



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:58 PM GMT

PDB ID : 4GTY
Title : Crystal structure of mouse Enpp1 in complex with GMP
Authors : Kato, K.; Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on : 2012-08-29
Resolution : 3.19 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

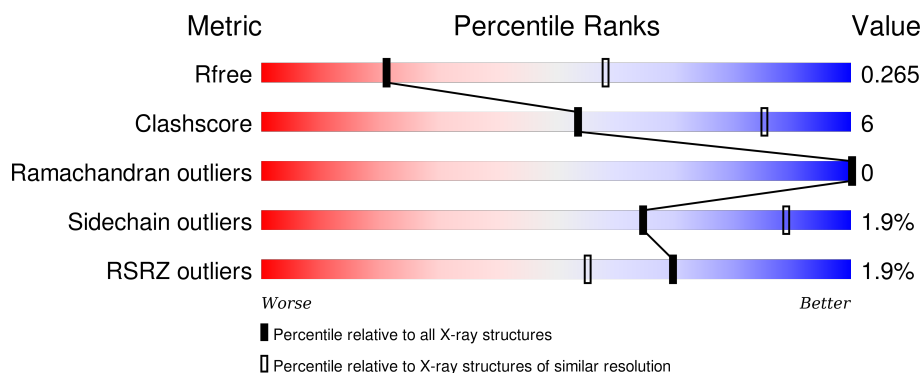
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 ≥ 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	823	<div> <div> <div></div> <div>71%</div> <div>14%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	823	<div> <div> <div>2%</div> <div>70%</div> <div>14%</div> <div>15%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11181 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 2, Alkaline phosphodiesterase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	706	Total	C	N	O	S	0	0	0
			5506	3546	909	1022	29			
1	B	697	Total	C	N	O	S	0	0	0
			5465	3517	897	1022	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	ARG	LYS	ENGINEERED MUTATION	UNP Q9R1E6
B	59	ARG	LYS	ENGINEERED MUTATION	UNP Q9R1E6

- Molecule 2 is a polymer of unknown type called SUGAR (6-MER).

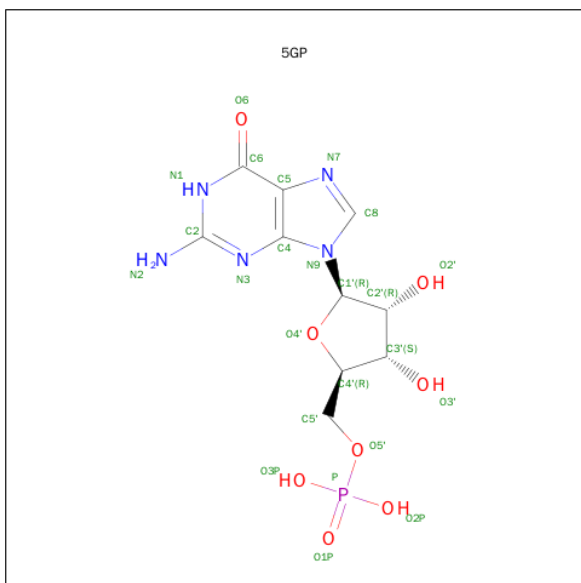
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
4	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Zn	0	0
			2	2		
5	A	2	Total	Zn	0	0
			2	2		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	A	1	Total	Ca	0	0
			1	1		

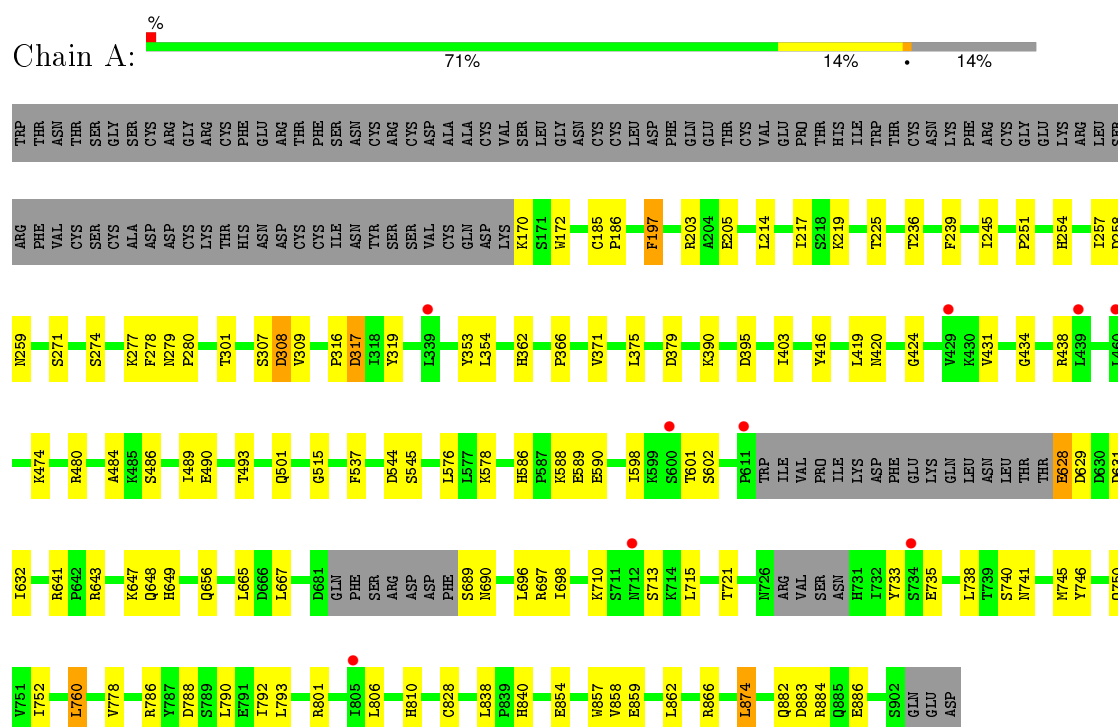
- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	2	Total	C	N	O	0	0
			28	16	2	10		

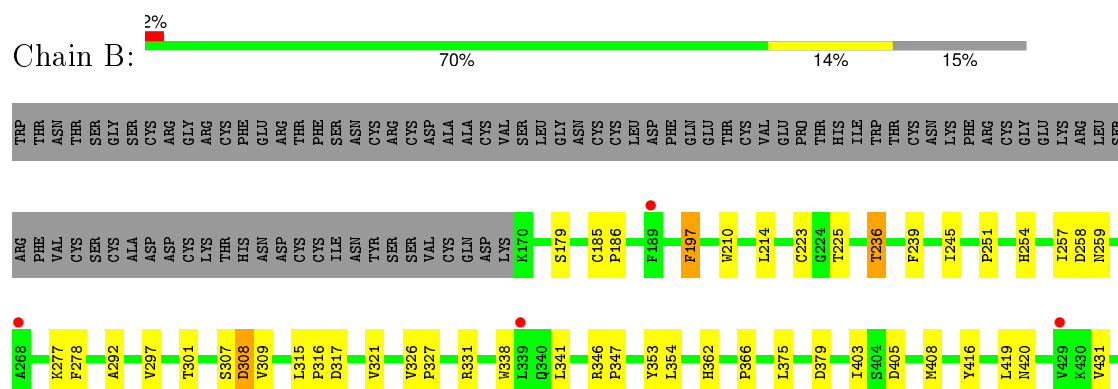
3 Residue-property plots

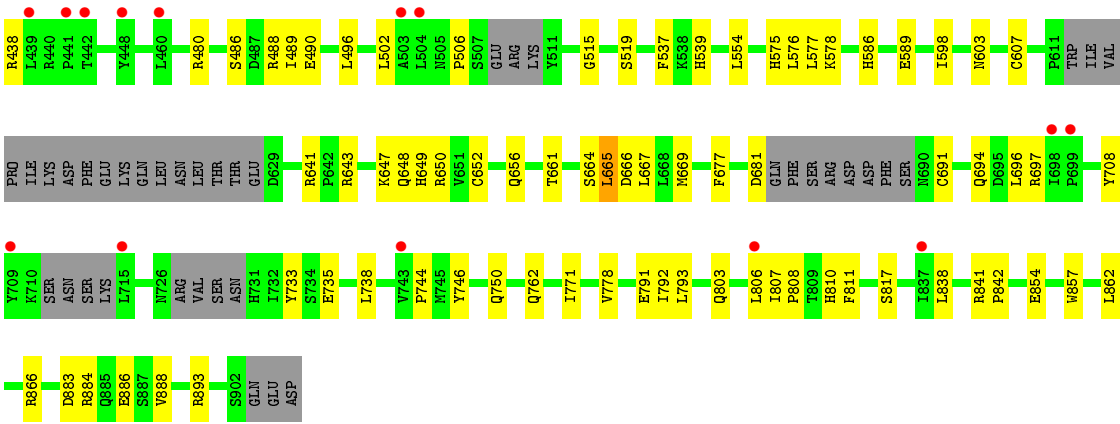
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2, Alkaline phosphodiesterase I



- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2, Alkaline phosphodiesterase I





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	104.86Å 104.86Å 174.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.05 – 3.19 49.05 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.05-3.19) 99.0 (49.05-3.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.258 , 0.281 0.242 , 0.265	Depositor DCC
R_{free} test set	1759 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	63.9	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.2	EDS
Estimated twinning fraction	0.095 for -h,-k,l 0.108 for h,-h-k,-l 0.089 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 35418 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11181	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CA, 5GP, MAN

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	0.23	0/5670	0.44	0/7749
1	B	0.23	0/5626	0.44	0/7685
All	All	0.23	0/11296	0.44	0/15434

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	5506	0	5164	71	0
1	B	5465	0	5121	70	0
2	A	72	0	61	0	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
4	A	24	0	12	3	0
4	B	24	0	12	4	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	28	0	25	0	0
All	All	11181	0	10447	140	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 6.

All (140) 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:649:HIS:HE2	1:B:664:SER:HG	1.07	0.95
1:B:301:THR:HG21	1:B:307:SER:HB2	1.70	0.72
1:A:715:LEU:O	1:A:801:ARG:NH2	2.23	0.70
1:B:603:ASN:H	1:B:694:GLN:HE22	1.40	0.69
1:B:259:ASN:ND2	4:B:1005:5GP:O3P	2.25	0.69
1:A:721:THR:HB	1:A:741:ASN:HD21	1.57	0.69
1:A:316:PRO:HG2	1:A:319:TYR:HB3	1.75	0.67
1:A:438:ARG:HG2	1:A:493:THR:HG22	1.77	0.66
1:A:760:LEU:HD21	1:A:859:GLU:HG2	1.75	0.66
1:A:589:GLU:OE2	1:A:641:ARG:NH2	2.29	0.66
1:B:650:ARG:NH1	1:B:666:ASP:OD1	2.29	0.65
1:A:828:CYS:O	1:A:884:ARG:NH2	2.26	0.62
1:A:643:ARG:NH2	1:A:883:ASP:OD2	2.32	0.62
1:B:537:PHE:O	1:B:578:LYS:NZ	2.27	0.61
1:B:744:PRO:HG2	1:B:808:PRO:HD3	1.82	0.61
1:B:225:THR:HG21	1:B:576:LEU:HG	1.82	0.61
1:A:308:ASP:OD2	1:A:308:ASP:N	2.33	0.61
1:A:733:TYR:CZ	1:A:735:GLU:HB2	2.36	0.60
1:B:733:TYR:CZ	1:B:735:GLU:HB2	2.37	0.60
1:A:793:LEU:HD22	1:A:806:LEU:HD21	1.84	0.59
1:A:486:SER:HB3	1:A:489:ILE:HG13	1.83	0.59
1:A:225:THR:HG21	1:A:576:LEU:HG	1.84	0.58
1:A:778:VAL:HB	1:A:810:HIS:HB2	1.84	0.58
1:A:735:GLU:HA	1:A:738:LEU:HD13	1.85	0.58
1:A:788:ASP:HB3	1:A:792:ILE:HG23	1.86	0.57
1:B:338:TRP:HA	1:B:341:LEU:HD13	1.86	0.57
1:B:315:LEU:HD12	1:B:316:PRO:HD2	1.86	0.57
1:B:292:ALA:HB1	1:B:297:VAL:HB	1.87	0.57
1:A:434:GLY:HA2	1:A:501:GLN:HE21	1.69	0.57
1:B:656:GLN:OE1	1:B:697:ARG:NH2	2.37	0.56
1:B:838:LEU:HD11	1:B:862:LEU:HD13	1.87	0.56
1:B:420:ASN:HD21	1:B:506:PRO:HD3	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:PHE:HE1	1:A:354:LEU:HD13	1.70	0.55
1:A:641:ARG:NH1	1:B:179:SER:OG	2.40	0.55
1:A:278:PHE:HA	1:A:309:VAL:HG22	1.89	0.55
1:B:554:LEU:HD11	1:B:577:LEU:HD21	1.88	0.55
1:A:172:TRP:O	1:A:219:LYS:NZ	2.36	0.55
1:B:277:LYS:HZ1	4:B:1005:5GP:HN1	1.54	0.55
1:A:733:TYR:OH	1:A:735:GLU:OE1	2.22	0.55
1:B:214:LEU:HD22	1:B:379:ASP:HB2	1.89	0.54
1:A:301:THR:HG21	1:A:307:SER:HB3	1.89	0.54
1:A:438:ARG:HB3	1:A:490:GLU:HB2	1.91	0.53
1:A:710:LYS:H	1:A:801:ARG:NH1	2.06	0.53
1:B:496:LEU:HD21	1:B:502:LEU:HB2	1.91	0.53
1:B:486:SER:HB3	1:B:489:ILE:HG13	1.91	0.52
1:A:537:PHE:O	1:A:578:LYS:NZ	2.41	0.51
1:B:667:LEU:HB3	1:B:669:MET:HG2	1.90	0.51
1:B:793:LEU:HD22	1:B:806:LEU:HD21	1.92	0.51
1:B:278:PHE:HA	1:B:309:VAL:HG22	1.93	0.51
1:A:203:ARG:NH2	1:A:205:GLU:OE1	2.44	0.51
1:B:598:ILE:HG23	1:B:696:LEU:HB3	1.91	0.51
1:B:362:HIS:ND1	1:B:515:GLY:O	2.41	0.51
1:A:752:ILE:HG23	1:A:858:VAL:HG13	1.94	0.50
1:A:598:ILE:HG23	1:A:696:LEU:HB3	1.92	0.50
1:B:405:ASP:N	1:B:405:ASP:OD1	2.37	0.49
1:B:778:VAL:HB	1:B:810:HIS:HB2	1.94	0.49
1:A:419:LEU:HD12	1:A:431:VAL:HG21	1.93	0.49
1:A:698:ILE:HD13	1:A:740:SER:HB3	1.94	0.49
1:B:197:PHE:HE1	1:B:354:LEU:HD13	1.76	0.48
1:A:746:TYR:O	1:A:750:GLN:HG3	2.14	0.48
1:B:480:ARG:HD3	1:B:866:ARG:O	2.13	0.48
1:A:838:LEU:HD21	1:A:862:LEU:HD13	1.96	0.48
1:A:544:ASP:OD1	1:A:545:SER:N	2.42	0.48
1:A:259:ASN:ND2	4:A:1009:5GP:O3P	2.40	0.48
1:B:366:PRO:HG3	1:B:408:MET:HG3	1.95	0.48
1:B:647:LYS:HA	1:B:648:GLN:HA	1.52	0.47
1:A:689:SER:O	1:A:690:ASN:HB3	2.14	0.47
1:B:258:ASP:OD1	1:B:259:ASN:N	2.47	0.47
1:B:643:ARG:NH2	1:B:883:ASP:OD2	2.48	0.47
1:B:331:ARG:NH1	1:B:353:TYR:O	2.46	0.46
1:A:245:ILE:HD13	1:A:403:ILE:HD13	1.97	0.46
1:B:884:ARG:HG3	1:B:886:GLU:OE1	2.16	0.45
1:A:170:LYS:O	1:A:390:LYS:NZ	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:GLU:HA	1:A:857:TRP:NE1	2.31	0.45
1:A:480:ARG:HD3	1:A:866:ARG:O	2.16	0.45
1:B:735:GLU:HA	1:B:738:LEU:HD13	1.98	0.45
1:B:245:ILE:HD13	1:B:403:ILE:HD13	1.99	0.45
1:B:277:LYS:NZ	4:B:1005:5GP:HN1	2.13	0.45
1:B:223:CYS:O	1:B:539:HIS:ND1	2.48	0.45
1:A:628:GLU:N	1:A:631:ASP:OD1	2.50	0.45
1:A:214:LEU:HD21	1:A:375:LEU:HB3	1.99	0.45
1:A:713:SER:HB3	1:A:801:ARG:NH1	2.32	0.45
1:B:771:ILE:HG22	1:B:817:SER:OG	2.17	0.45
1:B:681:ASP:N	1:B:681:ASP:OD1	2.50	0.44
1:A:474:LYS:HG2	1:A:484:ALA:HA	2.00	0.44
1:B:589:GLU:OE2	1:B:641:ARG:NH2	2.50	0.44
1:A:656:GLN:OE1	1:A:697:ARG:NH2	2.41	0.44
1:A:745:MET:HE2	1:A:750:GLN:HG2	2.00	0.44
1:A:586:HIS:ND1	1:A:882:GLN:HG2	2.32	0.44
1:B:236:THR:OG1	1:B:519:SER:O	2.35	0.44
1:B:438:ARG:HB3	1:B:490:GLU:HB2	1.99	0.44
1:A:884:ARG:HA	1:A:884:ARG:HD2	1.79	0.44
1:A:366:PRO:O	1:A:371:VAL:HG21	2.17	0.44
1:A:395:ASP:N	1:A:395:ASP:OD1	2.51	0.44
1:A:279:ASN:HA	1:A:280:PRO:HD3	1.83	0.44
1:A:647:LYS:HA	1:A:648:GLN:HA	1.49	0.43
1:A:258:ASP:OD1	1:A:259:ASN:N	2.51	0.43
1:A:317:ASP:N	1:A:317:ASP:OD2	2.52	0.43
1:B:677:PHE:HE2	1:B:762:GLN:HA	1.84	0.43
1:B:419:LEU:HD12	1:B:431:VAL:HG21	2.01	0.43
1:A:745:MET:HA	1:A:840:HIS:CE1	2.53	0.43
1:B:346:ARG:HA	1:B:347:PRO:HD3	1.89	0.42
1:B:652:CYS:SG	1:B:665:LEU:HD21	2.59	0.42
1:B:746:TYR:O	1:B:750:GLN:HG3	2.18	0.42
1:B:586:HIS:CD2	1:B:888:VAL:HG22	2.53	0.42
1:B:808:PRO:HG2	1:B:811:PHE:CZ	2.54	0.42
1:A:251:PRO:HA	1:A:254:HIS:NE2	2.35	0.42
1:B:807:ILE:HA	1:B:808:PRO:HD3	1.86	0.42
1:A:217:ILE:HG12	1:A:379:ASP:OD1	2.18	0.42
1:B:649:HIS:CD2	1:B:664:SER:HG	2.34	0.42
1:B:884:ARG:HA	1:B:884:ARG:HD2	1.81	0.42
1:A:643:ARG:HD3	1:A:643:ARG:HA	1.95	0.41
1:B:841:ARG:HA	1:B:842:PRO:HD3	1.87	0.41
1:A:271:SER:HB2	1:A:274:SER:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:HIS:HE1	1:A:667:LEU:HD13	1.85	0.41
1:B:353:TYR:OH	4:B:1005:5GP:H8	2.20	0.41
1:B:257:ILE:HD13	1:B:488:ARG:HB2	2.01	0.41
1:B:251:PRO:HA	1:B:254:HIS:NE2	2.36	0.41
1:A:362:HIS:ND1	1:A:515:GLY:O	2.53	0.41
1:B:326:VAL:HA	1:B:327:PRO:HD2	1.93	0.41
1:B:649:HIS:CE1	1:B:667:LEU:HD13	2.56	0.41
1:B:656:GLN:HE22	1:B:661:THR:HG22	1.85	0.41
1:A:353:TYR:OH	4:A:1009:5GP:H8	2.21	0.41
1:B:854:GLU:HA	1:B:857:TRP:NE1	2.36	0.41
1:A:786:ARG:HA	1:A:874:LEU:O	2.20	0.41
1:B:308:ASP:HB3	1:B:321:VAL:HA	2.01	0.41
1:A:185:CYS:HA	1:A:186:PRO:HD3	1.87	0.41
1:B:185:CYS:HA	1:B:186:PRO:HD3	1.86	0.41
1:A:214:LEU:HD22	1:A:379:ASP:HB2	2.03	0.41
1:A:629:ASP:O	1:A:632:ILE:HG22	2.21	0.41
1:B:708:TYR:HE2	1:B:803:GLN:HB2	1.86	0.41
1:A:420:ASN:O	1:A:424:GLY:N	2.50	0.41
1:A:588:LYS:HD3	1:A:588:LYS:HA	1.77	0.40
1:B:575:HIS:CE1	1:B:893:ARG:HD3	2.56	0.40
1:A:257:ILE:HG12	1:A:489:ILE:HG12	2.02	0.40
1:B:214:LEU:HD21	1:B:375:LEU:HB3	2.03	0.40
1:B:607:CYS:HB3	1:B:691:CYS:HA	2.03	0.40
1:B:210:TRP:O	1:B:214:LEU:HG	2.21	0.40
1:A:277:LYS:NZ	4:A:1009:5GP:HN1	2.20	0.40
1:A:601:THR:HA	1:A:602:SER:HA	1.92	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	698/823 (85%)	675 (97%)	23 (3%)	0	100	100
1	B	685/823 (83%)	660 (96%)	25 (4%)	0	100	100
All	All	1383/1646 (84%)	1335 (96%)	48 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	593/755 (78%)	580 (98%)	13 (2%)	60	87
1	B	592/755 (78%)	583 (98%)	9 (2%)	72	91
All	All	1185/1510 (78%)	1163 (98%)	22 (2%)	65	89

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	PHE
1	A	236	THR
1	A	239	PHE
1	A	308	ASP
1	A	317	ASP
1	A	416	TYR
1	A	590	GLU
1	A	628	GLU
1	A	665	LEU
1	A	760	LEU
1	A	790	LEU
1	A	874	LEU
1	A	886	GLU
1	B	197	PHE
1	B	236	THR
1	B	239	PHE
1	B	308	ASP
1	B	317	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	416	TYR
1	B	665	LEU
1	B	791	GLU
1	B	792	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	501	GLN
1	A	525	ASN
1	A	658	GLN
1	A	690	ASN
1	A	741	ASN
1	A	769	ASN
1	A	820	GLN
1	A	850	HIS
1	B	229	ASN
1	B	553	ASN
1	B	694	GLN
1	B	750	GLN
1	B	769	ASN
1	B	820	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](#)

8 carbohydrates 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	NAG	A	1001	1,2	14,14,15	0.52	0	15,19,21	0.86	0
2	NAG	A	1002	2	14,14,15	0.44	0	15,19,21	0.74	0
2	BMA	A	1003	2	11,11,12	0.61	0	14,15,17	1.04	2 (14%)
2	MAN	A	1004	2	11,11,12	0.71	0	14,15,17	1.20	1 (7%)
2	MAN	A	1005	2	11,11,12	0.58	0	14,15,17	1.81	5 (35%)
2	MAN	A	1006	2	11,11,12	0.55	0	14,15,17	1.13	2 (14%)
7	NAG	B	1001	1,7	14,14,15	0.51	0	15,19,21	1.00	0
7	NAG	B	1002	7	14,14,15	0.51	0	15,19,21	0.69	0

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	NAG	A	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1003	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1004	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1005	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1006	2	-	0/2/19/22	1/1/1/1
7	NAG	B	1001	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	1002	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1003	BMA	C1-O5-C5	-2.40	109.20	112.25
2	A	1005	MAN	O3-C3-C4	-2.02	105.80	110.34
2	A	1003	BMA	O5-C1-C2	-2.00	107.61	110.86
2	A	1006	MAN	C1-C2-C3	2.02	111.93	109.54
2	A	1005	MAN	O5-C5-C6	2.37	112.47	107.35
2	A	1005	MAN	C3-C4-C5	2.40	114.38	110.20
2	A	1006	MAN	C1-O5-C5	2.59	115.53	112.25
2	A	1004	MAN	C1-C2-C3	2.78	112.83	109.54
2	A	1005	MAN	C1-C2-C3	3.10	113.21	109.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1005	MAN	C1-O5-C5	4.01	117.34	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1006	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	NAG	A	1007	1	14,14,15	0.47	0	15,19,21	1.19	1 (6%)
3	NAG	A	1008	1	14,14,15	0.53	0	15,19,21	0.81	1 (6%)
4	5GP	A	1009	5	21,26,26	0.50	0	25,40,40	1.74	6 (24%)
3	NAG	B	1003	1	14,14,15	0.58	0	15,19,21	0.78	0
3	NAG	B	1004	1	14,14,15	0.53	0	15,19,21	0.76	0
4	5GP	B	1005	5	21,26,26	0.50	0	25,40,40	1.76	5 (20%)

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	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1008	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	5GP	A	1009	5	-	0/6/26/26	0/3/3/3
3	NAG	B	1003	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
4	5GP	B	1005	5	-	0/6/26/26	0/3/3/3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1005	5GP	N3-C2-N1	-4.54	120.53	127.44
4	A	1009	5GP	N3-C2-N1	-4.23	121.00	127.44
4	B	1005	5GP	C5-C6-N1	-3.20	119.22	123.59
4	A	1009	5GP	C5-C6-N1	-3.19	119.22	123.59
4	A	1009	5GP	O3P-P-O5'	-2.83	98.41	106.56
4	B	1005	5GP	O3P-P-O5'	-2.71	98.76	106.56
4	A	1009	5GP	C4-C5-N7	-2.15	107.50	109.48
3	A	1008	NAG	C1-O5-C5	2.08	114.89	112.25
4	A	1009	5GP	O2P-P-O1P	2.38	118.23	110.58
4	B	1005	5GP	O2P-P-O1P	2.40	118.29	110.58
3	A	1007	NAG	C1-O5-C5	3.47	116.65	112.25
4	A	1009	5GP	C6-N1-C2	3.67	121.03	115.94
4	B	1005	5GP	C6-N1-C2	3.86	121.29	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1009	5GP	3	0
4	B	1005	5GP	4	0

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, 95th 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 ²)	Q<0.9
1	A	706/823 (85%)	0.11	9 (1%) 79 67	52, 91, 130, 163	0
1	B	697/823 (84%)	0.15	18 (2%) 59 45	49, 94, 136, 167	0
All	All	1403/1646 (85%)	0.13	27 (1%) 70 55	49, 93, 132, 167	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	698	ILE	3.8
1	B	715	LEU	3.6
1	B	439	LEU	3.6
1	B	441	PRO	3.2
1	A	712	ASN	2.9
1	A	805	ILE	2.6
1	B	699	PRO	2.5
1	B	503	ALA	2.5
1	B	189	PHE	2.5
1	B	709	TYR	2.4
1	B	448	TYR	2.3
1	A	600	SER	2.3
1	B	442	THR	2.3
1	B	837	ILE	2.2
1	A	460	LEU	2.2
1	B	743	VAL	2.2
1	A	339	LEU	2.1
1	A	611	PRO	2.1
1	B	339	LEU	2.1
1	A	439	LEU	2.1
1	B	268	ALA	2.1
1	B	429	VAL	2.1
1	B	460	LEU	2.1
1	B	504	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	806	LEU	2.1
1	A	429	VAL	2.0
1	A	734	SER	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](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	NAG	B	1001	14/15	0.92	0.23	0.37	63,69,73,78	0
2	NAG	A	1001	14/15	0.96	0.21	0.03	58,63,65,70	0
2	NAG	A	1002	14/15	0.93	0.14	-	71,76,80,84	0
2	BMA	A	1003	11/12	0.85	0.13	-	87,90,94,97	0
2	MAN	A	1006	11/12	0.87	0.11	-	102,103,105,106	0
2	MAN	A	1004	11/12	0.93	0.13	-	87,89,91,91	0
7	NAG	B	1002	14/15	0.87	0.17	-	83,88,89,90	0
2	MAN	A	1005	11/12	0.83	0.13	-	97,98,100,102	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	ZN	A	1011	1/1	0.98	0.23	1.99	72,72,72,72	0
5	ZN	A	1010	1/1	0.91	0.25	1.76	90,90,90,90	0
5	ZN	B	1007	1/1	0.95	0.20	1.09	87,87,87,87	0
5	ZN	B	1006	1/1	0.94	0.21	0.38	89,89,89,89	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	CA	A	1012	1/1	0.98	0.15	-0.23	79,79,79,79	0
4	5GP	B	1005	24/24	0.93	0.17	-0.92	76,87,100,102	0
4	5GP	A	1009	24/24	0.95	0.15	-1.71	66,78,93,94	0
6	CA	B	1008	1/1	0.99	0.09	-1.78	97,97,97,97	0
3	NAG	B	1004	14/15	0.86	0.18	-	78,83,87,87	0
3	NAG	A	1007	14/15	0.83	0.22	-	93,101,103,104	0
3	NAG	A	1008	14/15	0.88	0.21	-	78,83,86,87	0
3	NAG	B	1003	14/15	0.76	0.27	-	89,95,98,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.