



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:34 PM GMT

PDB ID : 1G98  
Title : CRYSTAL STRUCTURE ANALYSIS OF RABBIT PHOSPHOGLUCOSE ISOMERASE COMPLEXED WITH 5-PHOSPHOARABINONATE, A TRANSITION STATE ANALOGUE  
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Deposited on : 2000-11-22  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

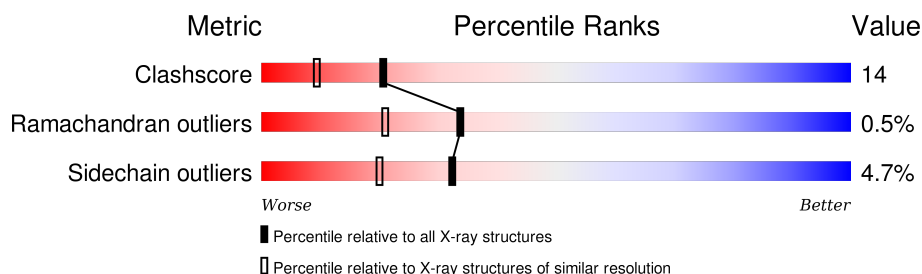
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	558	 75% 20% 5% •
1	B	558	 82% 15% ••

## 2 Entry composition [i](#)

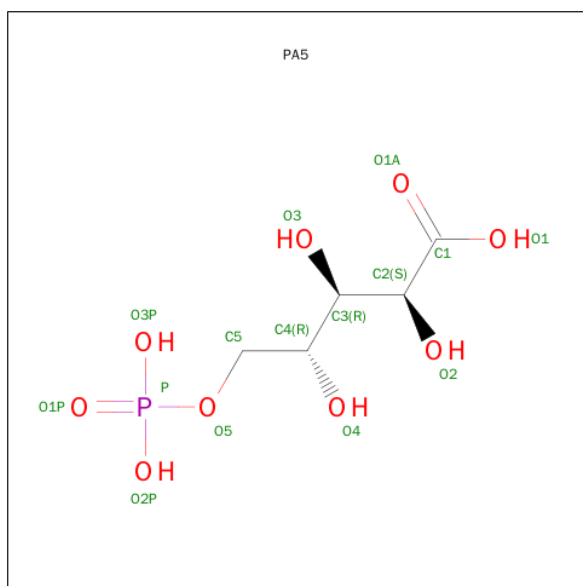
There are 3 unique types of molecules in this entry. The entry contains 9712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHOGLUCOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4395	2805	765	806	19			
1	B	555	Total	C	N	O	S	0	0	0
			4395	2805	765	806	19			

- Molecule 2 is 5-PHOSPHOARABINONIC ACID (three-letter code: PA5) (formula: C<sub>5</sub>H<sub>11</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			15	5	9	1		
2	B	1	Total	C	O	P	0	0
			15	5	9	1		

- Molecule 3 is water.

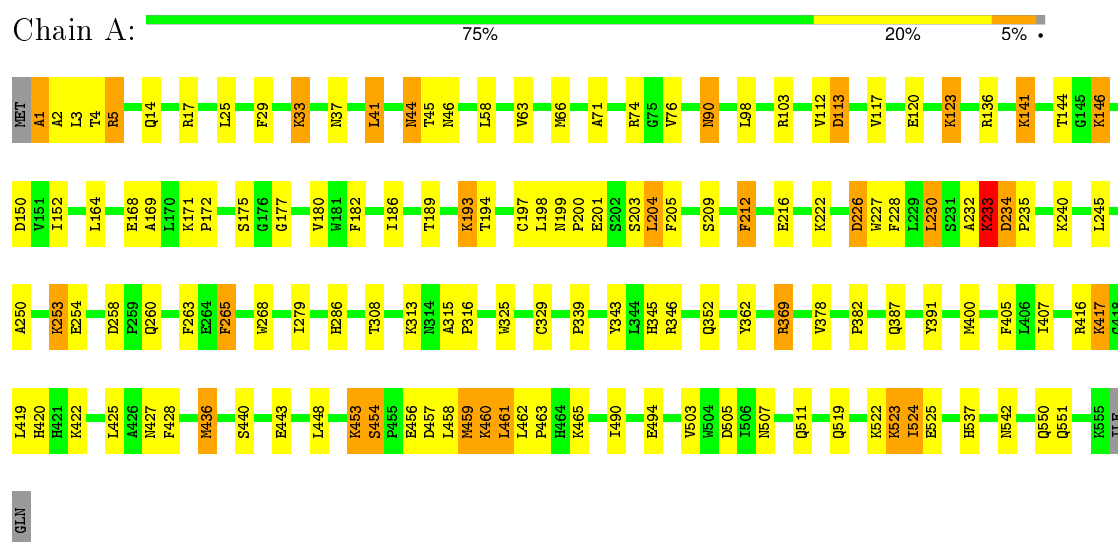
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	427	Total 427	O 427	0	0
3	B	465	Total 465	O 465	0	0

### 3 Residue-property plots

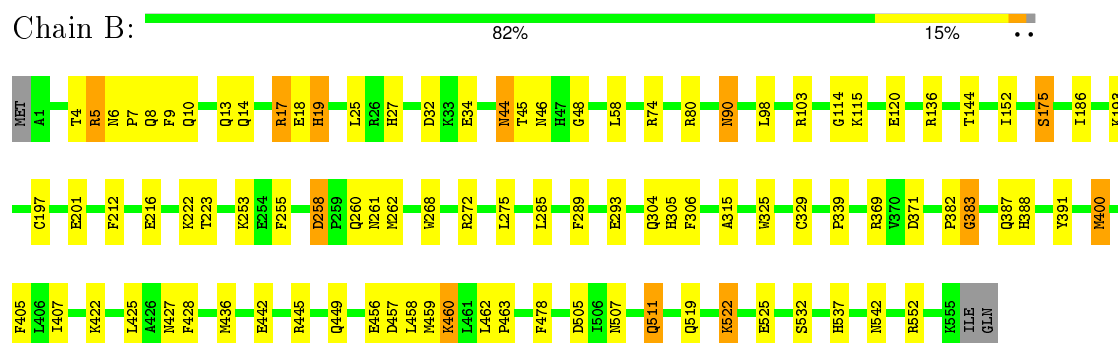
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: PHOSPHOGLUCOSE ISOMERASE



#### • Molecule 1: PHOSPHOGLUCOSE ISOMERASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.83 Å   116.55 Å   271.82 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	8.00 – 1.90	Depositor
% Data completeness (in resolution range)	93.6 (8.00-1.90)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.211 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9712	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PA5

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	0.44	0/4504	0.68	3/6101 (0.0%)
1	B	0.38	0/4504	0.62	3/6101 (0.0%)
All	All	0.41	0/9008	0.65	6/12202 (0.0%)

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	B	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	5	ARG	NE-CZ-NH2	6.63	123.61	120.30
1	B	262	MET	CG-SD-CE	6.12	110.00	100.20
1	A	459	MET	CG-SD-CE	6.08	109.93	100.20
1	B	400	MET	CG-SD-CE	5.60	109.16	100.20
1	A	1	ALA	N-CA-CB	-5.42	102.51	110.10
1	B	383	GLY	CA-C-O	-5.05	111.51	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	383	GLY	Mainchain

## 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	4395	0	4352	154	0
1	B	4395	0	4352	106	0
2	A	15	0	8	1	0
2	B	15	0	8	0	0
3	A	427	0	0	24	0
3	B	465	0	0	18	1
All	All	9712	0	8720	254	1

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 14.

All (254) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:LYS:CG	3:B:965:HOH:O	1.84	1.25
1:A:461:LEU:HD13	1:A:461:LEU:O	1.43	1.18
1:B:222:LYS:HE3	1:B:255:PHE:CE1	1.79	1.17
1:B:522:LYS:HG2	3:B:965:HOH:O	1.42	1.17
1:B:222:LYS:HE3	1:B:255:PHE:CD1	1.80	1.14
1:A:33:LYS:H	1:A:33:LYS:HE2	0.98	1.14
1:A:112:VAL:O	1:A:113:ASP:HB2	1.40	1.12
1:B:34:GLU:HB2	3:B:991:HOH:O	1.54	1.07
1:A:253:LYS:O	1:A:253:LYS:HD3	1.56	1.05
1:A:461:LEU:C	1:A:461:LEU:HD13	1.77	1.04
1:B:18:GLU:HG3	1:B:19:HIS:CE1	1.91	1.03
1:A:146:LYS:HE2	1:A:146:LYS:H	1.24	1.03
1:A:1:ALA:HB3	3:A:858:HOH:O	1.57	1.01
1:A:453:LYS:HD2	1:A:457:ASP:CB	1.94	0.98
1:A:2:ALA:N	3:A:806:HOH:O	1.95	0.97
1:A:33:LYS:HE2	1:A:33:LYS:N	1.82	0.95
1:A:33:LYS:CE	1:A:33:LYS:H	1.80	0.94
1:B:222:LYS:CE	1:B:255:PHE:CD1	2.51	0.93
1:A:453:LYS:O	1:A:454:SER:HB3	1.67	0.93
1:B:519:GLN:OE1	1:B:522:LYS:HE3	1.69	0.92
1:A:146:LYS:CE	1:A:146:LYS:H	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LYS:HG3	3:A:962:HOH:O	1.71	0.90
1:B:193:LYS:HE2	1:B:193:LYS:HA	1.54	0.90
1:B:552:ARG:O	3:B:1007:HOH:O	1.90	0.89
1:A:123:LYS:O	1:A:123:LYS:HE3	1.71	0.89
1:A:461:LEU:C	1:A:461:LEU:CD1	2.43	0.87
1:A:74:ARG:NH2	1:A:503:VAL:O	2.08	0.87
1:A:233:LYS:O	1:A:234:ASP:HB3	1.71	0.87
1:B:222:LYS:CE	1:B:255:PHE:CE1	2.58	0.86
1:A:461:LEU:HD11	1:A:465:LYS:CD	2.06	0.85
1:A:313:LYS:HG3	3:A:965:HOH:O	1.74	0.85
1:A:453:LYS:HD2	1:A:457:ASP:HB2	1.58	0.85
1:A:422:LYS:HE3	1:B:525:GLU:HG2	1.59	0.84
1:A:525:GLU:HG2	1:B:422:LYS:HE2	1.60	0.83
1:A:550:GLN:HE21	1:A:551:GLN:HE21	1.27	0.82
1:A:453:LYS:HD2	1:A:457:ASP:HB3	1.63	0.80
1:B:222:LYS:HE3	1:B:255:PHE:HD1	1.47	0.79
1:B:115:LYS:HA	1:B:115:LYS:HE3	1.63	0.79
1:A:253:LYS:HD3	1:A:253:LYS:C	2.01	0.78
1:B:305:HIS:HE1	1:B:315:ALA:H	1.28	0.78
1:A:194:THR:O	1:A:198:LEU:HD23	1.83	0.78
1:B:442:GLU:HG2	3:B:988:HOH:O	1.83	0.77
1:A:235:PRO:O	3:A:955:HOH:O	2.02	0.76
1:B:522:LYS:HG3	3:B:965:HOH:O	1.57	0.76
1:B:462:LEU:HB3	1:B:463:PRO:HD3	1.67	0.76
1:B:272:ARG:HH12	1:B:511:GLN:HE21	1.34	0.75
1:A:523:LYS:CE	3:A:749:HOH:O	2.35	0.75
1:A:200:PRO:HG3	1:A:227:TRP:CH2	2.22	0.74
1:A:74:ARG:HH22	1:A:505:ASP:HB2	1.52	0.73
1:A:461:LEU:HD11	1:A:465:LYS:CG	2.19	0.72
1:B:258:ASP:HB2	1:B:260:GLN:HE22	1.53	0.72
1:B:258:ASP:CB	1:B:260:GLN:HE22	2.03	0.72
1:B:222:LYS:HE3	1:B:255:PHE:HE1	1.45	0.71
1:A:461:LEU:HD11	1:A:465:LYS:HG3	1.73	0.71
1:A:537:HIS:H	1:A:542:ASN:HD21	1.36	0.70
1:B:10:GLN:NE2	1:B:10:GLN:HA	2.06	0.70
1:A:313:LYS:HG2	3:A:661:HOH:O	1.92	0.70
1:A:465:LYS:HE2	3:A:984:HOH:O	1.92	0.70
1:A:461:LEU:HD11	1:A:465:LYS:HD3	1.74	0.70
1:A:233:LYS:HE3	1:A:233:LYS:HA	1.73	0.69
1:B:32:ASP:OD2	3:B:991:HOH:O	2.08	0.69
1:A:14:GLN:OE1	1:A:17:ARG:HD2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:VAL:O	1:A:113:ASP:CB	2.25	0.68
1:B:120:GLU:OE2	3:B:840:HOH:O	2.11	0.68
1:A:233:LYS:O	1:A:234:ASP:CB	2.40	0.67
1:A:25:LEU:HD13	1:A:436:MET:HG3	1.76	0.67
1:B:519:GLN:O	1:B:522:LYS:HG3	1.94	0.66
1:A:146:LYS:CD	1:A:201:GLU:HB3	2.26	0.66
1:A:45:THR:O	1:A:46:ASN:HB2	1.95	0.66
1:B:445:ARG:O	1:B:449:GLN:HG3	1.94	0.66
1:B:114:GLY:O	1:B:115:LYS:HD2	1.95	0.66
1:B:10:GLN:HE21	1:B:10:GLN:HA	1.58	0.66
1:B:519:GLN:OE1	1:B:522:LYS:CE	2.43	0.65
1:B:6:ASN:HD22	1:B:9:PHE:H	1.41	0.65
1:A:523:LYS:HE3	3:A:749:HOH:O	1.96	0.65
1:A:14:GLN:O	1:A:17:ARG:HG2	1.98	0.64
1:B:45:THR:O	1:B:46:ASN:HB2	1.98	0.64
1:A:387:GLN:HE22	1:A:427:ASN:HB3	1.62	0.64
1:A:440:SER:OG	1:A:443:GLU:HG3	1.97	0.64
1:B:10:GLN:NE2	3:B:884:HOH:O	2.31	0.64
1:A:144:THR:OG1	1:A:146:LYS:HD3	1.98	0.63
1:A:144:THR:H	1:A:146:LYS:NZ	1.96	0.63
1:A:457:ASP:O	1:A:460:LYS:HG3	1.99	0.62
1:B:537:HIS:H	1:B:542:ASN:HD21	1.45	0.62
1:B:197:CYS:SG	3:B:930:HOH:O	2.56	0.62
1:B:6:ASN:HD21	1:B:8:GLN:HB2	1.65	0.62
1:A:4:THR:HG22	3:A:847:HOH:O	1.99	0.61
1:B:18:GLU:HG3	1:B:19:HIS:ND1	2.16	0.60
1:A:339:PRO:O	1:A:382:PRO:HA	2.02	0.60
1:A:345:HIS:HA	1:A:382:PRO:HG3	1.82	0.60
1:A:144:THR:H	1:A:146:LYS:HZ1	1.49	0.60
1:A:453:LYS:O	1:A:454:SER:CB	2.46	0.60
1:A:228:PHE:C	1:A:230:LEU:H	2.04	0.60
1:B:304:GLN:NE2	3:B:1023:HOH:O	2.35	0.60
1:B:4:THR:HG21	1:B:371:ASP:OD2	2.02	0.59
1:A:461:LEU:CD1	1:A:465:LYS:HG3	2.33	0.59
1:A:112:VAL:O	1:A:112:VAL:HG12	2.03	0.59
1:A:524:ILE:HG13	3:A:808:HOH:O	2.03	0.58
1:A:200:PRO:HG3	1:A:227:TRP:CZ2	2.37	0.58
1:B:14:GLN:O	1:B:18:GLU:HG2	2.02	0.58
1:B:460:LYS:HG3	3:B:903:HOH:O	2.02	0.58
1:A:232:ALA:O	1:A:233:LYS:HB2	2.03	0.58
1:A:44:ASN:ND2	1:A:46:ASN:H	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:THR:O	1:A:193:LYS:HG2	2.04	0.58
1:B:222:LYS:CE	1:B:255:PHE:HD1	2.05	0.57
1:B:5:ARG:HD2	1:B:5:ARG:O	2.04	0.57
1:B:44:ASN:ND2	1:B:46:ASN:H	2.02	0.57
1:A:422:LYS:CE	1:B:525:GLU:HG2	2.34	0.57
1:A:458:LEU:O	1:A:458:LEU:HD23	2.04	0.57
1:A:164:LEU:HD13	1:A:164:LEU:C	2.26	0.56
1:B:305:HIS:CE1	1:B:315:ALA:H	2.17	0.56
1:B:13:GLN:HG2	1:B:17:ARG:CZ	2.35	0.56
1:B:407:ILE:HD13	1:B:425:LEU:HD23	1.87	0.56
1:B:186:ILE:HB	1:B:216:GLU:HG3	1.87	0.56
1:A:362:TYR:HD1	1:A:369:ARG:CD	2.19	0.56
1:A:420:HIS:HE1	1:B:223:THR:OG1	1.88	0.55
1:B:74:ARG:NH2	1:B:505:ASP:HB2	2.21	0.55
1:B:90:ASN:ND2	1:B:507:ASN:HD21	2.04	0.55
1:A:90:ASN:ND2	1:A:507:ASN:HD21	2.04	0.55
1:B:449:GLN:HG2	1:B:458:LEU:HD11	1.90	0.54
1:B:272:ARG:HH12	1:B:511:GLN:NE2	2.03	0.54
1:A:416:ARG:NH1	1:A:419:LEU:HD23	2.22	0.54
1:B:325:TRP:O	1:B:329:CYS:HB2	2.07	0.54
1:A:198:LEU:HD12	1:A:203:SER:OG	2.08	0.54
1:A:171:LYS:N	1:A:172:PRO:HD2	2.22	0.54
1:A:146:LYS:HD2	1:A:201:GLU:HB3	1.89	0.53
1:A:189:THR:O	1:A:193:LYS:CG	2.56	0.53
1:A:258:ASP:N	1:A:258:ASP:OD2	2.41	0.53
1:B:387:GLN:HE22	1:B:427:ASN:HB3	1.74	0.53
1:A:228:PHE:C	1:A:230:LEU:N	2.61	0.52
1:A:186:ILE:HB	1:A:216:GLU:HG3	1.92	0.52
1:B:10:GLN:HE21	1:B:10:GLN:CA	2.18	0.52
1:A:146:LYS:CE	1:A:146:LYS:N	2.65	0.52
1:B:193:LYS:HE2	1:B:193:LYS:CA	2.36	0.52
1:B:445:ARG:HH11	1:B:445:ARG:HG2	1.74	0.52
1:A:4:THR:CG2	3:A:847:HOH:O	2.57	0.52
1:A:216:GLU:OE1	1:B:388:HIS:HE1	1.92	0.52
1:A:74:ARG:CZ	1:A:503:VAL:O	2.58	0.52
1:B:175:SER:HB3	3:B:694:HOH:O	2.10	0.52
1:A:152:ILE:N	1:A:152:ILE:HD12	2.25	0.52
1:B:258:ASP:HB2	1:B:260:GLN:NE2	2.24	0.51
1:A:417:LYS:HE2	1:A:417:LYS:N	2.26	0.51
1:B:18:GLU:CG	1:B:19:HIS:CE1	2.82	0.51
1:B:456:GLU:H	1:B:456:GLU:CD	2.15	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLY:C	1:B:115:LYS:HD2	2.31	0.50
1:A:117:VAL:O	1:A:120:GLU:HG2	2.11	0.50
1:A:233:LYS:CA	1:A:233:LYS:HE3	2.42	0.50
1:B:193:LYS:CE	1:B:193:LYS:HA	2.36	0.50
1:B:58:LEU:HD12	1:B:400:MET:HE3	1.94	0.50
1:A:462:LEU:HB3	1:A:463:PRO:CD	2.42	0.50
1:A:226:ASP:O	1:A:230:LEU:HB2	2.12	0.50
1:A:416:ARG:HD2	3:A:945:HOH:O	2.11	0.49
1:A:98:LEU:HB2	1:A:268:TRP:CE3	2.47	0.49
1:A:197:CYS:C	1:A:198:LEU:HD22	2.32	0.49
1:A:90:ASN:HD22	1:A:90:ASN:C	2.14	0.49
1:A:345:HIS:HD2	3:A:712:HOH:O	1.95	0.49
1:B:98:LEU:HB2	1:B:268:TRP:CE3	2.48	0.49
1:B:152:ILE:N	1:B:152:ILE:HD12	2.28	0.49
1:A:164:LEU:HD11	1:A:346:ARG:HG3	1.94	0.48
1:A:369:ARG:NH1	3:A:861:HOH:O	2.44	0.48
1:A:250:ALA:O	1:A:254:GLU:HB2	2.13	0.48
1:A:422:LYS:CE	3:A:836:HOH:O	2.60	0.48
1:B:27:HIS:CE1	3:B:960:HOH:O	2.65	0.48
1:B:369:ARG:HH11	1:B:369:ARG:HG2	1.77	0.48
1:B:449:GLN:HG2	1:B:458:LEU:CD1	2.44	0.48
1:A:168:GLU:OE2	1:A:345:HIS:HE1	1.95	0.48
1:A:417:LYS:CE	1:A:417:LYS:N	2.76	0.48
1:A:465:LYS:CE	3:A:984:HOH:O	2.55	0.48
2:A:558:PA5:O4	1:B:388:HIS:HD2	1.96	0.48
1:A:369:ARG:HH11	1:A:369:ARG:HG2	1.77	0.48
1:B:90:ASN:HD22	1:B:90:ASN:C	2.16	0.47
1:A:141:LYS:O	1:A:141:LYS:HD2	2.14	0.47
1:A:141:LYS:NZ	1:A:240:LYS:HE2	2.30	0.47
1:A:325:TRP:O	1:A:329:CYS:HB2	2.13	0.47
1:A:5:ARG:HG3	3:A:956:HOH:O	2.15	0.47
1:A:3:LEU:HD13	1:A:74:ARG:HE	1.80	0.47
1:A:146:LYS:HD3	1:A:201:GLU:HB3	1.95	0.47
1:A:417:LYS:NZ	1:A:417:LYS:H	2.12	0.47
1:B:405:PHE:HB3	1:B:428:PHE:CE1	2.50	0.47
1:B:462:LEU:HB3	1:B:463:PRO:CD	2.41	0.47
1:A:308:THR:HA	3:A:714:HOH:O	2.15	0.46
1:A:58:LEU:HD12	1:A:400:MET:CE	2.44	0.46
1:A:204:LEU:HD13	1:A:205:PHE:N	2.30	0.46
1:A:550:GLN:NE2	1:A:551:GLN:HE21	2.05	0.46
1:A:175:SER:C	1:A:177:GLY:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:GLN:OE1	1:B:522:LYS:HD2	2.16	0.46
1:A:2:ALA:HB3	3:A:806:HOH:O	2.15	0.46
1:A:141:LYS:HD3	3:A:888:HOH:O	2.16	0.46
1:A:150:ASP:CB	1:A:198:LEU:HD11	2.46	0.46
1:B:48:GLY:N	3:B:894:HOH:O	2.39	0.46
1:B:222:LYS:HA	1:B:222:LYS:HD3	1.72	0.45
1:A:227:TRP:O	1:A:230:LEU:HB3	2.16	0.45
1:A:199:ASN:OD1	1:A:201:GLU:HB2	2.17	0.45
1:A:245:LEU:HA	1:A:263:PHE:O	2.16	0.45
1:A:369:ARG:HH11	1:A:369:ARG:CG	2.30	0.45
1:A:453:LYS:HE2	1:A:460:LYS:HZ1	1.81	0.45
1:A:136:ARG:NH2	1:A:175:SER:OG	2.50	0.45
1:A:164:LEU:CD1	1:A:346:ARG:HG3	2.47	0.45
1:B:17:ARG:NH2	3:B:884:HOH:O	2.49	0.45
1:A:171:LYS:N	1:A:172:PRO:CD	2.80	0.45
1:A:417:LYS:CE	1:A:417:LYS:H	2.30	0.45
1:B:511:GLN:O	1:B:511:GLN:HG2	2.16	0.44
1:A:29:PHE:CE1	1:A:436:MET:SD	3.10	0.44
1:A:407:ILE:HD13	1:A:425:LEU:HD23	1.99	0.44
1:B:222:LYS:HE2	1:B:255:PHE:CD1	2.44	0.44
1:B:80:ARG:HG3	1:B:306:PHE:CE2	2.52	0.44
1:A:2:ALA:CA	3:A:806:HOH:O	2.56	0.43
1:A:180:VAL:HG21	1:A:286:HIS:HB2	1.98	0.43
1:B:522:LYS:HE2	3:B:944:HOH:O	2.18	0.43
1:A:420:HIS:HD2	1:B:186:ILE:O	2.01	0.43
1:B:253:LYS:HD3	1:B:253:LYS:O	2.19	0.43
1:A:523:LYS:HB3	1:A:523:LYS:HE3	1.69	0.43
1:B:305:HIS:HE1	1:B:315:ALA:N	2.06	0.43
1:B:387:GLN:HA	1:B:391:TYR:CG	2.53	0.43
1:B:25:LEU:HB3	1:B:436:MET:HG2	2.01	0.43
1:B:339:PRO:O	1:B:382:PRO:HA	2.18	0.43
1:A:141:LYS:H	1:A:141:LYS:HD2	1.84	0.42
1:B:289:PHE:O	1:B:293:GLU:HG3	2.19	0.42
1:A:490:ILE:O	1:A:494:GLU:HG3	2.19	0.42
1:A:511:GLN:HG2	1:A:511:GLN:O	2.19	0.42
1:B:460:LYS:HG3	1:B:460:LYS:O	2.20	0.42
1:A:164:LEU:HD23	1:A:182:PHE:CD1	2.54	0.42
1:A:254:GLU:HA	3:A:785:HOH:O	2.19	0.42
1:A:448:LEU:HD11	1:A:461:LEU:HD12	2.02	0.42
1:B:458:LEU:C	1:B:458:LEU:HD23	2.40	0.42
1:B:44:ASN:HD22	1:B:44:ASN:C	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:HD21	1:A:313:LYS:CG	2.50	0.42
1:A:458:LEU:HD23	1:A:458:LEU:C	2.40	0.42
1:A:416:ARG:HG2	1:A:419:LEU:HD23	2.01	0.41
1:A:387:GLN:HA	1:A:391:TYR:CG	2.55	0.41
1:A:209:SER:OG	1:A:212:PHE:HA	2.20	0.41
1:B:17:ARG:HB2	1:B:17:ARG:HE	1.72	0.41
1:B:6:ASN:HA	1:B:7:PRO:HD3	1.88	0.41
1:B:5:ARG:HG2	1:B:5:ARG:HH11	1.86	0.41
1:B:136:ARG:HD3	1:B:285:LEU:O	2.20	0.41
1:A:352:GLN:HA	1:A:378:VAL:HB	2.01	0.41
1:A:315:ALA:HB3	1:A:316:PRO:CD	2.50	0.41
1:A:71:ALA:O	1:A:76:VAL:HG23	2.21	0.41
1:A:405:PHE:HB3	1:A:428:PHE:CE1	2.55	0.41
1:B:115:LYS:HA	1:B:115:LYS:CE	2.42	0.41
1:A:169:ALA:HA	1:A:343:TYR:HB3	2.02	0.41
1:B:275:LEU:HD12	1:B:275:LEU:C	2.41	0.41
1:B:144:THR:HG21	1:B:201:GLU:OE2	2.20	0.41
1:B:519:GLN:OE1	1:B:522:LYS:CD	2.69	0.41
1:A:313:LYS:NZ	3:A:965:HOH:O	2.51	0.41
1:B:186:ILE:HB	1:B:216:GLU:CG	2.51	0.41
1:A:245:LEU:HD13	1:A:279:ILE:HA	2.02	0.41
1:A:33:LYS:CE	1:A:33:LYS:N	2.61	0.40
1:B:258:ASP:HB3	1:B:260:GLN:HE22	1.82	0.40
1:A:63:VAL:HA	1:A:66:MET:HE2	2.03	0.40
1:B:261:ASN:ND2	3:B:778:HOH:O	2.53	0.40
1:A:33:LYS:CD	1:A:33:LYS:H	2.34	0.40
1:A:265:PHE:CD2	1:A:265:PHE:N	2.90	0.40
1:A:33:LYS:CD	1:A:33:LYS:N	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:639:HOH:O	3:B:894:HOH:O[3_555]	1.19	1.01

## 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	553/558 (99%)	522 (94%)	26 (5%)	5 (1%)	21	9
1	B	553/558 (99%)	538 (97%)	15 (3%)	0	100	100
All	All	1106/1116 (99%)	1060 (96%)	41 (4%)	5 (0%)	34	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	453	LYS
1	A	454	SER
1	A	113	ASP
1	A	234	ASP
1	A	233	LYS

### 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	475/479 (99%)	446 (94%)	29 (6%)	23	11
1	B	475/479 (99%)	459 (97%)	16 (3%)	44	33
All	All	950/958 (99%)	905 (95%)	45 (5%)	32	20

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS

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Mol	Chain	Res	Type
1	A	37	ASN
1	A	41	LEU
1	A	44	ASN
1	A	90	ASN
1	A	103	ARG
1	A	123	LYS
1	A	141	LYS
1	A	146	LYS
1	A	193	LYS
1	A	204	LEU
1	A	212	PHE
1	A	222	LYS
1	A	226	ASP
1	A	230	LEU
1	A	233	LYS
1	A	253	LYS
1	A	260	GLN
1	A	265	PHE
1	A	369	ARG
1	A	417	LYS
1	A	436	MET
1	A	456	GLU
1	A	459	MET
1	A	460	LYS
1	A	461	LEU
1	A	519	GLN
1	A	523	LYS
1	A	524	ILE
1	B	5	ARG
1	B	17	ARG
1	B	19	HIS
1	B	44	ASN
1	B	90	ASN
1	B	103	ARG
1	B	175	SER
1	B	212	PHE
1	B	258	ASP
1	B	457	ASP
1	B	459	MET
1	B	460	LYS
1	B	478	PHE
1	B	511	GLN

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Mol	Chain	Res	Type
1	B	522	LYS
1	B	532	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	44	ASN
1	A	46	ASN
1	A	90	ASN
1	A	153	ASN
1	A	215	GLN
1	A	261	ASN
1	A	345	HIS
1	A	353	GLN
1	A	373	GLN
1	A	387	GLN
1	A	420	HIS
1	A	542	ASN
1	A	550	GLN
1	B	6	ASN
1	B	10	GLN
1	B	16	HIS
1	B	44	ASN
1	B	46	ASN
1	B	90	ASN
1	B	133	GLN
1	B	153	ASN
1	B	215	GLN
1	B	261	ASN
1	B	286	HIS
1	B	291	ASN
1	B	305	HIS
1	B	353	GLN
1	B	359	ASN
1	B	385	ASN
1	B	387	GLN
1	B	388	HIS
1	B	410	GLN
1	B	511	GLN
1	B	542	ASN
1	B	550	GLN

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Mol	Chain	Res	Type
1	B	551	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](#)

2 ligands are modelled in this entry.

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	PA5	A	558	-	10,14,14	1.28	1 (10%)	10,20,20	1.48	1 (10%)
2	PA5	B	558	-	10,14,14	1.26	1 (10%)	10,20,20	1.44	1 (10%)

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	PA5	A	558	-	-	0/14/18/18	0/0/0/0
2	PA5	B	558	-	-	0/14/18/18	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	558	PA5	C5-C4	2.68	1.55	1.51
2	B	558	PA5	C5-C4	2.71	1.55	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	558	PA5	O2-C2-C1	3.01	118.81	111.21
2	A	558	PA5	O2-C2-C1	3.03	118.86	111.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	558	PA5	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.