



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:13 PM GMT

PDB ID : 3WFZ
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
<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

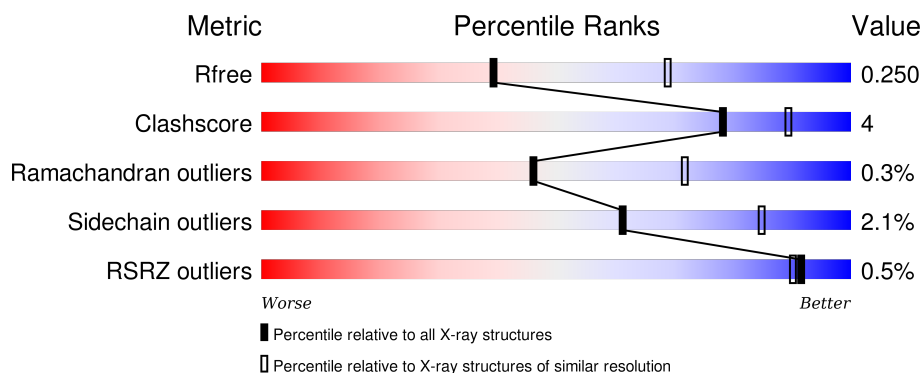
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 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	759	<div> <div>87%</div> <div>10% ..</div> </div>
1	B	759	<div> <div>%</div> <div>86%</div> <div>10% ..</div> </div>
1	C	759	<div> <div>%</div> <div>86%</div> <div>12% ..</div> </div>
1	D	759	<div> <div>%</div> <div>87%</div> <div>10% ..</div> </div>

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:

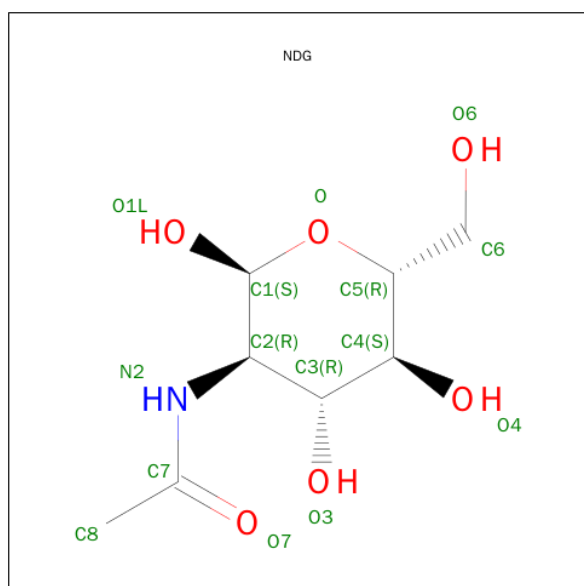
Chain	Residue	Modelled	Actual	Comment	Reference
A	236	TYR	CYS	ENGINEERED MUTATION	UNP E8MF13
A	752	LEU	-	EXPRESSION TAG	UNP E8MF13
A	753	GLU	-	EXPRESSION TAG	UNP E8MF13
A	754	HIS	-	EXPRESSION TAG	UNP E8MF13
A	755	HIS	-	EXPRESSION TAG	UNP E8MF13
A	756	HIS	-	EXPRESSION TAG	UNP E8MF13
A	757	HIS	-	EXPRESSION 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 SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: 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		

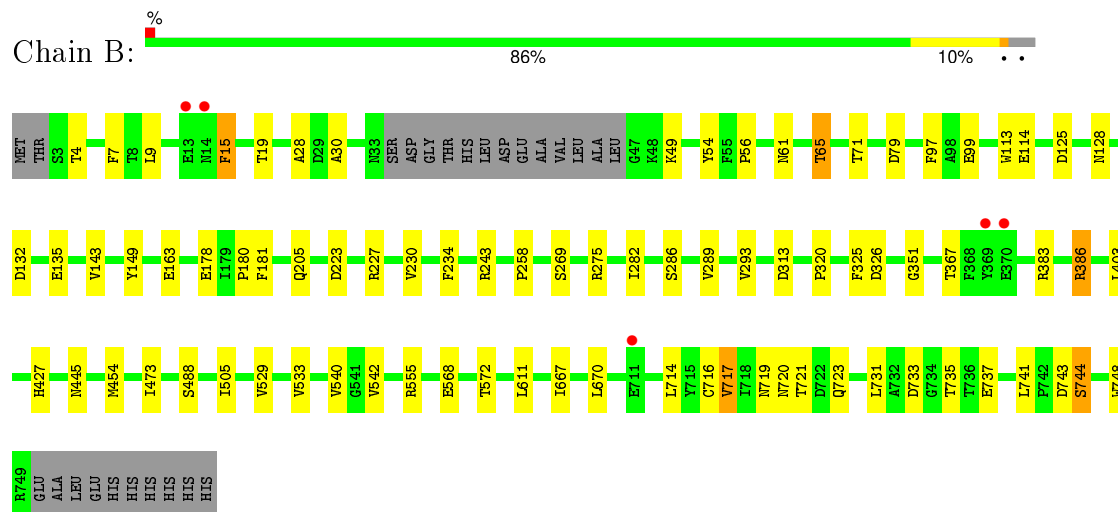
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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.

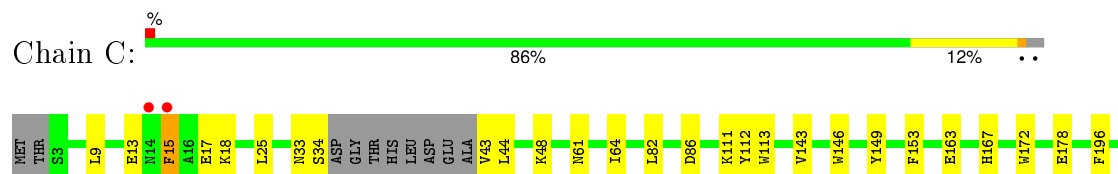
• Molecule 1: Lacto-N-biose phosphorylase



• Molecule 1: Lacto-N-biose phosphorylase



• Molecule 1: Lacto-N-biose phosphorylase



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 36.06 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.6 (36.09-2.60) 87.1 (36.06-2.60)	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 0.184 , 0.250	Depositor DCC
R_{free} test set	4869 reflections (5.25%)	DCC
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 , 34.2	EDS
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 97540 reflections	Xtriage
F_o, F_c correlation	0.93	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, 0.375 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: 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	0.65	0/6109	0.80	11/8321 (0.1%)
1	B	0.62	0/6019	0.77	3/8198 (0.0%)
1	C	0.61	0/6095	0.75	4/8302 (0.0%)
1	D	0.59	0/6041	0.75	2/8228 (0.0%)
All	All	0.62	0/24264	0.77	20/33049 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	ASP	CB-CG-OD1	7.99	125.49	118.30
1	A	79	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	A	79	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	534	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	D	275	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	326	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	344	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	C	247	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	339	ASP	CB-CG-OD1	5.84	123.55	118.30
1	C	485	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	275	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	555	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	A	646	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	591	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	189	ARG	NE-CZ-NH2	5.45	123.02	120.30
1	A	534	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	275	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	611	LEU	CA-CB-CG	5.16	127.17	115.30
1	C	283	ASP	CB-CG-OD1	5.14	122.93	118.30
1	C	611	LEU	CA-CB-CG	5.05	126.91	115.30

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	41	0
1	B	5851	0	5540	42	0
1	C	5926	0	5616	47	0
1	D	5873	0	5562	38	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
2	C	15	0	15	0	0
2	D	15	0	15	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	22405	166	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 (166) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:115:VAL:HG22	1:D:151:VAL:HG22	1.90	0.54
1:B:143:VAL:HB	1:B:149:TYR:CZ	2.43	0.54
1:B:473:ILE:HD11	1:B:542:VAL:HG11	1.90	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:B:143:VAL:HB	1:B:149:TYR:OH	2.09	0.53
1:D:568:GLU:OE1	1:D:572:THR:OG1	2.24	0.53
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:D:271:TRP:CZ2	1:D:467:THR:HG22	2.46	0.50
1:C:575:VAL:O	1:C:577:LYS:HE3	2.11	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:C:544:GLU:OE1	1:C:567:GLU:OE1	2.29	0.50
1:B:529:VAL:O	1:B:533:VAL:HG23	2.11	0.50
1:C:521:THR:HG22	1:C:551:PHE:CD2	2.47	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:D:663:ARG:NH2	3:D:937:HOH:O	2.42	0.49
1:C:441:VAL:HG21	1:C:684:LEU:HD13	1.95	0.49
1:A:33:ASN:HD22	1:A:52:ASN:CG	2.16	0.49
1:B:719:ASN:ND2	1:B:723:GLN:O	2.35	0.49
1:D:673:SER:O	1:D:674:ALA:C	2.51	0.48
1:C:44:LEU:HD11	1:C:205:GLN:HB2	1.94	0.48
1:C:542:VAL:HA	1:C:667:ILE:O	2.13	0.48
1:A:358:ARG:C	1:A:358:ARG:HD2	2.33	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:445:ASN:O	1:A:488:SER:HA	2.13	0.48
1:D:107:ALA:O	1:D:108:ASP:C	2.52	0.48
1:B:4:THR:HG23	1:B:4:THR:O	2.14	0.47
1:C:143:VAL:HB	1:C:149:TYR:CZ	2.49	0.47
1:B:733:ASP:OD1	1:B:735:THR:HG23	2.14	0.47
1:A:520:TRP:CE2	1:A:546:SER:HA	2.49	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:481:ARG:NH1	1:D:696:ALA:O	2.48	0.47
1:D:140:VAL:HG12	1:D:143:VAL:CG1	2.45	0.47
1:B:383:ARG:HH11	1:B:744:SER:HB3	1.79	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:272:ARG:O	1:C:513:ALA:HB2	2.15	0.47
1:C:15:PHE:CE2	1:C:18:LYS:HB2	2.50	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: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:C:526:VAL:HG12	1:C:530:ARG:HD2	1.98	0.45
1:B:227:ARG:HD3	3:B:1110:HOH:O	2.16	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
1:D:409:PHE:O	1:D:413:VAL:HG23	2.17	0.45
1:B:716:CYS:HB3	1:B:748:TRP:CE3	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LEU:HB2	1:A:482:VAL:HG12	1.97	0.45
1:C:389:ILE:HD11	1:C:394:ILE:HD11	1.99	0.44
1:B:505:ILE:HG12	1:B:540:VAL:HB	1.99	0.44
1:D:542:VAL:HA	1:D:667:ILE:O	2.17	0.44
1:C:236:TYR:CE2	1:C:282:ILE:HD12	2.52	0.44
1:A:574:SER:O	1:B:230:VAL:HA	2.17	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: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:B:383:ARG:HD2	1:B:720:ASN:C	2.38	0.44
1:B:386:ARG:NH1	1:B:744:SER:O	2.51	0.44
1:A:184:TYR:HA	1:A:288:PHE:CZ	2.53	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:C:281:TRP:O	1:C:282:ILE:C	2.56	0.43
1:D:566:ASP:O	1:D:635:THR:HA	2.19	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:A:742:PRO:O	1:A:743:ASP:C	2.56	0.43
1:D:714:LEU:HD23	1:D:749:ARG:O	2.18	0.43
1:C:555:ARG:HD3	1:C:560:ALA:HB3	1.99	0.43
1:B:326:ASP:HB3	1:B:351:GLY:HA2	1.99	0.43
1:C:364:PHE:CG	1:C:365:PRO:HD2	2.53	0.43
1:D:19:THR:O	1:D:20:LYS:C	2.57	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:C:452:SER:O	1:C:454:MET:HG3	2.19	0.43
1:A:665:VAL:HG21	1:A:683:VAL:HG13	2.00	0.43
1:A:78:THR:HG23	1:A:151:VAL:O	2.19	0.43
1:C:15:PHE:CE2	1:C:18:LYS:CB	3.02	0.42
1:B:205:GLN:CD	1:B:205:GLN:H	2.22	0.42
1:D:191:PHE:O	1:D:195:THR:OG1	2.36	0.42
1:B:97:PHE:HB2	1:B:223:ASP:O	2.20	0.42
1:B:71:THR:HG22	1:B:180:PRO:O	2.19	0.42
1:C:282:ILE:O	1:C:286:SER:HB2	2.19	0.42
1:B:163:GLU:HG3	1:B:178:GLU:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:TYR:O	1:B:56:PRO:HD3	2.20	0.42
1:A:680:LEU:O	1:A:684:LEU:HG	2.19	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:D:229:LYS:HG2	1:D:230:VAL:HG23	2.00	0.42
1:B:234:PHE:CE1	1:B:454:MET:HB3	2.54	0.42
1:D:448:GLY:HA3	3:D:913:HOH:O	2.20	0.42
1:C:608:ARG:HD2	3:C:1002:HOH:O	2.20	0.42
1:C:113:TRP:CE2	1:C:153:PHE:HB2	2.55	0.42
1:B:445:ASN:O	1:B:488:SER:HA	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:D:522:ASN:C	1:D:522:ASN:OD1	2.57	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:C:196:PHE:CE2	1:C:200:LEU:HD11	2.56	0.41
1:A:369:TYR:CZ	1:A:372:ASN:HB2	2.56	0.41
1:A:43:VAL:HA	1:A:46:LEU:HD12	2.03	0.41
1:B:113:TRP:N	1:B:113:TRP:CD1	2.87	0.41
1:D:680:LEU:O	1:D:684:LEU:HG	2.21	0.41
1:D:608:ARG:HD2	3:D:952:HOH:O	2.21	0.41
1:C:539:PHE:O	1:C:664:GLY:HA2	2.20	0.41
1:B:61:ASN:O	1:B:65:THR:OG1	2.17	0.41
1:B:234:PHE:CZ	1:B:454:MET:HB3	2.56	0.40
1:A:368:PHE:CE1	1:A:406:ALA:HA	2.56	0.40
1:D:592:VAL:O	1:D:593:PRO:C	2.58	0.40
1:C:521:THR:HG22	1:C:551:PHE:CG	2.55	0.40
1:B:97:PHE:CZ	1:B:99:GLU:HB2	2.56	0.40
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:344:ARG:O	1:C:345:MET:C	2.60	0.40

There are no symmetry-related clashes.

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	742/759 (98%)	705 (95%)	35 (5%)	2 (0%)	46	72
1	B	730/759 (96%)	689 (94%)	37 (5%)	4 (0%)	34	60
1	C	740/759 (98%)	697 (94%)	41 (6%)	2 (0%)	46	72
1	D	733/759 (97%)	688 (94%)	45 (6%)	0	100	100
All	All	2945/3036 (97%)	2779 (94%)	158 (5%)	8 (0%)	46	72

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%)	614 (99%)	8 (1%)	76	91
1	B	613/634 (97%)	599 (98%)	14 (2%)	58	83
1	C	621/634 (98%)	607 (98%)	14 (2%)	58	83
1	D	615/634 (97%)	599 (97%)	16 (3%)	54	80
All	All	2471/2536 (97%)	2419 (98%)	52 (2%)	61	85

All (52) 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	358	ARG
1	A	555	ARG
1	A	611	LEU
1	A	752	LEU
1	B	15	PHE
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	670	LEU
1	B	714	LEU
1	B	717	VAL
1	B	721	THR
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	226	ARG
1	C	353	LYS
1	C	364	PHE
1	C	367	THR
1	C	405	LEU
1	C	430	THR
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	141	SER
1	D	181	PHE
1	D	195	THR
1	D	205	GLN

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Mol	Chain	Res	Type
1	D	322	LYS
1	D	358	ARG
1	D	414	ASP
1	D	555	ARG
1	D	611	LEU
1	D	663	ARG
1	D	711	GLU
1	D	726	LYS
1	D	731	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	33	ASN
1	B	177	HIS
1	C	52	ASN
1	D	128	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	17,21,21	0.87	1 (5%)
2	NDG	B	801	-	15,15,15	0.51	0	17,21,21	0.81	1 (5%)
2	NDG	C	801	-	15,15,15	0.67	0	17,21,21	1.48	1 (5%)
2	NDG	D	801	-	15,15,15	0.48	0	17,21,21	0.95	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	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	C	801	-	-	0/6/26/26	0/1/1/1
2	NDG	D	801	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	NDG	C4-C3-C2	-4.71	103.90	110.43
2	A	4001	NDG	C4-C3-C2	-2.11	107.51	110.43
2	B	801	NDG	C3-C2-N2	2.01	114.83	110.66

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%)	-0.70	1 (0%) 95 95	11, 23, 42, 84	0
1	B	734/759 (96%)	-0.58	5 (0%) 89 87	12, 25, 58, 80	0
1	C	744/759 (98%)	-0.59	6 (0%) 87 85	15, 29, 52, 85	0
1	D	737/759 (97%)	-0.49	4 (0%) 91 90	17, 30, 66, 91	0
All	All	2961/3036 (97%)	-0.59	16 (0%) 91 90	11, 27, 57, 91	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	GLU	3.3
1	D	13	GLU	3.2
1	A	754	HIS	2.9
1	B	14	ASN	2.9
1	C	754	HIS	2.8
1	D	14	ASN	2.7
1	B	369	TYR	2.6
1	C	711	GLU	2.6
1	B	370	GLU	2.6
1	C	302	ALA	2.5
1	C	371	GLY	2.4
1	C	15	PHE	2.4
1	B	711	GLU	2.3
1	C	14	ASN	2.3
1	D	17	GLU	2.3
1	D	20	LYS	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 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, 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(\AA^2)	Q<0.9
2	NDG	A	4001	15/15	0.97	0.14	-0.27	19,21,23,27	0
2	NDG	C	801	15/15	0.97	0.14	-0.40	25,26,28,29	0
2	NDG	B	801	15/15	0.96	0.11	-1.00	19,22,23,25	0
2	NDG	D	801	15/15	0.96	0.10	-1.72	26,27,31,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.