



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:49 PM UTC

PDB ID : 3WFZ / pdb_00003wfz
Title : Crystal structure of Galacto-N-Biose/Lacto-N-Biose I Phosphorylase C236Y Mutant
Authors : Koyama, Y.; Hidaka, M.; Kawakami, M.; Nishimoto, M.; Kitaoka, M.
Deposited on : 2013-07-25
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

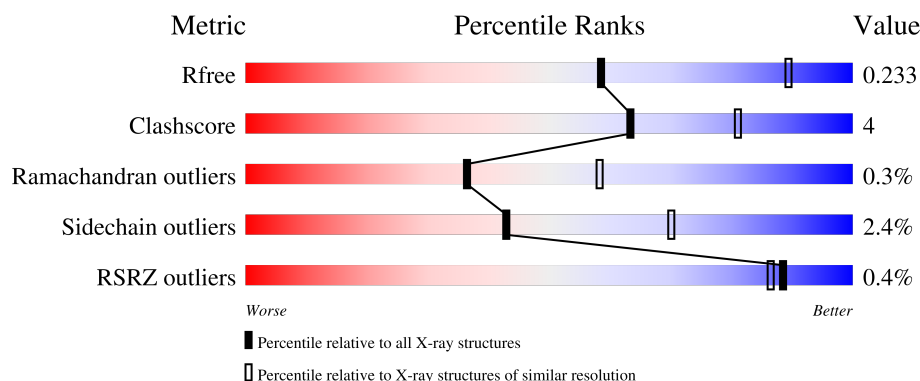
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	759	 87% 10% ..
1	B	759	 85% 11% ..
1	C	759	 85% 13% .
1	D	759	 84% 12% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24550 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 Lacto-N-biose phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	746	Total	C	N	O	S	0	0	0
			5940	3793	998	1134	15			
1	B	734	Total	C	N	O	S	0	0	0
			5851	3737	984	1115	15			
1	C	744	Total	C	N	O	S	0	0	0
			5926	3785	996	1130	15			
1	D	737	Total	C	N	O	S	0	0	0
			5873	3751	987	1120	15			

There are 36 discrepancies between the modelled and reference sequences:

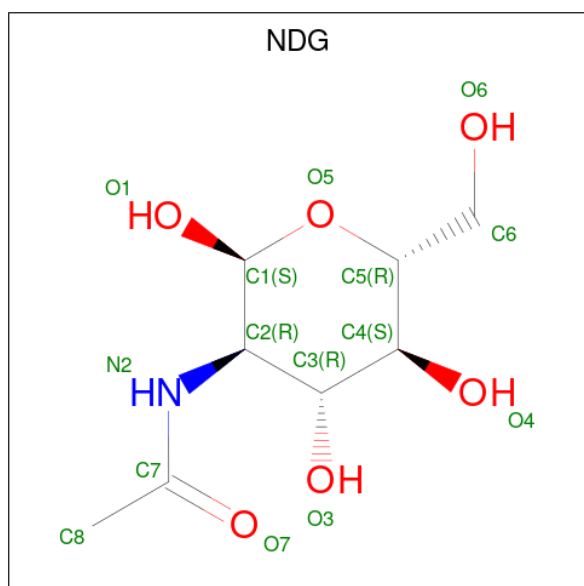
Chain	Residue	Modelled	Actual	Comment	Reference
A	236	TYR	CYS	engineered mutation	UNP E8MF13
A	752	LEU	-	expression tag	UNP E8MF13
A	753	GLU	-	expression tag	UNP E8MF13
A	754	HIS	-	expression tag	UNP E8MF13
A	755	HIS	-	expression tag	UNP E8MF13
A	756	HIS	-	expression tag	UNP E8MF13
A	757	HIS	-	expression tag	UNP E8MF13
A	758	HIS	-	expression tag	UNP E8MF13
A	759	HIS	-	expression tag	UNP E8MF13
B	236	TYR	CYS	engineered mutation	UNP E8MF13
B	752	LEU	-	expression tag	UNP E8MF13
B	753	GLU	-	expression tag	UNP E8MF13
B	754	HIS	-	expression tag	UNP E8MF13
B	755	HIS	-	expression tag	UNP E8MF13
B	756	HIS	-	expression tag	UNP E8MF13
B	757	HIS	-	expression tag	UNP E8MF13
B	758	HIS	-	expression tag	UNP E8MF13
B	759	HIS	-	expression tag	UNP E8MF13
C	236	TYR	CYS	engineered mutation	UNP E8MF13
C	752	LEU	-	expression tag	UNP E8MF13
C	753	GLU	-	expression tag	UNP E8MF13

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Chain	Residue	Modelled	Actual	Comment	Reference
C	754	HIS	-	expression tag	UNP E8MF13
C	755	HIS	-	expression tag	UNP E8MF13
C	756	HIS	-	expression tag	UNP E8MF13
C	757	HIS	-	expression tag	UNP E8MF13
C	758	HIS	-	expression tag	UNP E8MF13
C	759	HIS	-	expression tag	UNP E8MF13
D	236	TYR	CYS	engineered mutation	UNP E8MF13
D	752	LEU	-	expression tag	UNP E8MF13
D	753	GLU	-	expression tag	UNP E8MF13
D	754	HIS	-	expression tag	UNP E8MF13
D	755	HIS	-	expression tag	UNP E8MF13
D	756	HIS	-	expression tag	UNP E8MF13
D	757	HIS	-	expression tag	UNP E8MF13
D	758	HIS	-	expression tag	UNP E8MF13
D	759	HIS	-	expression tag	UNP E8MF13

- Molecule 2 is 2-acetamido-2-deoxy- α -D-glucopyranose (CCD ID: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	C	1	Total	C	N	O	0	0
			15	8	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			15	8	1	6		

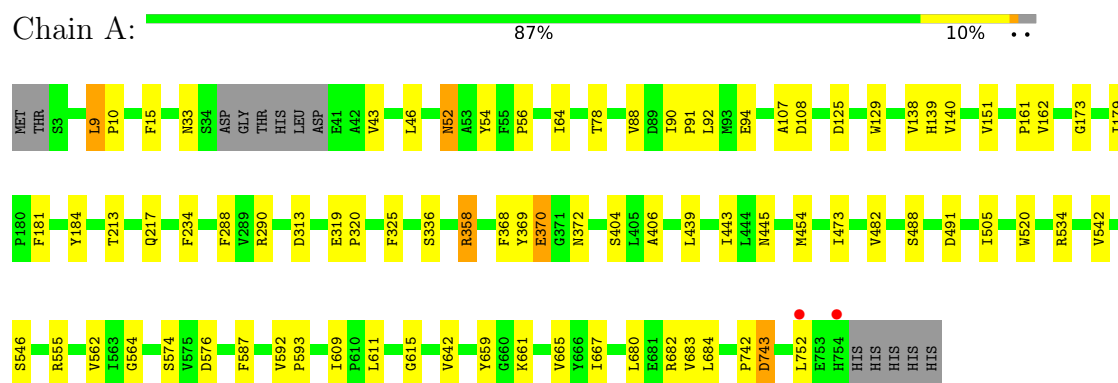
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	268	Total	O	0	0
			268	268		
3	B	225	Total	O	0	0
			225	225		
3	C	224	Total	O	0	0
			224	224		
3	D	183	Total	O	0	0
			183	183		

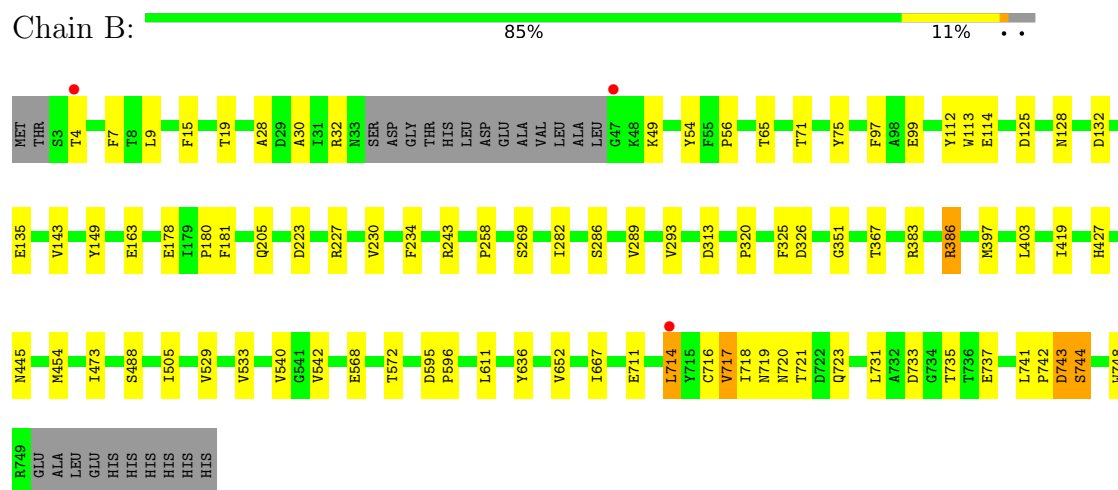
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

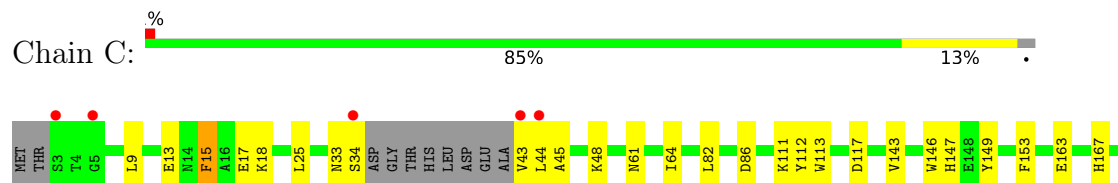
• Molecule 1: Lacto-N-biose phosphorylase



• Molecule 1: Lacto-N-biose phosphorylase



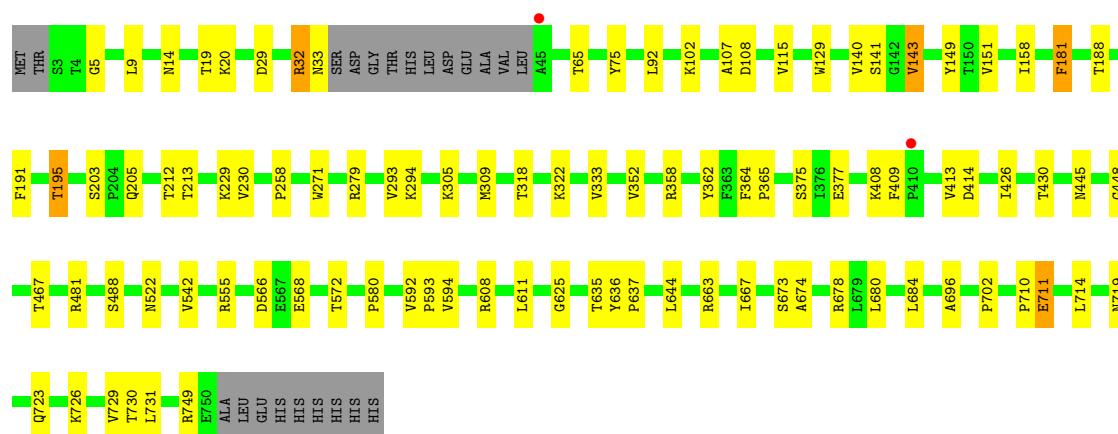
• Molecule 1: Lacto-N-biose phosphorylase





• Molecule 1: Lacto-N-biose phosphorylase

Chain D: 84% 12% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.62Å 113.00Å 118.93Å 105.48° 90.88° 106.73°	Depositor
Resolution (Å)	36.09 – 2.60 36.09 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.6 (36.09-2.60) 96.6 (36.09-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.179 , 0.249 (Not available) , 0.233	Depositor DCC
R_{free} test set	4869 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24550	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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, 0.333 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: NDG

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	0.87	0/6109	0.99	1/8321 (0.0%)
1	B	0.84	0/6019	0.95	2/8198 (0.0%)
1	C	0.81	0/6095	0.94	4/8302 (0.0%)
1	D	0.79	0/6041	0.93	5/8228 (0.1%)
All	All	0.83	0/24264	0.95	12/33049 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	279	ARG	N-CA-C	-6.27	104.53	111.36
1	C	319	GLU	CA-C-N	5.88	125.74	119.28
1	C	319	GLU	C-N-CA	5.88	125.74	119.28
1	A	90	ILE	N-CA-C	5.76	113.85	108.15
1	D	129	TRP	N-CA-C	5.60	117.78	108.99
1	D	580	PRO	O-C-N	5.30	123.64	121.15
1	D	102	LYS	CA-C-N	-5.29	114.31	119.76
1	D	102	LYS	C-N-CA	-5.29	114.31	119.76
1	C	282	ILE	N-CA-CB	5.22	116.10	110.62
1	B	714	LEU	N-CA-C	5.09	117.13	109.23
1	C	282	ILE	CB-CA-C	-5.04	105.25	111.70
1	B	652	VAL	N-CA-C	5.03	115.55	108.36

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	5940	0	5627	43	0
1	B	5851	0	5540	47	0
1	C	5926	0	5616	51	0
1	D	5873	0	5562	43	0
2	A	15	0	12	0	0
2	B	15	0	12	0	0
2	C	15	0	12	0	0
2	D	15	0	12	0	0
3	A	268	0	0	0	0
3	B	225	0	0	1	0
3	C	224	0	0	2	0
3	D	183	0	0	5	0
All	All	24550	0	22393	182	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 4.

All (182) 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:C:43:VAL:HG13	1:C:44:LEU:H	1.55	0.70
1:B:383:ARG:HD3	1:B:744:SER:HB3	1.74	0.69
1:B:282:ILE:O	1:B:286:SER:HB2	1.93	0.69
1:D:32:ARG:O	1:D:33:ASN:HB2	1.94	0.66
1:C:33:ASN:OD1	1:C:34:SER:N	2.29	0.65
1:A:162:VAL:HG21	1:A:313:ASP:OD1	1.98	0.64
1:D:333:VAL:HG23	1:D:352:VAL:HG11	1.80	0.62
1:B:542:VAL:HA	1:B:667:ILE:O	2.00	0.61
1:A:9:LEU:HD23	1:A:10:PRO:HD2	1.84	0.60
1:C:464:ASN:OD1	1:C:467:THR:HG23	2.03	0.59
1:A:320:PRO:HA	1:A:325:PHE:CD1	2.38	0.58
1:C:592:VAL:HG21	1:C:626:ILE:HD11	1.87	0.57
1:B:15:PHE:O	1:B:19:THR:OG1	2.14	0.55
1:A:92:LEU:HD21	1:A:138:VAL:HG23	1.89	0.55
1:B:568:GLU:OE1	1:B:572:THR:OG1	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:VAL:HB	1:B:149:TYR:CZ	2.43	0.54
1:D:115:VAL:HG22	1:D:151:VAL:HG22	1.90	0.54
1:B:473:ILE:HD11	1:B:542:VAL:HG11	1.90	0.54
1:A:33:ASN:HD22	1:A:52:ASN:CG	2.16	0.54
1:B:125:ASP:HB3	1:B:128:ASN:OD1	2.09	0.54
1:B:114:GLU:HB2	1:B:258:PRO:HG2	1.90	0.53
1:C:61:ASN:HA	1:C:64:ILE:HG22	1.90	0.53
1:D:673:SER:O	1:D:674:ALA:C	2.51	0.53
1:B:143:VAL:HB	1:B:149:TYR:OH	2.09	0.53
1:A:358:ARG:C	1:A:358:ARG:HD2	2.33	0.53
1:D:568:GLU:OE1	1:D:572:THR:OG1	2.24	0.53
1:D:107:ALA:O	1:D:108:ASP:C	2.52	0.52
1:A:488:SER:O	1:A:491:ASP:HB2	2.09	0.52
1:B:320:PRO:HA	1:B:325:PHE:CD1	2.44	0.52
1:B:717:VAL:HG22	1:B:741:LEU:HD11	1.91	0.52
1:C:17:GLU:OE2	1:C:17:GLU:HA	2.07	0.52
1:C:234:PHE:CE1	1:C:454:MET:HB3	2.45	0.51
1:A:564:GLY:O	1:A:642:VAL:HG21	2.10	0.51
1:C:234:PHE:CZ	1:C:454:MET:HB3	2.46	0.50
1:C:575:VAL:O	1:C:577:LYS:HE3	2.11	0.50
1:D:271:TRP:CZ2	1:D:467:THR:HG22	2.46	0.50
1:A:64:ILE:HG21	1:A:179:ILE:HB	1.93	0.50
1:A:9:LEU:HD22	1:A:10:PRO:O	2.11	0.50
1:C:716:CYS:HB3	1:C:748:TRP:CE3	2.47	0.50
1:B:529:VAL:O	1:B:533:VAL:HG23	2.11	0.50
1:C:544:GLU:OE1	1:C:567:GLU:OE1	2.29	0.50
1:C:521:THR:HG22	1:C:551:PHE:CD2	2.47	0.50
1:D:309:MET:HE1	1:D:318:THR:OG1	2.11	0.50
1:B:9:LEU:HD21	1:B:403:LEU:HD22	1.94	0.49
1:A:290:ARG:NH2	1:A:319:GLU:O	2.45	0.49
1:A:576:ASP:HB3	1:A:615:GLY:HA2	1.93	0.49
1:B:719:ASN:ND2	1:B:723:GLN:O	2.35	0.49
1:C:441:VAL:HG21	1:C:684:LEU:HD13	1.95	0.49
1:D:663:ARG:NH2	3:D:937:HOH:O	2.42	0.49
1:B:397:MET:HE1	1:B:419:ILE:HG22	1.93	0.48
1:C:44:LEU:HD11	1:C:205:GLN:HB2	1.94	0.48
1:B:383:ARG:HD2	1:B:720:ASN:C	2.38	0.48
1:C:542:VAL:HA	1:C:667:ILE:O	2.13	0.48
1:A:542:VAL:HA	1:A:667:ILE:O	2.13	0.48
1:C:373:ASP:OD2	1:C:411:LYS:NZ	2.47	0.48
1:A:15:PHE:CZ	1:A:404:SER:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:PHE:CZ	1:A:454:MET:HB3	2.49	0.48
1:A:742:PRO:O	1:A:743:ASP:C	2.56	0.48
1:C:281:TRP:O	1:C:282:ILE:C	2.56	0.48
1:A:445:ASN:O	1:A:488:SER:HA	2.13	0.48
1:D:19:THR:O	1:D:20:LYS:C	2.57	0.48
1:B:4:THR:O	1:B:4:THR:HG23	2.14	0.47
1:C:143:VAL:HB	1:C:149:TYR:CZ	2.49	0.47
1:A:520:TRP:CE2	1:A:546:SER:HA	2.49	0.47
1:B:205:GLN:H	1:B:205:GLN:CD	2.22	0.47
1:B:733:ASP:OD1	1:B:735:THR:HG23	2.14	0.47
1:B:7:PHE:HB3	1:B:28:ALA:HA	1.96	0.47
1:B:30:ALA:HA	1:B:49:LYS:O	2.15	0.47
1:B:289:VAL:O	1:B:293:VAL:HG23	2.15	0.47
1:D:140:VAL:HG12	1:D:143:VAL:CG1	2.45	0.47
1:D:481:ARG:NH1	1:D:696:ALA:O	2.48	0.47
1:B:383:ARG:HH11	1:B:744:SER:HB3	1.79	0.47
1:C:15:PHE:CE2	1:C:18:LYS:HB2	2.50	0.47
1:C:272:ARG:O	1:C:513:ALA:HB2	2.15	0.47
1:D:143:VAL:HB	1:D:149:TYR:CZ	2.50	0.47
1:D:426:ILE:O	1:D:430:THR:OG1	2.16	0.47
1:C:347:ALA:HB2	1:C:394:ILE:HG23	1.97	0.46
1:A:64:ILE:HD13	1:A:181:PHE:HB3	1.97	0.46
1:D:212:THR:N	1:D:213:THR:HA	2.30	0.46
1:B:282:ILE:O	1:B:286:SER:CB	2.63	0.46
1:A:443:ILE:HD13	1:A:505:ILE:HB	1.97	0.46
1:C:111:LYS:HD3	1:C:112:TYR:CE2	2.50	0.46
1:C:552:GLN:NE2	1:C:558:GLN:OE1	2.48	0.46
1:D:5:GLY:HA2	1:D:29:ASP:HB3	1.97	0.46
1:C:163:GLU:HG3	1:C:178:GLU:HG3	1.98	0.46
1:D:377:GLU:OE2	1:D:377:GLU:N	2.45	0.46
1:D:522:ASN:OD1	1:D:522:ASN:C	2.57	0.46
1:D:364:PHE:CD2	1:D:365:PRO:HD2	2.51	0.46
1:D:181:PHE:HB2	1:D:188:THR:HG21	1.98	0.45
1:B:383:ARG:HD3	1:B:744:SER:CB	2.44	0.45
1:D:678:ARG:NH2	1:D:702:PRO:HA	2.32	0.45
1:B:227:ARG:HD3	3:B:1110:HOH:O	2.16	0.45
1:C:526:VAL:HG12	1:C:530:ARG:HD2	1.98	0.45
1:A:473:ILE:HD11	1:A:542:VAL:HG11	1.99	0.45
1:D:637:PRO:HB3	1:D:644:LEU:HD21	1.98	0.45
1:C:340:GLY:O	1:C:343:THR:HB	2.16	0.45
1:D:75:TYR:CE2	1:D:258:PRO:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:PHE:O	1:D:413:VAL:HG23	2.17	0.45
1:A:439:LEU:HB2	1:A:482:VAL:HG12	1.97	0.45
1:B:716:CYS:HB3	1:B:748:TRP:CE3	2.52	0.45
1:C:344:ARG:O	1:C:345:MET:C	2.60	0.45
1:D:719:ASN:ND2	1:D:723:GLN:O	2.46	0.45
1:D:729:VAL:HG12	1:D:730:THR:N	2.32	0.45
1:B:505:ILE:HG12	1:B:540:VAL:HB	1.99	0.44
1:C:389:ILE:HD11	1:C:394:ILE:HD11	1.99	0.44
1:A:107:ALA:O	1:A:108:ASP:C	2.60	0.44
1:C:236:TYR:CE2	1:C:282:ILE:HD12	2.52	0.44
1:D:542:VAL:HA	1:D:667:ILE:O	2.17	0.44
1:A:574:SER:O	1:B:230:VAL:HA	2.17	0.44
1:B:742:PRO:O	1:B:743:ASP:C	2.60	0.44
1:C:680:LEU:O	1:C:684:LEU:HG	2.17	0.44
1:D:362:TYR:HA	3:D:918:HOH:O	2.16	0.44
1:A:562:VAL:HG22	1:A:659:TYR:CZ	2.52	0.44
1:C:43:VAL:C	1:C:45:ALA:H	2.25	0.44
1:C:520:TRP:CE2	1:C:546:SER:HA	2.53	0.44
1:D:445:ASN:O	1:D:488:SER:HA	2.17	0.44
1:A:91:PRO:CB	1:A:94:GLU:HG3	2.47	0.44
1:D:92:LEU:N	3:D:947:HOH:O	2.51	0.44
1:A:184:TYR:HA	1:A:288:PHE:CZ	2.53	0.44
1:B:386:ARG:NH1	1:B:744:SER:O	2.51	0.44
1:A:234:PHE:CE1	1:A:454:MET:HB3	2.53	0.43
1:C:709:PHE:HB3	1:C:712:GLN:OE1	2.18	0.43
1:C:82:LEU:HD11	1:C:146:TRP:HA	2.00	0.43
1:B:132:ASP:HB3	1:B:135:GLU:O	2.18	0.43
1:C:325:PHE:CD1	1:C:328:LEU:HD12	2.53	0.43
1:D:566:ASP:O	1:D:635:THR:HA	2.19	0.43
1:B:326:ASP:HB3	1:B:351:GLY:HA2	1.99	0.43
1:C:555:ARG:HD3	1:C:560:ALA:HB3	1.99	0.43
1:D:592:VAL:O	1:D:593:PRO:C	2.58	0.43
1:D:714:LEU:HD23	1:D:749:ARG:O	2.18	0.43
1:C:364:PHE:CG	1:C:365:PRO:HD2	2.53	0.43
1:B:75:TYR:OH	1:B:112:TYR:O	2.26	0.43
1:C:167:HIS:HA	1:C:172:TRP:CE3	2.54	0.43
1:A:54:TYR:O	1:A:56:PRO:HD3	2.19	0.43
1:D:710:PRO:O	1:D:711:GLU:C	2.61	0.43
1:A:78:THR:HG23	1:A:151:VAL:O	2.19	0.43
1:A:665:VAL:HG21	1:A:683:VAL:HG13	2.00	0.43
1:B:636:TYR:CD1	1:B:636:TYR:C	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:SER:O	1:C:454:MET:HG3	2.19	0.43
1:C:15:PHE:CE2	1:C:18:LYS:CB	3.02	0.42
1:B:71:THR:HG22	1:B:180:PRO:O	2.19	0.42
1:B:97:PHE:HB2	1:B:223:ASP:O	2.20	0.42
1:D:191:PHE:O	1:D:195:THR:OG1	2.36	0.42
1:B:163:GLU:HG3	1:B:178:GLU:HG3	2.00	0.42
1:C:282:ILE:O	1:C:286:SER:HB2	2.19	0.42
1:B:54:TYR:O	1:B:56:PRO:HD3	2.20	0.42
1:B:743:ASP:C	1:B:743:ASP:OD1	2.61	0.42
1:A:680:LEU:O	1:A:684:LEU:HG	2.19	0.42
1:B:595:ASP:O	1:B:596:PRO:C	2.61	0.42
1:A:91:PRO:HB2	1:A:94:GLU:HG3	2.01	0.42
1:A:129:TRP:HA	1:A:139:HIS:O	2.20	0.42
1:A:370:GLU:OE1	1:D:625:GLY:N	2.42	0.42
1:B:234:PHE:CE1	1:B:454:MET:HB3	2.54	0.42
1:D:229:LYS:HG2	1:D:230:VAL:HG23	2.00	0.42
1:B:445:ASN:O	1:B:488:SER:HA	2.20	0.42
1:C:113:TRP:CE2	1:C:153:PHE:HB2	2.55	0.42
1:C:608:ARG:HD2	3:C:1002:HOH:O	2.20	0.42
1:D:448:GLY:HA3	3:D:913:HOH:O	2.20	0.42
1:C:43:VAL:HG13	1:C:44:LEU:N	2.31	0.41
1:A:534:ARG:O	1:A:661:LYS:HB2	2.20	0.41
1:A:592:VAL:O	1:A:593:PRO:C	2.61	0.41
1:D:203:SER:O	1:D:305:LYS:NZ	2.51	0.41
1:A:88:VAL:HG12	1:A:140:VAL:HB	2.01	0.41
1:A:587:PHE:O	1:A:682:ARG:HD3	2.20	0.41
1:A:43:VAL:HA	1:A:46:LEU:HD12	2.03	0.41
1:A:369:TYR:CZ	1:A:372:ASN:HB2	2.56	0.41
1:C:196:PHE:CE2	1:C:200:LEU:HD11	2.56	0.41
1:B:113:TRP:CD1	1:B:113:TRP:N	2.87	0.41
1:C:742:PRO:O	1:C:743:ASP:C	2.63	0.41
1:D:636:TYR:CD1	1:D:636:TYR:C	2.99	0.41
1:D:293:VAL:O	1:D:294:LYS:C	2.64	0.41
1:D:680:LEU:O	1:D:684:LEU:HG	2.21	0.41
1:C:539:PHE:O	1:C:664:GLY:HA2	2.20	0.41
1:D:608:ARG:HD2	3:D:952:HOH:O	2.21	0.41
1:A:368:PHE:CE1	1:A:406:ALA:HA	2.56	0.40
1:B:234:PHE:CZ	1:B:454:MET:HB3	2.56	0.40
1:C:117:ASP:CG	1:C:147:HIS:HD1	2.29	0.40
1:B:97:PHE:CZ	1:B:99:GLU:HB2	2.56	0.40
1:C:521:THR:HG22	1:C:551:PHE:CG	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:711:GLU:HG2	3:C:983:HOH:O	2.20	0.40
1:A:161:PRO:HG2	1:A:217:GLN:HG2	2.04	0.40
1:C:497:ILE:O	1:C:498:ASP:C	2.65	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	742/759 (98%)	705 (95%)	35 (5%)	2 (0%)	36	58
1	B	730/759 (96%)	689 (94%)	37 (5%)	4 (0%)	24	46
1	C	740/759 (98%)	697 (94%)	41 (6%)	2 (0%)	36	58
1	D	733/759 (97%)	688 (94%)	45 (6%)	0	100	100
All	All	2945/3036 (97%)	2779 (94%)	158 (5%)	8 (0%)	36	58

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	GLY
1	C	15	PHE
1	A	743	ASP
1	B	744	SER
1	B	269	SER
1	B	743	ASP
1	C	13	GLU
1	B	313	ASP

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	622/634 (98%)	611 (98%)	11 (2%)	51	76
1	B	613/634 (97%)	598 (98%)	15 (2%)	43	70
1	C	621/634 (98%)	608 (98%)	13 (2%)	47	73
1	D	615/634 (97%)	594 (97%)	21 (3%)	32	60
All	All	2471/2536 (97%)	2411 (98%)	60 (2%)	43	70

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	52	ASN
1	A	125	ASP
1	A	213	THR
1	A	336	SER
1	A	358	ARG
1	A	370	GLU
1	A	555	ARG
1	A	609	ILE
1	A	611	LEU
1	A	752	LEU
1	B	32	ARG
1	B	65	THR
1	B	181	PHE
1	B	243	ARG
1	B	367	THR
1	B	386	ARG
1	B	427	HIS
1	B	611	LEU
1	B	711	GLU
1	B	714	LEU
1	B	717	VAL
1	B	718	ILE
1	B	721	THR

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Mol	Chain	Res	Type
1	B	731	LEU
1	B	737	GLU
1	C	9	LEU
1	C	25	LEU
1	C	48	LYS
1	C	86	ASP
1	C	353	LYS
1	C	367	THR
1	C	405	LEU
1	C	430	THR
1	C	449	LYS
1	C	555	ARG
1	C	611	LEU
1	C	731	LEU
1	C	750	GLU
1	D	9	LEU
1	D	14	ASN
1	D	32	ARG
1	D	65	THR
1	D	141	SER
1	D	143	VAL
1	D	158	ILE
1	D	181	PHE
1	D	195	THR
1	D	205	GLN
1	D	322	LYS
1	D	358	ARG
1	D	375	SER
1	D	408	LYS
1	D	414	ASP
1	D	555	ARG
1	D	594	VAL
1	D	611	LEU
1	D	711	GLU
1	D	726	LYS
1	D	731	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	421	ASN

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Mol	Chain	Res	Type
1	A	483	ASN
1	B	33	ASN
1	B	166	ASN
1	B	177	HIS
1	B	427	HIS
1	B	460	HIS
1	B	495	HIS
1	B	690	ASN
1	C	14	ASN
1	C	166	ASN
1	C	418	HIS
1	C	657	ASN
1	C	720	ASN
1	D	52	ASN
1	D	128	ASN
1	D	295	GLN
1	D	723	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	NDG	A	4001	-	15,15,15	0.41	0	21,21,21	1.19	1 (4%)
2	NDG	B	801	-	15,15,15	0.54	0	21,21,21	1.06	2 (9%)
2	NDG	D	801	-	15,15,15	0.51	0	21,21,21	1.20	1 (4%)
2	NDG	C	801	-	15,15,15	0.67	0	21,21,21	1.54	2 (9%)

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	NDG	A	4001	-	-	0/6/26/26	0/1/1/1
2	NDG	B	801	-	-	0/6/26/26	0/1/1/1
2	NDG	D	801	-	-	0/6/26/26	0/1/1/1
2	NDG	C	801	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	NDG	C4-C3-C2	-4.46	103.90	110.40
2	A	4001	NDG	O5-C1-C2	3.49	113.03	109.52
2	C	801	NDG	O5-C1-C2	3.27	112.80	109.52
2	D	801	NDG	O5-C1-C2	3.01	112.54	109.52
2	B	801	NDG	C1-C2-N2	-2.88	107.39	110.73
2	B	801	NDG	C3-C2-N2	2.29	114.83	110.62

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, 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	746/759 (98%)	-0.54	2 (0%) 90 88	11, 23, 42, 84	0
1	B	734/759 (96%)	-0.41	3 (0%) 88 86	12, 25, 58, 80	0
1	C	744/759 (98%)	-0.36	6 (0%) 82 80	15, 29, 52, 85	0
1	D	737/759 (97%)	-0.23	2 (0%) 90 88	17, 30, 66, 91	0
All	All	2961/3036 (97%)	-0.39	13 (0%) 88 86	11, 27, 57, 91	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	43	VAL	4.0
1	A	752	LEU	3.1
1	C	44	LEU	2.8
1	B	4	THR	2.7
1	D	410	PRO	2.7
1	D	45	ALA	2.5
1	B	47	GLY	2.4
1	C	5	GLY	2.4
1	C	3	SER	2.3
1	B	714	LEU	2.3
1	A	754	HIS	2.2
1	C	34	SER	2.1
1	C	754	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	NDG	A	4001	15/15	0.94	0.07	19,21,23,27	0
2	NDG	C	801	15/15	0.95	0.07	25,26,28,29	0
2	NDG	D	801	15/15	0.95	0.07	26,27,31,33	0
2	NDG	B	801	15/15	0.96	0.07	19,22,23,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.