA	1:A:434:THR:HG22	1.74	0.69
1:A:61:ILE:HG23	1:A:152:VAL:HB	1.74	0.68
1:A:534:THR:O	1:A:535:SER:HB2	1.93	0.67
1:A:551:TRP:CZ3	1:A:554:PHE:HD2	2.12	0.67
1:A:164:LEU:HD13	1:A:166:GLN:NE2	2.04	0.67
1:A:169:ASN:HB3	1:A:172:LEU:H	1.58	0.67
1:A:526:PHE:O	1:A:526:PHE:HD2	1.77	0.67
1:A:161:GLN:HG3	1:A:161:GLN:O	1.94	0.67
1:A:159:GLU:HA	1:A:162:VAL:HG12	1.77	0.66
1:A:295:MET:HG2	1:A:319:VAL:HG22	1.77	0.66
1:A:165:TYR:CD2	1:A:165:TYR:N	2.58	0.66
1:A:545:LYS:HE3	1:A:548:PHE:CD2	2.31	0.66
1:A:534:THR:HB	1:A:539:ASN:CG	2.17	0.65
1:A:147:LEU:HD12	1:A:179:VAL:HG12	1.78	0.64
1:A:527:GLY:O	1:A:529:ASP:N	2.30	0.64
1:A:159:GLU:CA	1:A:162:VAL:HG12	2.28	0.64
1:A:633:ASP:HB3	1:A:636:LEU:HB2	1.80	0.63
1:A:534:THR:CB	1:A:539:ASN:HD21	2.01	0.63
1:A:412:LEU:HB3	1:A:439:LEU:HD11	1.81	0.62
1:A:529:ASP:O	1:A:529:ASP:CG	2.38	0.62
1:A:46:ILE:HD12	1:A:294:THR:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ILE:HD12	1:A:98:ILE:HD12	1.80	0.61
1:A:453:GLN:NE2	4:A:808:HOH:O	2.33	0.61
1:A:507:PRO:HA	1:A:511:THR:HG21	1.83	0.61
1:A:594:GLN:OE1	1:A:595:ASP:N	2.33	0.61
1:A:544:GLU:O	1:A:547:LYS:HB2	2.01	0.61
1:A:518:GLN:OE1	1:A:519:PHE:N	2.34	0.60
1:A:51:PRO:C	1:A:53:ASP:H	2.04	0.60
1:A:141:LYS:HE3	1:A:305:GLU:HA	1.84	0.60
1:A:534:THR:OG1	1:A:535:SER:N	2.35	0.59
1:A:597:GLU:OE2	1:A:679:TYR:OH	2.19	0.59
1:A:526:PHE:C	1:A:526:PHE:CD2	2.74	0.59
1:A:551:TRP:CZ3	1:A:554:PHE:CD2	2.91	0.59
1:A:635:LYS:O	1:A:639:GLN:HB3	2.03	0.59
1:A:54:VAL:HB	1:A:290:ILE:HG21	1.85	0.59
1:A:38:PHE:CE2	1:A:298:GLU:HG2	2.37	0.58
1:A:428:PHE:C	1:A:531:GLY:O	2.41	0.58
1:A:540:GLN:HA	1:A:543:ILE:HD12	1.84	0.58
1:A:526:PHE:HE2	1:A:543:ILE:CB	2.15	0.58
1:A:164:LEU:HB2	1:A:166:GLN:CG	2.28	0.58
1:A:159:GLU:HA	1:A:162:VAL:CG1	2.33	0.58
1:A:158:TRP:N	1:A:158:TRP:CD1	2.68	0.58
1:A:278:GLU:O	1:A:278:GLU:HG2	2.04	0.57
1:A:44:ASP:O	1:A:48:LYS:HG2	2.04	0.57
1:A:499:SER:CB	1:A:518:GLN:HE21	2.17	0.57
1:A:419:ASP:HA	1:A:422:ALA:HB3	1.86	0.57
1:A:551:TRP:HZ3	1:A:554:PHE:CD2	2.23	0.57
1:A:518:GLN:OE1	1:A:518:GLN:C	2.42	0.57
1:A:61:ILE:HD11	1:A:280:PHE:HZ	1.70	0.57
1:A:43:LEU:HA	1:A:294:THR:HG21	1.86	0.57
1:A:161:GLN:NE2	1:A:166:GLN:HG3	2.19	0.57
1:A:526:PHE:CE2	1:A:543:ILE:HG12	2.39	0.56
1:A:159:GLU:C	1:A:162:VAL:HG12	2.25	0.56
1:A:51:PRO:O	1:A:53:ASP:N	2.38	0.56
1:A:416:PHE:CE2	1:A:472:ILE:HD11	2.40	0.56
1:A:165:TYR:CZ	1:A:170:MET:HB2	2.41	0.55
1:A:311:ASP:OD2	1:A:314:THR:HG23	2.07	0.55
1:A:527:GLY:C	1:A:529:ASP:H	2.10	0.55
1:A:406:LYS:HG3	1:A:409:CYS:HB2	1.88	0.55
1:A:423:LEU:HB3	1:A:428:PHE:HE1	1.72	0.55
1:A:57:ASN:OD1	1:A:117:SER:CB	2.55	0.55
1:A:423:LEU:O	1:A:425:GLY:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ASN:CB	1:A:172:LEU:HB2	2.36	0.54
1:A:530:PHE:CD1	1:A:530:PHE:N	2.73	0.54
1:A:294:THR:HG23	4:A:811:HOH:O	2.07	0.54
1:A:496:LEU:HD21	1:A:554:PHE:HA	1.88	0.54
1:A:427:ASP:O	1:A:431:ASN:HB2	2.08	0.54
1:A:421:VAL:HA	1:A:476:GLN:HE22	1.74	0.53
1:A:633:ASP:O	1:A:637:ARG:HG3	2.08	0.53
1:A:161:GLN:HE21	1:A:167:GLY:HA3	1.69	0.52
1:A:508:ASN:H	1:A:511:THR:HG23	1.74	0.52
1:A:527:GLY:C	1:A:529:ASP:N	2.63	0.52
1:A:401:PHE:HE1	1:A:450:MET:HG3	1.73	0.52
1:A:527:GLY:HA2	1:A:530:PHE:CZ	2.45	0.52
1:A:499:SER:HB3	1:A:518:GLN:HE21	1.75	0.52
1:A:299:ARG:HH21	1:A:318:LEU:HD13	1.75	0.52
1:A:335:PHE:CZ	1:A:393:ILE:HG23	2.45	0.51
1:A:541:GLN:HA	1:A:544:GLU:HB2	1.93	0.51
1:A:531:GLY:O	1:A:532:LEU:HD22	2.03	0.51
1:A:507:PRO:HB2	1:A:610:VAL:HG22	1.91	0.51
1:A:545:LYS:NZ	1:A:640:PHE:CD2	2.72	0.51
1:A:417:GLU:HA	1:A:420:LEU:HD12	1.93	0.50
1:A:51:PRO:C	1:A:53:ASP:N	2.64	0.50
1:A:52:ALA:O	1:A:376:ARG:NH2	2.42	0.50
1:A:652:ASP:O	1:A:652:ASP:OD1	2.30	0.50
1:A:529:ASP:OD1	1:A:529:ASP:O	2.30	0.50
1:A:475:LYS:O	1:A:478:VAL:HG22	2.12	0.50
1:A:164:LEU:CD1	1:A:166:GLN:CD	2.75	0.49
1:A:193:ASN:O	1:A:193:ASN:OD1	2.29	0.49
1:A:652:ASP:O	1:A:653:HIS:O	2.30	0.49
1:A:161:GLN:OE1	1:A:161:GLN:O	2.30	0.49
1:A:545:LYS:CE	1:A:548:PHE:CD2	2.95	0.49
1:A:551:TRP:HE1	1:A:628:ASP:HB2	1.78	0.49
1:A:155:ILE:HG21	1:A:173:LEU:HD21	1.95	0.49
1:A:592:ASN:OD1	1:A:593:GLU:N	2.46	0.49
1:A:303:GLN:HE21	1:A:310:LEU:HA	1.78	0.48
1:A:423:LEU:HB3	1:A:428:PHE:CE1	2.48	0.48
1:A:512:TRP:CE2	1:A:617:ALA:HA	2.48	0.48
1:A:554:PHE:CD2	1:A:655:PHE:HZ	2.31	0.48
1:A:631:ILE:HG22	1:A:632:PHE:N	2.20	0.48
1:A:639:GLN:NE2	1:A:640:PHE:CZ	2.81	0.48
1:A:156:ASN:ND2	1:A:204:ARG:HH21	2.11	0.48
1:A:169:ASN:HB3	1:A:172:LEU:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:PHE:CD2	1:A:472:ILE:HD11	2.48	0.48
1:A:401:PHE:CE1	1:A:450:MET:HG3	2.49	0.47
1:A:544:GLU:O	1:A:545:LYS:HG3	2.14	0.47
1:A:548:PHE:O	1:A:551:TRP:N	2.47	0.47
1:A:213:GLU:O	1:A:217:LYS:HG3	2.14	0.47
1:A:439:LEU:HD23	1:A:469:ILE:HD11	1.95	0.47
1:A:540:GLN:O	1:A:543:ILE:HB	2.14	0.47
1:A:431:ASN:HA	1:A:434:THR:CG2	2.44	0.47
1:A:496:LEU:CA	1:A:518:GLN:HE22	2.10	0.47
1:A:492:LEU:HD23	1:A:522:VAL:HG12	1.96	0.47
1:A:415:LYS:O	1:A:415:LYS:HD2	2.15	0.47
1:A:159:GLU:C	1:A:162:VAL:CG1	2.78	0.47
1:A:491:LYS:HA	1:A:494:ALA:HB3	1.95	0.47
1:A:406:LYS:HA	1:A:409:CYS:HB2	1.97	0.47
1:A:59:HIS:HA	1:A:151:GLU:OE2	2.15	0.47
1:A:159:GLU:O	1:A:160:THR:C	2.52	0.47
1:A:513:ASP:HA	1:A:619:LEU:HD22	1.97	0.47
1:A:489:VAL:O	1:A:492:LEU:HB3	2.15	0.46
1:A:548:PHE:O	1:A:552:CYS:N	2.35	0.46
1:A:535:SER:O	1:A:538:GLN:N	2.48	0.46
1:A:551:TRP:HB3	1:A:631:ILE:HD11	1.98	0.45
1:A:531:GLY:CA	1:A:532:LEU:HD23	2.24	0.45
1:A:638:GLU:HA	1:A:641:LEU:H	1.80	0.45
1:A:165:TYR:O	1:A:166:GLN:C	2.56	0.45
1:A:592:ASN:OD1	1:A:594:GLN:N	2.33	0.45
1:A:472:ILE:CA	1:A:475:LYS:HB2	2.43	0.45
1:A:193:ASN:C	1:A:193:ASN:OD1	2.55	0.44
1:A:545:LYS:HA	1:A:547:LYS:N	2.33	0.44
1:A:549:LYS:O	1:A:553:GLN:HG2	2.17	0.44
1:A:421:VAL:HG22	1:A:476:GLN:HE22	1.83	0.44
1:A:367:PHE:HZ	1:A:390:ARG:HG3	1.82	0.44
1:A:388:LYS:O	1:A:392:LEU:HG	2.18	0.43
1:A:658:ILE:HG22	1:A:659:ILE:HG12	2.00	0.43
1:A:639:GLN:HG2	1:A:640:PHE:CD2	2.54	0.43
1:A:159:GLU:CA	1:A:162:VAL:CG1	2.93	0.43
1:A:161:GLN:NE2	1:A:168:ALA:N	2.66	0.43
1:A:303:GLN:NE2	1:A:310:LEU:HA	2.33	0.43
1:A:545:LYS:HE2	1:A:640:PHE:CD2	2.51	0.43
1:A:415:LYS:NZ	1:A:419:ASP:OD2	2.52	0.43
1:A:71:LYS:NZ	3:A:702:GDP:O2B	2.38	0.43
1:A:134:GLU:OE1	1:A:136:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:HG21	1:A:112:HIS:HB3	1.99	0.43
1:A:63:VAL:HG23	1:A:154:ILE:HB	1.99	0.43
1:A:115:SER:HB2	4:A:876:HOH:O	2.19	0.42
1:A:579:PHE:HB2	1:A:603:ALA:CB	2.49	0.42
1:A:165:TYR:O	1:A:168:ALA:N	2.52	0.42
1:A:426:LYS:H	1:A:426:LYS:HG2	1.58	0.42
1:A:600:PHE:HE1	1:A:675:VAL:HG13	1.84	0.42
1:A:549:LYS:HE2	1:A:549:LYS:HB3	1.68	0.42
1:A:255:LYS:HB2	3:A:702:GDP:C6	2.54	0.42
1:A:157:ILE:HG13	1:A:157:ILE:O	2.20	0.42
1:A:206:HIS:CE1	1:A:208:GLY:HA2	2.54	0.42
1:A:343:PHE:HZ	1:A:358:LEU:HD23	1.84	0.42
1:A:676:ASP:O	1:A:679:TYR:HB3	2.20	0.42
1:A:678:LYS:O	1:A:682:THR:HG23	2.20	0.42
1:A:545:LYS:NZ	1:A:548:PHE:CD2	2.87	0.42
1:A:541:GLN:OE1	1:A:544:GLU:HG3	2.20	0.42
1:A:681:GLU:C	1:A:683:LYS:H	2.24	0.42
1:A:136:GLN:H	1:A:136:GLN:CD	2.23	0.41
1:A:64:PHE:CZ	1:A:143:ALA:HB2	2.55	0.41
1:A:499:SER:O	1:A:503:GLU:HG2	2.20	0.41
1:A:545:LYS:O	1:A:549:LYS:HG3	2.19	0.41
1:A:656:ALA:O	1:A:658:ILE:HD12	2.20	0.41
1:A:299:ARG:NH2	1:A:318:LEU:HD13	2.34	0.41
1:A:508:ASN:OD1	1:A:510:GLU:N	2.51	0.41
1:A:526:PHE:CE2	1:A:543:ILE:CG1	3.04	0.41
1:A:461:ILE:HA	1:A:461:ILE:HD13	1.88	0.41
1:A:600:PHE:CE1	1:A:675:VAL:HG13	2.56	0.41
1:A:452:LEU:O	1:A:454:GLY:N	2.52	0.41
1:A:499:SER:HB2	1:A:518:GLN:HG3	2.03	0.41
1:A:551:TRP:CE3	1:A:554:PHE:HD2	2.38	0.41
1:A:420:LEU:O	1:A:428:PHE:HZ	2.03	0.41
1:A:458:LEU:HD23	1:A:458:LEU:HA	1.75	0.41
1:A:398:LYS:HB2	1:A:456:LEU:HD22	2.02	0.40
1:A:476:GLN:O	1:A:480:GLU:HG2	2.21	0.40
1:A:81:THR:O	1:A:82:ASN:HB3	2.21	0.40
1:A:116:LYS:HD2	1:A:116:LYS:HA	1.71	0.40
1:A:233:PRO:HB2	1:A:236:LEU:HD13	2.03	0.40
1:A:348:ALA:O	1:A:350:PRO:HD3	2.21	0.40
1:A:439:LEU:HD12	1:A:439:LEU:HA	1.92	0.40
1:A:165:TYR:C	1:A:167:GLY:N	2.73	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLN:O	1:A:166:GLN:OE1[2_656]	1.45	0.75
1:A:166:GLN:CB	1:A:166:GLN:CB[2_656]	2.16	0.04
1:A:427:ASP:OD2	1:A:433:LYS:NZ[2_555]	2.18	0.02

## 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	628/692 (91%)	583 (93%)	32 (5%)	13 (2%)	<b>8</b> <b>6</b>

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	424	LYS
1	A	535	SER
1	A	536	SER
1	A	653	HIS
1	A	528	GLY
1	A	534	THR
1	A	549	LYS
1	A	427	ASP
1	A	164	LEU
1	A	277	ASN
1	A	167	GLY
1	A	631	ILE

### 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	570/621 (92%)	536 (94%)	34 (6%)	22	30

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASP
1	A	50	SER
1	A	53	ASP
1	A	62	SER
1	A	85	VAL
1	A	105	VAL
1	A	116	LYS
1	A	125	GLU
1	A	161	GLN
1	A	164	LEU
1	A	165	TYR
1	A	221	LEU
1	A	247	VAL
1	A	303	GLN
1	A	336	LEU
1	A	345	GLU
1	A	347	ASP
1	A	353	GLU
1	A	396	LYS
1	A	431	ASN
1	A	433	LYS
1	A	452	LEU
1	A	457	SER
1	A	472	ILE
1	A	518	GLN
1	A	524	GLU
1	A	525	LYS
1	A	526	PHE
1	A	529	ASP
1	A	532	LEU
1	A	544	GLU
1	A	594	GLN
1	A	675	VAL
1	A	686	ILE



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	166	GLN
1	A	277	ASN
1	A	303	GLN
1	A	476	GLN
1	A	539	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 2 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
3	GDP	A	702	2	25,30,30	1.16	2 (8%)	26,47,47	1.98	6 (23%)

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	GDP	A	702	2	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	GDP	C5-C4	3.05	1.47	1.40
3	A	702	GDP	C6-C5	3.84	1.48	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	GDP	C5-C6-N1	-3.95	117.85	123.48
3	A	702	GDP	C6-C5-C4	-3.72	117.15	120.84
3	A	702	GDP	N3-C2-N1	-3.22	122.75	127.46
3	A	702	GDP	C4-C5-N7	-2.97	106.54	109.41
3	A	702	GDP	C6-N1-C2	4.49	122.51	116.06
3	A	702	GDP	C2-N3-C4	4.90	120.88	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	GDP	2	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	636/692 (91%)	0.88	69 (10%) 6 9	26, 71, 134, 210	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	GLY	19.9
1	A	166	GLN	18.2
1	A	168	ALA	11.4
1	A	165	TYR	6.3
1	A	551	TRP	6.0
1	A	447	VAL	5.5
1	A	343	PHE	5.4
1	A	545	LYS	5.3
1	A	443	VAL	5.2
1	A	359	PHE	5.1
1	A	337	THR	5.0
1	A	640	PHE	4.9
1	A	423	LEU	4.7
1	A	405	ALA	4.5
1	A	335	PHE	4.4
1	A	428	PHE	4.3
1	A	641	LEU	4.3
1	A	629	TYR	4.1
1	A	549	LYS	3.9
1	A	52	ALA	3.9
1	A	429	ALA	3.6
1	A	51	PRO	3.6
1	A	355	LEU	3.6
1	A	457	SER	3.5
1	A	430	VAL	3.5
1	A	161	GLN	3.5
1	A	164	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	412	LEU	3.4
1	A	543	ILE	3.3
1	A	634	SER	3.1
1	A	544	GLU	3.0
1	A	391	TRP	3.0
1	A	398	LYS	2.9
1	A	344	LYS	2.8
1	A	481	LEU	2.8
1	A	635	LYS	2.8
1	A	639	GLN	2.7
1	A	163	GLY	2.7
1	A	432	VAL	2.7
1	A	435	LEU	2.7
1	A	482	ASN	2.7
1	A	632	PHE	2.7
1	A	331	VAL	2.6
1	A	354	GLU	2.6
1	A	636	LEU	2.5
1	A	346	VAL	2.5
1	A	515	VAL	2.5
1	A	538	GLN	2.4
1	A	591	LEU	2.4
1	A	487	LYS	2.4
1	A	348	ALA	2.4
1	A	332	PHE	2.4
1	A	352	PHE	2.4
1	A	37	HIS	2.3
1	A	534	THR	2.3
1	A	445	PHE	2.3
1	A	456	LEU	2.2
1	A	360	ALA	2.2
1	A	221	LEU	2.2
1	A	138	PHE	2.2
1	A	401	PHE	2.2
1	A	548	PHE	2.1
1	A	451	SER	2.1
1	A	247	VAL	2.1
1	A	489	VAL	2.1
1	A	450	MET	2.0
1	A	490	LYS	2.0
1	A	126	GLY	2.0
1	A	136	GLN	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( $\text{\AA}^2$ )	Q<0.9
3	GDP	A	702	28/28	0.95	0.11	-0.75	44,49,52,52	0
2	MG	A	701	1/1	0.88	0.16	-	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.