



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 3, 2017 – 01:26 PM EDT

PDB ID : 1HE8  
Title : Ras G12V - PI 3-kinase gamma complex  
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Deposited on : unknown  
Resolution : 3.00 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 : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

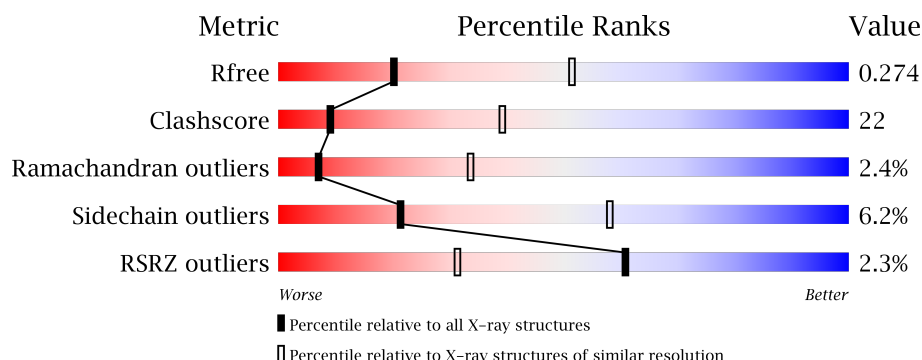
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	965	<div> <div>2%</div> <div>42%</div> <div>31%</div> <div>•</div> <div>22%</div> </div>
2	B	166	<div> <div>%</div> <div>57%</div> <div>39%</div> <div>•</div> </div>

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
3	MG	B	201	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7434 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 PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUB-UNIT, GAMMA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	749	Total	C	N	O	S	0	0	0
			6069	3894	1033	1107	35			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	LYS	VAL	engineered mutation	UNP P48736
A	326	ALA	VAL	engineered mutation	UNP P48736

- Molecule 2 is a protein called TRANSFORMING PROTEIN P21/H-RAS-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1326	827	228	264	7			

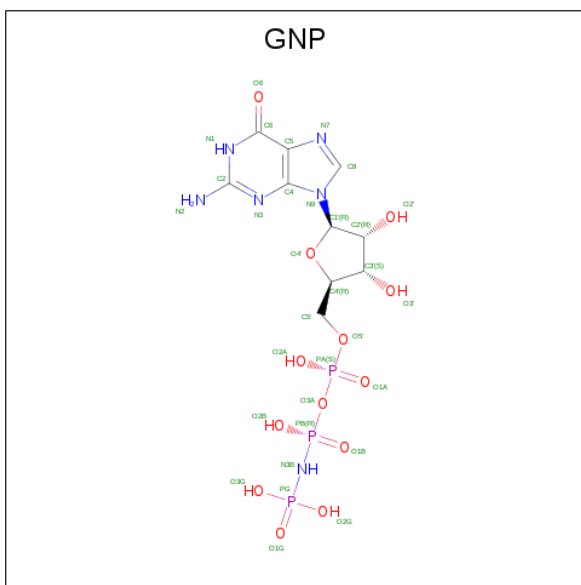
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	12	VAL	GLY	engineered mutation	UNP P01112

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

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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	B	5	Total O 5 5	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.64Å 113.64Å 183.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.03 – 3.00 52.03 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.5 (52.03-3.00) 91.6 (52.03-3.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.212 , 0.280 0.210 , 0.274	Depositor DCC
$R_{free}$ test set	1510 reflections (5.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.0	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 108.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: 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	0.45	0/6192	0.60	0/8364
2	B	0.53	0/1345	0.69	0/1815
All	All	0.46	0/7537	0.61	0/10179

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	6069	0	6121	277	0
2	B	1326	0	1301	54	0
3	B	1	0	0	0	0
4	B	32	0	13	0	0
5	A	1	0	0	0	0
5	B	5	0	0	1	0
All	All	7434	0	7435	330	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 22.

All (330) 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:228:THR:HB	2:B:41:ARG:HB3	1.36	1.06
1:A:843:LEU:HG	1:A:1034:MET:HG3	1.53	0.89
1:A:372:VAL:HG12	1:A:373:LEU:H	1.42	0.84
1:A:693:HIS:CD2	1:A:789:PRO:HG3	2.13	0.84
1:A:745:VAL:HG21	1:A:774:LEU:HD11	1.58	0.83
1:A:255:LYS:HD3	1:A:258:LEU:HD12	1.64	0.80
2:B:133:LEU:HD11	2:B:137:TYR:CZ	2.17	0.78
2:B:19:LEU:HD12	2:B:146:ALA:HB2	1.66	0.77
1:A:895:THR:HG22	1:A:902:PHE:HB2	1.68	0.75
1:A:479:GLU:HG2	1:A:519:LEU:HD13	1.68	0.75
1:A:917:THR:HG23	1:A:920:LYS:HB2	1.68	0.74
1:A:750:LYS:HE3	1:A:809:LYS:HG2	1.70	0.73
1:A:366:ARG:HB2	1:A:517:SER:HB3	1.72	0.72
1:A:903:LYS:O	1:A:906:VAL:HG23	1.90	0.72
1:A:989:PRO:HG2	1:A:1080:TRP:NE1	2.05	0.72
1:A:420:ILE:HD12	1:A:475:LEU:CD2	2.21	0.70
1:A:736:VAL:O	1:A:740:GLU:HB2	1.91	0.70
1:A:420:ILE:HG23	1:A:475:LEU:HD22	1.74	0.69
1:A:907:LEU:HD12	1:A:994:VAL:HG21	1.74	0.69
1:A:1048:ILE:HD13	1:A:1048:ILE:O	1.92	0.68
1:A:761:SER:HB3	1:A:764:ILE:HG13	1.74	0.68
1:A:208:PRO:HD2	1:A:211:LEU:HD12	1.75	0.68
1:A:245:LEU:HD21	1:A:307:LEU:HD13	1.75	0.68
1:A:356:ASP:HB3	1:A:359:ARG:HG3	1.76	0.68
1:A:779:LEU:HD23	1:A:780:PRO:HD2	1.76	0.67
1:A:355:TRP:HB3	1:A:359:ARG:CZ	2.25	0.67
1:A:457:LYS:HD3	1:A:459:ARG:HH21	1.57	0.67
1:A:498:ASN:HD21	1:A:500:ASP:HB2	1.61	0.66
1:A:364:LYS:HE2	1:A:366:ARG:NH2	2.12	0.65
1:A:184:ARG:O	1:A:188:VAL:HG23	1.97	0.65
1:A:860:LEU:HD21	1:A:1015:LYS:HD3	1.79	0.64
1:A:816:LYS:NZ	1:A:816:LYS:HB2	2.13	0.64
1:A:240:THR:HG22	1:A:242:GLY:N	2.12	0.64
1:A:518:ILE:HD12	1:A:520:LEU:CD1	2.28	0.64
1:A:921:PHE:O	1:A:925:VAL:HG23	1.98	0.64
1:A:796:LEU:HD22	1:A:798:ILE:HG13	1.80	0.63
1:A:947:ARG:NH2	1:A:963:ILE:O	2.30	0.63
2:B:97:ARG:HD3	2:B:101:LYS:HE2	1.80	0.63
1:A:518:ILE:HD12	1:A:520:LEU:HD11	1.78	0.63
1:A:761:SER:OG	1:A:763:VAL:HG12	1.98	0.63
2:B:68:ARG:O	2:B:72:MET:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ARG:HA	1:A:366:ARG:HE	1.62	0.62
2:B:45:VAL:HA	2:B:50:THR:HA	1.82	0.61
1:A:355:TRP:HB3	1:A:359:ARG:NH2	2.15	0.61
1:A:1006:PHE:O	1:A:1010:GLN:HG3	2.01	0.61
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.83	0.61
1:A:840:GLN:OE1	1:A:966:GLY:HA2	2.01	0.60
1:A:743:GLN:HA	1:A:832:PHE:HE2	1.67	0.60
1:A:887:THR:HG23	1:A:953:MET:HG2	1.83	0.60
1:A:168:VAL:HG12	1:A:170:ASP:H	1.67	0.60
2:B:92:ASP:HA	2:B:95:GLN:HG2	1.84	0.60
1:A:766:GLN:O	1:A:770:LYS:HG3	2.01	0.60
1:A:852:GLU:HG3	1:A:864:LEU:HD12	1.83	0.60
1:A:182:THR:OG1	1:A:183:PRO:HD3	2.02	0.60
1:A:743:GLN:HA	1:A:832:PHE:CE2	2.37	0.59
1:A:420:ILE:HD12	1:A:475:LEU:HD21	1.84	0.59
1:A:373:LEU:HG	1:A:374:PRO:HD2	1.82	0.59
1:A:843:LEU:HG	1:A:1034:MET:CG	2.31	0.59
1:A:169:HIS:CD2	1:A:476:ARG:HH12	2.21	0.59
1:A:379:LEU:HG	1:A:380:THR:H	1.66	0.59
2:B:64:TYR:O	2:B:67:MET:HG2	2.00	0.59
1:A:483:HIS:CD2	1:A:510:LYS:HA	2.36	0.59
2:B:113:LEU:HD23	2:B:134:ALA:HB2	1.83	0.59
1:A:193:PRO:HB2	1:A:313:PRO:HB3	1.84	0.59
1:A:397:ARG:HG2	1:A:416:PHE:CD2	2.37	0.58
1:A:771:LEU:HD12	1:A:798:ILE:HG23	1.85	0.58
1:A:287:ILE:O	1:A:293:VAL:HG21	2.03	0.58
1:A:370:ILE:HD12	1:A:514:MET:HE2	1.85	0.58
1:A:255:LYS:HG2	1:A:258:LEU:HB2	1.85	0.58
1:A:169:HIS:HD2	1:A:476:ARG:HH12	1.51	0.58
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.85	0.58
1:A:371:PRO:HG2	1:A:512:ASN:HA	1.86	0.57
1:A:622:LEU:HD11	1:A:854:ILE:HA	1.86	0.57
1:A:240:THR:HG22	1:A:242:GLY:H	1.67	0.57
1:A:432:GLN:HB3	1:A:460:LEU:HD11	1.86	0.57
1:A:476:ARG:HD2	1:A:480:TYR:OH	2.04	0.57
1:A:302:GLU:HB2	1:A:304:HIS:HE1	1.69	0.57
1:A:262:PRO:HB2	1:A:265:GLN:HB2	1.86	0.57
1:A:359:ARG:O	1:A:420:ILE:HG12	2.05	0.57
1:A:271:VAL:HB	1:A:310:PRO:HG3	1.87	0.57
1:A:880:GLU:HG2	1:A:881:ILE:N	2.17	0.57
2:B:19:LEU:CD1	2:B:146:ALA:HB2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:LYS:HG2	1:A:728:MET:HE2	1.87	0.56
1:A:367:GLY:HA3	1:A:409:LEU:HD23	1.87	0.56
1:A:657:LEU:HD11	1:A:690:ARG:HE	1.70	0.56
1:A:766:GLN:HA	1:A:769:GLN:OE1	2.05	0.56
1:A:271:VAL:HG23	1:A:282:VAL:CG1	2.35	0.55
1:A:936:CYS:O	1:A:939:THR:HG22	2.06	0.55
1:A:241:PRO:HD3	1:A:285:THR:O	2.06	0.55
1:A:236:SER:HB3	1:A:239:ASP:OD2	2.07	0.55
1:A:660:LEU:HD23	1:A:698:PHE:CE2	2.41	0.55
1:A:201:TRP:NE1	1:A:291:GLN:HG3	2.21	0.55
1:A:420:ILE:HD12	1:A:475:LEU:HD22	1.89	0.55
1:A:703:ILE:HD12	1:A:717:LEU:HD12	1.89	0.55
1:A:981:GLU:HG2	1:A:982:ARG:H	1.72	0.55
1:A:779:LEU:HD23	1:A:780:PRO:CD	2.37	0.54
1:A:146:GLU:HG2	1:A:319:ARG:HH21	1.73	0.54
1:A:798:ILE:HD12	1:A:798:ILE:H	1.72	0.54
2:B:118:CYS:SG	2:B:143:GLU:HB3	2.47	0.54
1:A:200:PRO:HG3	1:A:282:VAL:CG2	2.37	0.54
1:A:1065:LYS:O	1:A:1069:LEU:HG	2.08	0.54
2:B:123:ARG:HG2	2:B:124:THR:N	2.23	0.54
1:A:209:GLU:OE1	1:A:209:GLU:HA	2.07	0.53
1:A:768:LYS:O	1:A:772:GLU:HG2	2.08	0.53
1:A:838:LEU:O	1:A:842:MET:HG3	2.09	0.53
1:A:838:LEU:HD21	1:A:879:ILE:HD11	1.89	0.53
1:A:281:LEU:HD22	1:A:305:VAL:HG11	1.91	0.53
2:B:42:LYS:HG2	2:B:44:VAL:HG23	1.91	0.53
1:A:366:ARG:HH21	1:A:411:ASN:HB3	1.74	0.53
1:A:1073:GLU:HA	1:A:1076:ARG:HB2	1.91	0.53
2:B:72:MET:SD	2:B:99:GLN:HG2	2.49	0.53
1:A:652:GLU:HG2	1:A:655:ASP:OD2	2.09	0.52
1:A:916:PRO:HD2	1:A:920:LYS:HG2	1.91	0.52
2:B:46:ILE:HG12	2:B:51:CYS:SG	2.50	0.52
1:A:312:ASP:HB3	1:A:315:LEU:HG	1.90	0.52
1:A:396:GLN:O	1:A:397:ARG:HD3	2.09	0.52
1:A:693:HIS:CG	1:A:789:PRO:HG3	2.44	0.52
1:A:874:ASP:OD1	1:A:875:LYS:HG3	2.10	0.52
2:B:126:GLU:HB2	2:B:129:GLN:HG3	1.91	0.52
1:A:750:LYS:NZ	1:A:808:LYS:HB3	2.25	0.52
2:B:28:PHE:HA	5:B:304:HOH:O	2.09	0.52
1:A:997:THR:HG22	1:A:998:SER:N	2.25	0.52
1:A:1025:ASN:O	1:A:1029:ILE:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:MET:O	1:A:260:ASP:HB3	2.09	0.52
1:A:403:PRO:O	1:A:405:THR:HG23	2.10	0.52
1:A:917:THR:OG1	1:A:919:GLU:HG3	2.09	0.51
1:A:379:LEU:CG	1:A:380:THR:H	2.23	0.51
2:B:46:ILE:HG22	2:B:47:ASP:N	2.26	0.51
1:A:862:LEU:HD11	1:A:1012:ILE:HG22	1.92	0.51
2:B:87:THR:O	2:B:90:PHE:HB3	2.09	0.51
1:A:920:LYS:O	1:A:923:ALA:HB3	2.11	0.51
2:B:86:ASN:ND2	2:B:89:SER:HB3	2.26	0.51
1:A:870:ILE:HD13	1:A:871:SER:N	2.26	0.51
1:A:364:LYS:HD2	1:A:413:TRP:CZ2	2.47	0.50
2:B:116:ASN:O	2:B:117:LYS:HB2	2.11	0.50
1:A:739:ILE:HD13	1:A:872:THR:HB	1.91	0.50
1:A:854:ILE:HG23	1:A:1023:HIS:HD2	1.77	0.50
1:A:480:TYR:HB2	1:A:518:ILE:HG13	1.94	0.50
1:A:246:GLN:O	1:A:250:THR:HG23	2.12	0.50
1:A:1034:MET:SD	1:A:1035:LEU:HD13	2.53	0.49
1:A:207:LEU:HD21	1:A:211:LEU:HB3	1.95	0.49
1:A:357:CYS:HB2	1:A:421:LYS:HB2	1.94	0.49
1:A:837:ASP:OD2	1:A:839:ARG:HB2	2.12	0.49
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.93	0.49
1:A:860:LEU:HD11	1:A:1015:LYS:HG2	1.94	0.49
1:A:154:LEU:O	1:A:158:ILE:HG12	2.12	0.49
1:A:221:PHE:CE1	1:A:234:LYS:HD2	2.46	0.49
1:A:854:ILE:HG23	1:A:1023:HIS:CD2	2.46	0.49
2:B:96:TYR:O	2:B:100:ILE:HG13	2.11	0.49
1:A:249:PHE:CD2	1:A:267:GLU:HB3	2.48	0.49
2:B:63:GLU:O	2:B:63:GLU:HG2	2.13	0.49
1:A:184:ARG:HD3	1:A:719:ALA:O	2.13	0.49
1:A:240:THR:O	1:A:244:ILE:HG13	2.12	0.49
1:A:772:GLU:HA	1:A:775:GLN:HB3	1.94	0.48
1:A:793:ALA:HA	1:A:828:ILE:HD12	1.95	0.48
2:B:97:ARG:HH11	2:B:97:ARG:HG2	1.78	0.48
1:A:197:ALA:HA	1:A:689:LYS:NZ	2.29	0.48
2:B:142:ILE:HD12	2:B:155:ALA:HA	1.94	0.48
1:A:1007:GLN:HA	1:A:1010:GLN:HE21	1.78	0.48
1:A:372:VAL:HG12	1:A:373:LEU:N	2.20	0.48
1:A:741:MET:SD	1:A:779:LEU:HG	2.54	0.48
2:B:23:LEU:HD13	2:B:156:PHE:CG	2.49	0.48
1:A:173:LEU:HD23	1:A:673:HIS:CD2	2.48	0.48
1:A:988:THR:HG21	1:A:1083:GLN:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:ARG:O	1:A:1057:VAL:HG23	2.14	0.48
1:A:1056:THR:HG22	1:A:1059:LYS:HD2	1.94	0.48
1:A:768:LYS:HZ2	1:A:768:LYS:HB2	1.79	0.48
1:A:862:LEU:HB3	1:A:934:GLY:HA3	1.95	0.48
1:A:273:ARG:NH2	1:A:819:ASP:OD2	2.45	0.47
1:A:838:LEU:HD22	1:A:877:GLY:HA3	1.96	0.47
1:A:215:ILE:O	1:A:215:ILE:HD12	2.14	0.47
1:A:262:PRO:HB2	1:A:265:GLN:CB	2.44	0.47
1:A:771:LEU:CD1	1:A:798:ILE:HG23	2.44	0.47
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.14	0.47
1:A:235:VAL:HG11	1:A:244:ILE:CD1	2.44	0.47
2:B:22:GLN:O	2:B:26:ASN:N	2.46	0.47
1:A:198:MET:HG3	1:A:280:TYR:CG	2.49	0.47
1:A:739:ILE:O	1:A:743:GLN:HB2	2.13	0.47
1:A:865:LEU:HD23	1:A:961:PHE:CD1	2.50	0.47
2:B:94:HIS:H	2:B:94:HIS:HD1	1.62	0.47
1:A:908:ASN:HB2	1:A:994:VAL:HG22	1.96	0.47
1:A:1026:LEU:HD13	1:A:1030:LEU:HD12	1.96	0.47
1:A:384:GLU:HG3	1:A:398:ARG:HG2	1.95	0.47
1:A:235:VAL:HG11	1:A:244:ILE:HD13	1.96	0.47
1:A:738:VAL:O	1:A:741:MET:N	2.45	0.47
1:A:215:ILE:O	1:A:215:ILE:CG1	2.63	0.47
1:A:511:GLU:HB3	1:A:512:ASN:OD1	2.15	0.47
1:A:1034:MET:SD	1:A:1035:LEU:N	2.89	0.46
1:A:848:LEU:HG	1:A:864:LEU:HD13	1.96	0.46
1:A:865:LEU:HD23	1:A:961:PHE:CG	2.51	0.46
2:B:97:ARG:HG3	2:B:137:TYR:CE2	2.50	0.46
2:B:5:LYS:HA	2:B:54:ASP:HB2	1.98	0.46
1:A:1014:VAL:O	1:A:1018:LEU:HG	2.16	0.46
1:A:215:ILE:HG13	1:A:215:ILE:O	2.16	0.46
1:A:240:THR:HG23	1:A:241:PRO:HD2	1.96	0.46
1:A:196:TYR:O	1:A:689:LYS:HD2	2.16	0.46
1:A:852:GLU:CD	1:A:864:LEU:HB2	2.36	0.46
2:B:5:LYS:O	2:B:76:GLU:HB2	2.16	0.46
1:A:1070:ASP:O	1:A:1074:VAL:HG23	2.16	0.46
1:A:945:GLY:O	1:A:986:VAL:HG23	2.16	0.46
1:A:354:LEU:N	1:A:354:LEU:HD22	2.31	0.46
1:A:927:ARG:HD3	1:A:959:ASN:HB2	1.98	0.46
1:A:397:ARG:HG2	1:A:416:PHE:CE2	2.51	0.46
1:A:660:LEU:O	1:A:664:VAL:HG23	2.16	0.46
1:A:944:ILE:HG22	1:A:967:HIS:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PRO:HG3	1:A:282:VAL:HG23	1.97	0.46
1:A:750:LYS:HG3	1:A:809:LYS:CG	2.46	0.46
1:A:180:LEU:C	1:A:183:PRO:HD2	2.36	0.45
1:A:699:LEU:O	1:A:703:ILE:HG13	2.16	0.45
1:A:209:GLU:O	1:A:213:LYS:HG3	2.15	0.45
1:A:848:LEU:HD12	1:A:848:LEU:HA	1.81	0.45
1:A:368:ILE:CG2	1:A:433:ILE:HD11	2.47	0.45
2:B:68:ARG:HB3	2:B:72:MET:HE3	1.98	0.45
1:A:1001:LYS:HB2	1:A:1001:LYS:NZ	2.31	0.45
1:A:172:GLU:HG2	1:A:673:HIS:CD2	2.52	0.45
1:A:768:LYS:NZ	1:A:768:LYS:HB2	2.31	0.45
1:A:770:LYS:O	1:A:774:LEU:HG	2.16	0.45
1:A:903:LYS:C	1:A:905:GLU:H	2.19	0.45
2:B:36:ILE:O	2:B:37:GLU:HB2	2.17	0.45
1:A:227:SER:C	1:A:229:THR:H	2.20	0.45
1:A:221:PHE:HE1	1:A:234:LYS:HD2	1.81	0.45
1:A:388:GLN:HG2	1:A:393:VAL:HA	1.99	0.45
1:A:364:LYS:O	1:A:518:ILE:HA	2.17	0.45
2:B:91:GLU:O	2:B:94:HIS:ND1	2.50	0.45
1:A:255:LYS:CD	1:A:258:LEU:HD12	2.43	0.45
1:A:879:ILE:N	1:A:879:ILE:HD12	2.32	0.45
1:A:838:LEU:HD21	1:A:879:ILE:CD1	2.47	0.44
1:A:242:GLY:O	1:A:246:GLN:HG3	2.17	0.44
1:A:364:LYS:HB3	1:A:519:LEU:HB3	1.98	0.44
1:A:832:PHE:CE2	1:A:876:ILE:HD11	2.52	0.44
1:A:990:ASP:O	1:A:994:VAL:HG23	2.17	0.44
1:A:703:ILE:CD1	1:A:717:LEU:HD12	2.48	0.44
1:A:745:VAL:O	1:A:749:ILE:HG22	2.17	0.44
1:A:1017:TYR:O	1:A:1021:ARG:HG3	2.18	0.44
1:A:367:GLY:HA3	1:A:409:LEU:CD2	2.47	0.44
1:A:460:LEU:HG	1:A:487:ILE:HD11	1.99	0.44
1:A:431:LEU:HD11	1:A:518:ILE:HG21	2.00	0.44
1:A:935:TYR:CE1	1:A:961:PHE:HA	2.53	0.44
2:B:22:GLN:O	2:B:26:ASN:HA	2.18	0.44
1:A:843:LEU:CG	1:A:1034:MET:HG3	2.36	0.44
2:B:41:ARG:HG3	2:B:52:LEU:HD11	2.00	0.44
1:A:364:LYS:HD2	1:A:413:TRP:CE2	2.52	0.44
1:A:741:MET:HE1	1:A:778:GLN:O	2.17	0.44
2:B:77:GLY:HA3	2:B:163:ILE:HD11	1.99	0.44
2:B:84:ILE:HG13	2:B:116:ASN:O	2.17	0.44
1:A:989:PRO:HD2	1:A:1080:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:LYS:O	1:A:1012:ILE:HG13	2.18	0.43
1:A:1017:TYR:CE2	1:A:1021:ARG:HD2	2.53	0.43
1:A:283:GLY:O	1:A:285:THR:N	2.51	0.43
1:A:309:THR:HA	1:A:310:PRO:HD3	1.85	0.43
1:A:469:ILE:N	1:A:469:ILE:HD12	2.33	0.43
1:A:826:GLU:HG2	1:A:883:LYS:HZ3	1.83	0.43
1:A:891:ILE:HG22	1:A:906:VAL:HG12	1.99	0.43
1:A:684:ARG:HD3	1:A:687:ARG:HH21	1.84	0.43
1:A:982:ARG:HH11	1:A:982:ARG:HG3	1.82	0.43
2:B:101:LYS:O	2:B:105:ASP:N	2.51	0.43
2:B:41:ARG:CD	2:B:52:LEU:HD11	2.49	0.43
1:A:428:LEU:HD23	1:A:467:LEU:HA	2.01	0.43
1:A:741:MET:CG	1:A:774:LEU:HD22	2.49	0.43
1:A:903:LYS:O	1:A:905:GLU:N	2.52	0.43
2:B:71:TYR:CD1	2:B:72:MET:N	2.87	0.43
1:A:1059:LYS:HD3	1:A:1063:ASP:OD1	2.18	0.42
1:A:208:PRO:HB3	1:A:210:TYR:CE2	2.55	0.42
2:B:80:CYS:HB3	2:B:93:ILE:HD11	2.01	0.42
1:A:850:ILE:O	1:A:854:ILE:HG13	2.19	0.42
1:A:870:ILE:HD13	1:A:871:SER:H	1.84	0.42
1:A:911:LEU:HD23	1:A:911:LEU:HA	1.82	0.42
1:A:1056:THR:HG23	1:A:1067:TYR:CD2	2.55	0.42
1:A:384:GLU:CD	1:A:396:GLN:HE21	2.22	0.42
2:B:99:GLN:O	2:B:103:VAL:HG23	2.20	0.42
1:A:1074:VAL:O	1:A:1078:LYS:HG2	2.19	0.42
1:A:271:VAL:HG23	1:A:282:VAL:HG12	2.01	0.42
1:A:1080:TRP:CE3	1:A:1084:PHE:HE1	2.37	0.42
1:A:306:VAL:O	1:A:306:VAL:HG13	2.19	0.42
1:A:428:LEU:HA	1:A:428:LEU:HD23	1.79	0.42
1:A:480:TYR:HB2	1:A:518:ILE:CG1	2.48	0.42
2:B:133:LEU:HD11	2:B:137:TYR:OH	2.20	0.42
2:B:84:ILE:HD11	2:B:117:LYS:O	2.19	0.42
1:A:989:PRO:HB2	1:A:1080:TRP:CZ2	2.55	0.42
1:A:196:TYR:CE2	1:A:689:LYS:HE3	2.54	0.42
1:A:259:MET:O	1:A:260:ASP:CB	2.67	0.42
1:A:381:VAL:CG1	1:A:433:ILE:HG23	2.49	0.42
1:A:816:LYS:HB2	1:A:816:LYS:HZ2	1.83	0.42
1:A:215:ILE:HD12	1:A:216:ALA:O	2.19	0.42
1:A:365:ILE:HD13	1:A:518:ILE:HG22	2.02	0.42
1:A:675:SER:O	1:A:679:ARG:HG3	2.20	0.42
1:A:800:LYS:CB	1:A:814:GLU:HG3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:THR:HG22	1:A:998:SER:H	1.83	0.42
1:A:286:PRO:HD2	1:A:289:ASN:HD22	1.85	0.42
1:A:851:MET:HG2	1:A:1020:LEU:HD21	2.02	0.42
1:A:464:VAL:HG21	1:A:482:LEU:HB3	2.02	0.42
1:A:226:ARG:HG2	1:A:259:MET:O	2.20	0.41
1:A:395:CYS:SG	1:A:416:PHE:HB3	2.60	0.41
1:A:158:ILE:HD11	1:A:721:LEU:HD12	2.02	0.41
1:A:779:LEU:HD23	1:A:780:PRO:N	2.35	0.41
1:A:826:GLU:OE1	1:A:883:LYS:HD3	2.20	0.41
1:A:952:ILE:HD11	1:A:986:VAL:HG21	2.02	0.41
1:A:464:VAL:HB	1:A:484:MET:HA	2.03	0.41
2:B:104:LYS:O	2:B:105:ASP:C	2.57	0.41
1:A:1024:THR:HG21	1:A:1057:VAL:HG22	2.02	0.41
1:A:464:VAL:HG12	1:A:484:MET:HE3	2.01	0.41
1:A:750:LYS:HZ1	1:A:808:LYS:HB3	1.86	0.41
1:A:856:GLU:C	1:A:858:GLU:H	2.24	0.41
2:B:88:LYS:O	2:B:91:GLU:N	2.53	0.41
1:A:207:LEU:HA	1:A:294:ARG:NH1	2.35	0.41
1:A:360:LYS:HA	1:A:419:LYS:HA	2.02	0.41
1:A:362:ARG:HB3	1:A:415:GLU:HG3	2.03	0.41
1:A:862:LEU:HD22	1:A:862:LEU:N	2.36	0.41
2:B:24:ILE:HD13	2:B:24:ILE:HA	1.89	0.41
1:A:700:ARG:HG2	1:A:700:ARG:HH11	1.86	0.41
2:B:92:ASP:HA	2:B:95:GLN:CG	2.51	0.41
1:A:1026:LEU:HA	1:A:1029:ILE:CG2	2.50	0.41
1:A:834:HIS:ND1	1:A:835:GLY:N	2.69	0.41
2:B:52:LEU:C	2:B:52:LEU:HD13	2.41	0.41
2:B:123:ARG:CG	2:B:124:THR:N	2.84	0.41
2:B:93:ILE:HA	2:B:93:ILE:HD12	1.87	0.41
1:A:312:ASP:OD1	1:A:314:ALA:HB3	2.21	0.41
1:A:394:LEU:HB2	1:A:395:CYS:H	1.74	0.41
1:A:665:GLN:HB3	1:A:1037:THR:HG21	2.03	0.41
1:A:710:GLN:HG3	1:A:711:GLN:N	2.35	0.41
1:A:842:MET:HE1	1:A:871:SER:HB3	2.04	0.40
2:B:6:LEU:HG	2:B:159:LEU:HD23	2.02	0.40
1:A:356:ASP:HB3	1:A:359:ARG:CG	2.47	0.40
1:A:433:ILE:HB	1:A:462:TYR:HB2	2.04	0.40
1:A:637:ASP:O	1:A:638:GLU:C	2.59	0.40
1:A:887:THR:CG2	1:A:953:MET:HG2	2.49	0.40
2:B:23:LEU:HD23	2:B:23:LEU:C	2.41	0.40
1:A:854:ILE:HG21	1:A:1020:LEU:HD23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ARG:HD3	1:A:476:ARG:HA	1.88	0.40
1:A:484:MET:HE3	1:A:516:ILE:HG21	2.03	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	729/965 (76%)	625 (86%)	87 (12%)	17 (2%)	7	35
2	B	164/166 (99%)	141 (86%)	19 (12%)	4 (2%)	7	34
All	All	893/1131 (79%)	766 (86%)	106 (12%)	21 (2%)	7	34

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ALA
2	B	46	ILE
1	A	260	ASP
1	A	778	GLN
1	A	906	VAL
1	A	916	PRO
1	A	170	ASP
1	A	284	GLU
1	A	405	THR
1	A	904	ASP
1	A	964	ASP
2	B	37	GLU
1	A	218	ASN
1	A	371	PRO
1	A	777	SER
2	B	11	ALA

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Mol	Chain	Res	Type
2	B	50	THR
1	A	247	SER
1	A	298	LYS
1	A	944	ILE
1	A	526	PRO

### 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	679/862 (79%)	635 (94%)	44 (6%)	20	56
2	B	145/145 (100%)	138 (95%)	7 (5%)	30	69
All	All	824/1007 (82%)	773 (94%)	51 (6%)	21	58

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	THR
1	A	198	MET
1	A	207	LEU
1	A	212	TRP
1	A	234	LYS
1	A	247	SER
1	A	252	MET
1	A	258	LEU
1	A	277	ARG
1	A	305	VAL
1	A	319	ARG
1	A	355	TRP
1	A	366	ARG
1	A	407	GLU
1	A	512	ASN
1	A	521	ASP
1	A	522	ASN
1	A	646	GLN

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Mol	Chain	Res	Type
1	A	657	LEU
1	A	682	LEU
1	A	717	LEU
1	A	728	MET
1	A	748	ASP
1	A	768	LYS
1	A	816	LYS
1	A	846	GLN
1	A	870	ILE
1	A	887	THR
1	A	905	GLU
1	A	917	THR
1	A	927	ARG
1	A	985	PHE
1	A	988	THR
1	A	1000	LYS
1	A	1001	LYS
1	A	1005	HIS
1	A	1025	ASN
1	A	1026	LEU
1	A	1029	ILE
1	A	1031	PHE
1	A	1033	MET
1	A	1034	MET
1	A	1048	ILE
1	A	1056	THR
2	B	12	VAL
2	B	19	LEU
2	B	27	HIS
2	B	44	VAL
2	B	70	GLN
2	B	74	THR
2	B	97	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	295	HIS
1	A	299	ASN
1	A	304	HIS
1	A	388	GLN

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Mol	Chain	Res	Type
1	A	389	HIS
1	A	392	GLN
1	A	396	GLN
1	A	432	GLN
1	A	471	HIS
1	A	483	HIS
1	A	498	ASN
1	A	629	GLN
1	A	646	GLN
1	A	705	GLN
1	A	710	GLN
1	A	766	GLN
1	A	773	ASN
1	A	846	GLN
1	A	892	GLN
1	A	908	ASN
1	A	922	GLN
1	A	951	ASN
1	A	1010	GLN
1	A	1023	HIS
1	A	1025	ASN
2	B	25	GLN
2	B	61	GLN

### 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	$\# Z  > 2$
4	GNP	B	202	3	27,34,34	3.37	8 (29%)	26,54,54	1.82	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
4	GNP	B	202	3	-	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)
4	B	202	GNP	C4-N9	-7.40	1.37	1.47
4	B	202	GNP	C5-C6	-4.93	1.44	1.53
4	B	202	GNP	PG-O3G	-4.55	1.44	1.56
4	B	202	GNP	PB-O2B	-3.69	1.46	1.56
4	B	202	GNP	PG-O2G	-3.30	1.47	1.56
4	B	202	GNP	C8-N9	-2.94	1.37	1.46
4	B	202	GNP	C6-N1	5.53	1.42	1.33
4	B	202	GNP	PG-O1G	11.62	1.59	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	202	GNP	O3G-PG-O1G	-4.77	101.30	113.41
4	B	202	GNP	O1G-PG-N3B	-2.58	107.93	111.79
4	B	202	GNP	O2G-PG-O1G	-2.42	107.25	113.41
4	B	202	GNP	O6-C6-N1	-2.06	119.96	122.70
4	B	202	GNP	O1B-PB-N3B	2.62	115.70	111.79
4	B	202	GNP	O6-C6-C5	4.35	128.00	119.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	749/965 (77%)	0.01	19 (2%) 58 29	23, 68, 122, 170	0
2	B	166/166 (100%)	-0.07	2 (1%) 79 53	23, 51, 102, 132	0
All	All	915/1131 (80%)	-0.00	21 (2%) 61 31	23, 66, 119, 170	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	778	GLN	3.9
1	A	777	SER	3.8
1	A	1037	THR	3.3
1	A	764	ILE	2.8
1	A	774	LEU	2.8
1	A	408	VAL	2.7
1	A	400	SER	2.4
1	A	404	PHE	2.4
2	B	49	GLU	2.4
2	B	1	MET	2.3
1	A	999	GLY	2.2
1	A	414	LEU	2.2
1	A	753	SER	2.2
1	A	776	ASN	2.2
1	A	998	SER	2.2
1	A	399	THR	2.2
1	A	807	LYS	2.1
1	A	967	HIS	2.1
1	A	997	THR	2.1
1	A	525	HIS	2.1
1	A	763	VAL	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	MG	B	201	1/1	0.95	0.39	11.19	67,67,67,67	0
4	GNP	B	202	32/32	0.98	0.20	0.35	39,42,47,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.