



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:16 PM UTC

PDB ID : 4DRF / pdb_00004drf
Title : Crystal Structure of Bacterial Pnkp-C/Hen1-N Heterodimer
Authors : Huang, R.H.; Wang, P.
Deposited on : 2012-02-17
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

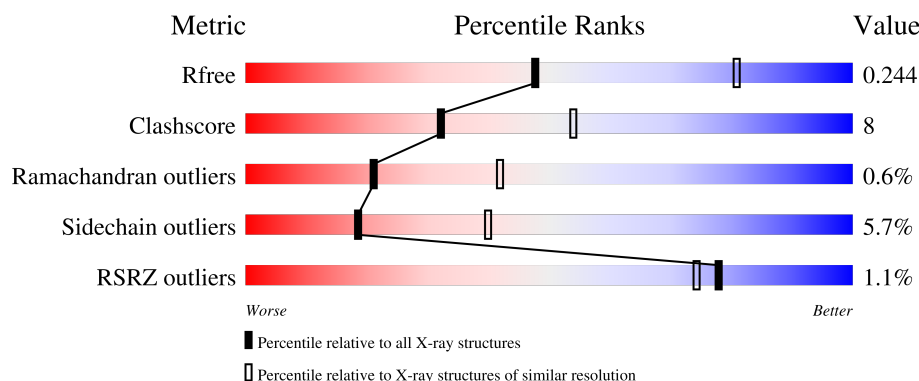
1 Overall quality at a glance

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	427	% 76% 18% ..
1	C	427	% 77% 17% ..
2	B	230	% 64% 22% . 10%
2	D	230	% 63% 22% .. 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10046 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 Metallophosphoesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3276	2076	570	606	24			
1	C	408	Total	C	N	O	S	0	0	0
			3276	2076	570	606	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	444	MET	-	initiating methionine	UNP A3DJ38
C	444	MET	-	initiating methionine	UNP A3DJ38

- Molecule 2 is a protein called Methyltransferase type 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	206	Total	C	N	O	S	0	0	0
			1667	1085	269	304	9			
2	D	206	Total	C	N	O	S	0	0	0
			1667	1085	269	304	9			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

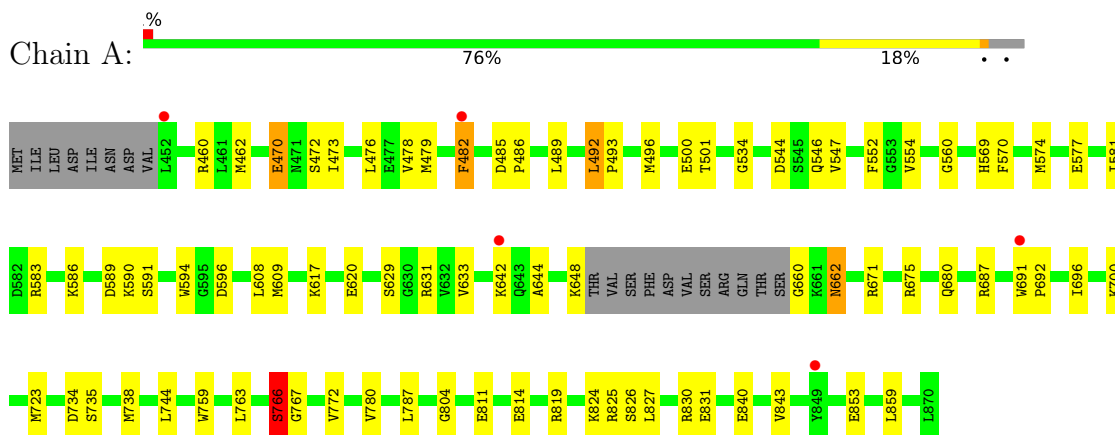
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	B	28	Total	O	0	0
			28	28		
4	C	52	Total	O	0	0
			52	52		
4	D	20	Total	O	0	0
			20	20		

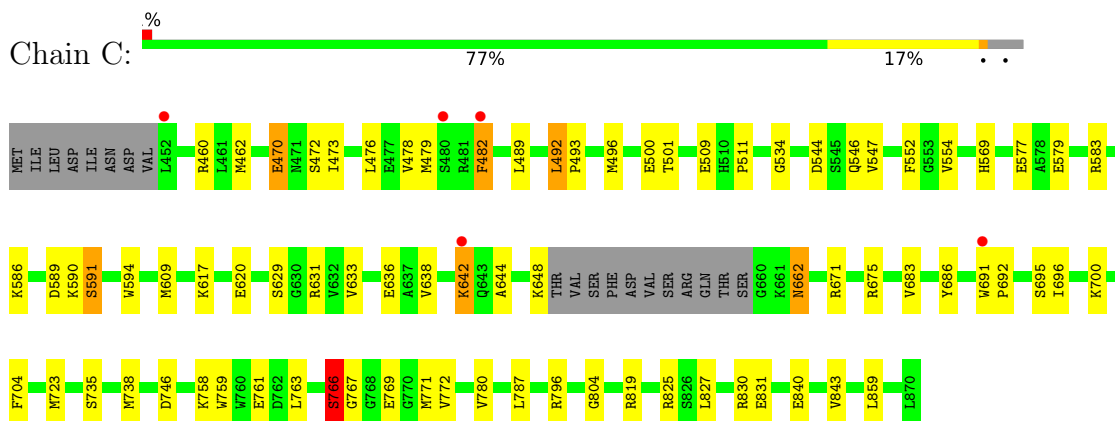
3 Residue-property plots [i](#)

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.

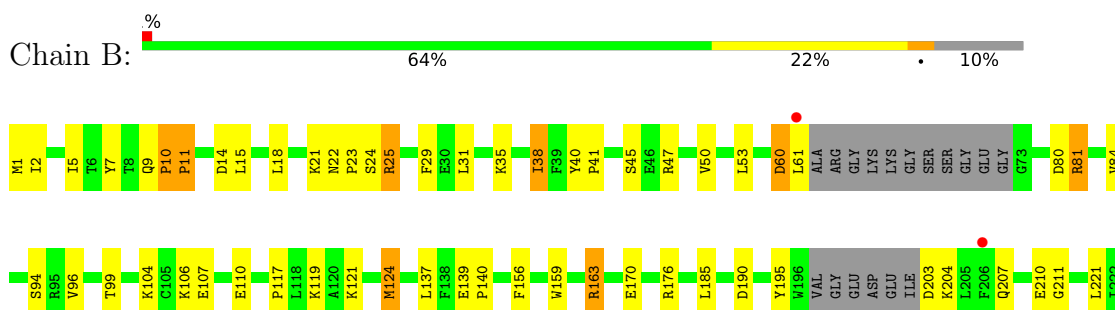
- Molecule 1: Metallophosphoesterase



- Molecule 1: Metallophosphoesterase



- Molecule 2: Methyltransferase type 12



T223
GLY
ARG
TYR
LEU
ILE
ARG
LYS

• Molecule 2: Methyltransferase type 12



M1	I2	I5	T6	Y7	T8	Q9	P10	P11	D14	L15	L18	H20	K21	N22	P23	S24	R25	F29	F30	L31	K35	I38	F39	Y40	P41	R47	V50	L53	D60	L61	ALA	ARG	GLY	LYS	LYS	GLY	SER	SER	GLY	GLU	GLY	G73	Y77	R81	R95
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V96	T99	A100	M101	K104	C105	K106	E107	E110	K119	A120	K121	I122	M123	M124	I133	L137	F138	E139	P140	K144	W159	R163	Y164	L169	E170	R176	N180	L185	D190	Y195	W196	VAL	GLY	GLU	ASP	GLU	ILE	D203	K204	L205	F206	Q207	L221
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T222
T223
GLY
ARG
TYR
LEU
ILE
ARG
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.67Å 59.71Å 101.54Å 81.27° 87.67° 88.39°	Depositor
Resolution (Å)	42.40 – 2.60 42.40 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.2 (42.40-2.60) 96.5 (42.40-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.79 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.184 , 0.245 0.184 , 0.244	Depositor DCC
R_{free} test set	2011 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10046	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.59% 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: GOL

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	0.60	1/3342 (0.0%)	0.94	5/4506 (0.1%)
1	C	0.60	2/3342 (0.1%)	0.95	6/4506 (0.1%)
2	B	0.60	0/1711	0.97	0/2318
2	D	0.62	0/1711	1.00	5/2318 (0.2%)
All	All	0.61	3/10106 (0.0%)	0.96	16/13648 (0.1%)

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
2	B	0	1
2	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	662	ASN	CG-ND2	-7.01	1.18	1.33
1	C	662	ASN	CG-ND2	-6.43	1.19	1.33
1	C	662	ASN	CG-OD1	-5.26	1.13	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	492	LEU	CA-C-N	10.09	127.02	119.66
1	C	492	LEU	C-N-CA	10.09	127.02	119.66
1	A	492	LEU	CA-C-N	9.67	126.72	119.66
1	A	492	LEU	C-N-CA	9.67	126.72	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	804	GLY	CA-C-N	7.75	128.16	119.32
1	A	804	GLY	C-N-CA	7.75	128.16	119.32
1	C	804	GLY	CA-C-N	7.51	127.89	119.32
1	C	804	GLY	C-N-CA	7.51	127.89	119.32
1	C	766	SER	N-CA-C	6.57	118.10	111.07
2	D	10	PRO	N-CA-C	6.38	118.48	110.70
2	D	110	GLU	N-CA-C	-6.19	106.05	113.97
1	A	766	SER	N-CA-C	5.86	118.14	111.11
2	D	77	TYR	N-CA-C	-5.44	107.65	114.56
2	D	110	GLU	CA-CB-CG	-5.34	103.41	114.10
2	D	11	PRO	N-CA-C	-5.13	101.91	112.47
1	C	617	LYS	N-CA-C	-5.06	106.28	112.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	10	PRO	Peptide
2	D	10	PRO	Peptide

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	3276	0	3273	51	0
1	C	3276	0	3273	47	0
2	B	1667	0	1667	36	0
2	D	1667	0	1667	40	0
3	B	6	0	8	2	0
4	A	54	0	0	13	0
4	B	28	0	0	4	0
4	C	52	0	0	10	0
4	D	20	0	0	3	0
All	All	10046	0	9888	158	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 8.

All (158) 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:761:GLU:OE1	4:C:921:HOH:O	1.85	0.94
2:B:117:PRO:O	4:B:424:HOH:O	1.91	0.89
1:C:692:PRO:O	4:C:913:HOH:O	1.88	0.88
1:A:500:GLU:OE1	4:A:937:HOH:O	1.92	0.85
2:B:47:ARG:NH2	4:B:420:HOH:O	2.05	0.83
1:C:509:GLU:O	4:C:910:HOH:O	2.00	0.80
1:A:633:VAL:HB	2:B:1:MET:HG2	1.68	0.76
1:C:633:VAL:HB	2:D:1:MET:HG2	1.67	0.76
1:A:660:GLY:N	4:A:941:HOH:O	2.24	0.71
2:B:210:GLU:HA	3:B:301:GOL:H2	1.73	0.71
1:A:591:SER:O	4:A:951:HOH:O	2.07	0.70
1:A:492:LEU:O	4:A:946:HOH:O	2.10	0.69
1:A:824:LYS:NZ	4:A:911:HOH:O	2.01	0.69
1:A:596:ASP:OD2	4:A:951:HOH:O	2.10	0.69
2:D:164:TYR:O	4:D:302:HOH:O	2.10	0.68
1:C:644:ALA:HB2	2:D:41:PRO:HA	1.75	0.67
1:C:769:GLU:OE2	4:C:945:HOH:O	2.13	0.66
1:A:853:GLU:OE2	4:A:932:HOH:O	2.14	0.65
1:C:746:ASP:OD2	4:C:952:HOH:O	2.13	0.65
1:A:617:LYS:NZ	4:A:936:HOH:O	2.29	0.64
2:B:137:LEU:HB3	2:B:185:LEU:HD13	1.78	0.64
1:A:644:ALA:HB2	2:B:41:PRO:HA	1.80	0.63
1:A:814:GLU:OE1	2:D:25:ARG:NH2	2.32	0.62
2:D:137:LEU:HB3	2:D:185:LEU:HD13	1.81	0.62
2:B:1:MET:HE1	4:B:401:HOH:O	2.00	0.62
1:A:629:SER:HA	2:B:124:MET:HE2	1.82	0.61
2:D:21:LYS:NZ	2:D:96:VAL:O	2.33	0.60
1:C:629:SER:HA	2:D:124:MET:HE2	1.84	0.60
1:A:631:ARG:NH2	4:A:903:HOH:O	2.07	0.59
2:D:21:LYS:HG3	2:D:38:ILE:HD12	1.84	0.59
2:B:21:LYS:HG3	2:B:38:ILE:HD12	1.85	0.59
2:B:203:ASP:OD2	4:B:409:HOH:O	2.16	0.59
1:A:482:PHE:N	1:A:482:PHE:CD2	2.70	0.58
1:C:620:GLU:HG2	2:D:159:TRP:CG	2.38	0.58
1:C:695:SER:OG	4:C:930:HOH:O	2.17	0.58
1:A:662:ASN:HD21	2:B:25:ARG:HH21	1.51	0.58
1:C:482:PHE:CD2	1:C:482:PHE:N	2.72	0.57
2:D:163:ARG:HH11	2:D:163:ARG:HG2	1.69	0.57
1:A:620:GLU:HG2	2:B:159:TRP:CG	2.39	0.57
2:B:21:LYS:NZ	2:B:96:VAL:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:PRO:HA	2:D:40:TYR:CD2	2.41	0.56
1:C:723:MET:HA	1:C:723:MET:HE2	1.87	0.56
2:D:22:ASN:OD1	2:D:24:SER:OG	2.20	0.56
2:D:81:ARG:NH2	2:D:190:ASP:OD1	2.39	0.55
2:D:1:MET:HE1	4:D:301:HOH:O	2.06	0.55
2:B:7:TYR:CZ	2:B:9:GLN:HB2	2.41	0.55
1:A:700:LYS:HD2	1:A:738:MET:HE3	1.88	0.55
2:B:23:PRO:HA	2:B:40:TYR:CD2	2.42	0.55
1:A:723:MET:HA	1:A:723:MET:HE2	1.88	0.54
1:C:759:TRP:CH2	1:C:763:LEU:HD11	2.42	0.54
2:D:15:LEU:HA	2:D:18:LEU:HD12	1.90	0.54
2:D:7:TYR:CZ	2:D:9:GLN:HB2	2.42	0.54
2:B:15:LEU:HA	2:B:18:LEU:HD12	1.89	0.53
1:A:734:ASP:O	4:A:933:HOH:O	2.18	0.53
1:A:766:SER:N	1:A:767:GLY:HA2	2.24	0.53
1:C:766:SER:N	1:C:767:GLY:HA2	2.24	0.53
2:B:81:ARG:NH2	2:B:190:ASP:OD1	2.41	0.52
1:C:700:LYS:HD2	1:C:738:MET:HE3	1.90	0.52
2:B:163:ARG:HG2	2:B:163:ARG:HH11	1.75	0.52
1:C:704:PHE:O	4:C:943:HOH:O	2.19	0.51
1:A:569:HIS:ND1	1:A:577:GLU:OE2	2.41	0.50
1:A:589:ASP:OD1	1:A:594:TRP:NE1	2.44	0.50
1:A:470:GLU:HA	1:A:473:ILE:HG12	1.94	0.50
1:A:759:TRP:CH2	1:A:763:LEU:HD11	2.46	0.50
1:C:470:GLU:HA	1:C:473:ILE:HG12	1.93	0.50
1:A:583:ARG:NH1	1:A:696:ILE:HD13	2.27	0.49
1:C:583:ARG:NH1	1:C:696:ILE:HD13	2.26	0.49
1:C:460:ARG:NH1	1:C:840:GLU:OE2	2.45	0.49
1:C:500:GLU:CD	1:C:825:ARG:HH22	2.21	0.49
1:A:780:VAL:HG23	1:A:787:LEU:HB2	1.93	0.49
1:A:460:ARG:NH1	1:A:840:GLU:OE2	2.45	0.49
1:A:827:LEU:O	1:A:831:GLU:HG3	2.12	0.48
1:C:589:ASP:OD1	1:C:594:TRP:NE1	2.46	0.48
1:A:814:GLU:HG2	2:D:25:ARG:NH1	2.29	0.48
2:D:110:GLU:H	2:D:110:GLU:HG2	1.52	0.48
2:B:10:PRO:HA	2:B:45:SER:O	2.14	0.47
1:A:500:GLU:CD	1:A:825:ARG:HH22	2.23	0.47
2:B:11:PRO:HG2	2:B:14:ASP:OD2	2.14	0.47
2:D:47:ARG:NH2	4:D:312:HOH:O	2.46	0.47
2:B:80:ASP:O	2:B:84:VAL:HG13	2.13	0.47
2:D:163:ARG:HG2	2:D:163:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:ASP:OD1	1:C:547:VAL:HG23	2.14	0.47
2:B:1:MET:HE3	2:B:1:MET:HB2	1.53	0.47
1:C:827:LEU:O	1:C:831:GLU:HG3	2.15	0.46
1:C:671:ARG:O	1:C:675:ARG:HG3	2.15	0.46
2:B:22:ASN:OD1	2:B:24:SER:OG	2.20	0.46
1:C:511:PRO:HB3	1:C:771:MET:HE1	1.97	0.46
2:B:221:LEU:O	2:B:221:LEU:HD23	2.16	0.46
1:A:544:ASP:OD1	1:A:547:VAL:HG23	2.16	0.46
2:D:1:MET:HG3	2:D:2:ILE:HG13	1.98	0.46
2:D:81:ARG:HD2	2:D:81:ARG:HA	1.55	0.45
1:A:552:PHE:HB2	1:A:554:VAL:HG23	1.98	0.45
1:A:589:ASP:O	1:A:591:SER:N	2.44	0.45
1:C:620:GLU:HG2	2:D:159:TRP:CD1	2.50	0.45
1:C:780:VAL:HG23	1:C:787:LEU:HB2	1.99	0.45
2:D:11:PRO:HG2	2:D:14:ASP:OD2	2.16	0.45
1:C:589:ASP:O	1:C:591:SER:N	2.42	0.44
1:A:577:GLU:HB2	4:A:908:HOH:O	2.16	0.44
1:C:569:HIS:ND1	1:C:577:GLU:OE2	2.45	0.44
1:C:700:LYS:HE2	1:C:735:SER:O	2.17	0.44
1:C:638:VAL:O	1:C:642:LYS:HB2	2.18	0.44
1:A:560:GLY:HA3	1:A:581:ILE:HG21	1.99	0.44
1:A:691:TRP:HA	1:A:692:PRO:HD3	1.71	0.44
1:C:758:LYS:HD2	4:C:921:HOH:O	2.16	0.44
1:A:570:PHE:CZ	1:A:608:LEU:HD22	2.52	0.43
2:D:29:PHE:O	2:D:35:LYS:HB2	2.18	0.43
2:B:211:GLY:H	3:B:301:GOL:H2	1.83	0.43
1:A:501:THR:HG22	1:A:819:ARG:NE	2.33	0.43
1:A:671:ARG:O	1:A:675:ARG:HG3	2.18	0.43
2:B:139:GLU:N	2:B:140:PRO:HD2	2.33	0.43
1:C:796:ARG:NH1	4:C:931:HOH:O	2.45	0.43
2:D:20:HIS:HD2	2:D:99:THR:HG23	1.84	0.43
2:D:204:LYS:HB2	2:D:207:GLN:OE1	2.19	0.43
1:A:687:ARG:HG2	2:B:156:PHE:HE2	1.84	0.43
1:C:631:ARG:NH2	4:C:902:HOH:O	2.24	0.43
1:A:462:MET:HE1	1:A:830:ARG:HG2	2.01	0.43
1:C:552:PHE:HB2	1:C:554:VAL:HG23	1.99	0.43
2:B:5:ILE:HB	2:B:50:VAL:HG12	2.00	0.43
2:B:9:GLN:HA	2:B:10:PRO:HD3	1.80	0.43
1:C:492:LEU:HA	1:C:493:PRO:HD2	1.84	0.43
2:D:221:LEU:HD23	2:D:221:LEU:O	2.19	0.43
1:A:479:MET:HE1	1:A:489:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:662:ASN:HD21	2:D:25:ARG:HH21	1.67	0.43
1:A:680:GLN:OE1	4:A:953:HOH:O	2.21	0.43
1:C:501:THR:HG22	1:C:819:ARG:NE	2.34	0.43
1:C:636:GLU:HG2	2:D:123:MET:SD	2.59	0.43
2:D:20:HIS:HD2	2:D:99:THR:CG2	2.32	0.43
2:D:5:ILE:HB	2:D:50:VAL:HG12	2.00	0.42
1:C:496:MET:SD	1:C:772:VAL:HG13	2.59	0.42
2:D:9:GLN:HA	2:D:10:PRO:HD3	1.80	0.42
1:A:700:LYS:HE2	1:A:735:SER:O	2.19	0.42
1:C:691:TRP:HA	1:C:692:PRO:HD3	1.71	0.42
1:A:496:MET:SD	1:A:772:VAL:HG13	2.60	0.42
1:A:534:GLY:HA3	1:A:609:MET:HG3	2.00	0.42
2:B:81:ARG:HA	2:B:81:ARG:HD2	1.57	0.42
2:D:119:LYS:HG2	2:D:170:GLU:HG3	2.01	0.42
1:A:574:MET:HG3	4:A:954:HOH:O	2.19	0.42
1:C:683:VAL:HA	1:C:686:TYR:CE2	2.55	0.42
1:A:620:GLU:HG2	2:B:159:TRP:CD1	2.53	0.42
1:C:579:GLU:HG2	1:C:696:ILE:HD12	2.02	0.42
2:D:119:LYS:HA	2:D:169:LEU:O	2.20	0.41
2:D:139:GLU:N	2:D:140:PRO:HD2	2.34	0.41
2:B:163:ARG:HG2	2:B:163:ARG:NH1	2.34	0.41
2:B:204:LYS:HB2	2:B:207:GLN:OE1	2.20	0.41
1:C:859:LEU:HD23	1:C:859:LEU:HA	1.81	0.41
2:D:20:HIS:CD2	2:D:99:THR:HG23	2.56	0.41
1:A:492:LEU:HA	1:A:493:PRO:HD2	1.84	0.41
1:C:462:MET:HE1	1:C:830:ARG:HG2	2.03	0.41
2:B:29:PHE:O	2:B:35:LYS:HB2	2.21	0.41
2:B:119:LYS:HG2	2:B:170:GLU:HG3	2.03	0.41
2:D:2:ILE:HG12	2:D:53:LEU:CD1	2.50	0.41
2:D:101:MET:HB3	2:D:180:ASN:HD21	1.85	0.41
1:A:859:LEU:HD23	1:A:859:LEU:HA	1.81	0.41
2:B:2:ILE:HG12	2:B:53:LEU:CD1	2.51	0.41
1:C:534:GLY:HA3	1:C:609:MET:HG3	2.01	0.41
1:A:485:ASP:HA	1:A:486:PRO:HD3	1.94	0.41
2:D:133:ILE:HD12	2:D:133:ILE:HA	1.81	0.41
1:C:479:MET:HE1	1:C:489:LEU:HD12	2.03	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	404/427 (95%)	394 (98%)	9 (2%)	1 (0%)	43	66
1	C	404/427 (95%)	394 (98%)	8 (2%)	2 (0%)	24	46
2	B	200/230 (87%)	185 (92%)	13 (6%)	2 (1%)	12	28
2	D	200/230 (87%)	186 (93%)	12 (6%)	2 (1%)	12	28
All	All	1208/1314 (92%)	1159 (96%)	42 (4%)	7 (1%)	21	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	590	LYS
1	C	590	LYS
2	D	11	PRO
2	D	60	ASP
2	B	60	ASP
2	B	11	PRO
1	C	591	SER

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	356/375 (95%)	342 (96%)	14 (4%)	28	55
1	C	356/375 (95%)	345 (97%)	11 (3%)	35	63
2	B	184/201 (92%)	166 (90%)	18 (10%)	7	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	184/201 (92%)	165 (90%)	19 (10%)	7	15
All	All	1080/1152 (94%)	1018 (94%)	62 (6%)	18	40

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	470	GLU
1	A	472	SER
1	A	476	LEU
1	A	478	VAL
1	A	482	PHE
1	A	546	GLN
1	A	586	LYS
1	A	642	LYS
1	A	648	LYS
1	A	744	LEU
1	A	766	SER
1	A	811	GLU
1	A	826	SER
1	A	843	VAL
2	B	25	ARG
2	B	31	LEU
2	B	38	ILE
2	B	60	ASP
2	B	61	LEU
2	B	81	ARG
2	B	94	SER
2	B	99	THR
2	B	104	LYS
2	B	106	LYS
2	B	107	GLU
2	B	110	GLU
2	B	121	LYS
2	B	124	MET
2	B	163	ARG
2	B	176	ARG
2	B	195	TYR
2	B	223	THR
1	C	470	GLU
1	C	472	SER
1	C	476	LEU
1	C	478	VAL

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Mol	Chain	Res	Type
1	C	482	PHE
1	C	546	GLN
1	C	586	LYS
1	C	642	LYS
1	C	648	LYS
1	C	766	SER
1	C	843	VAL
2	D	1	MET
2	D	31	LEU
2	D	38	ILE
2	D	60	ASP
2	D	61	LEU
2	D	81	ARG
2	D	95	ARG
2	D	99	THR
2	D	104	LYS
2	D	106	LYS
2	D	107	GLU
2	D	110	GLU
2	D	121	LYS
2	D	124	MET
2	D	144	LYS
2	D	163	ARG
2	D	176	ARG
2	D	195	TYR
2	D	223	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	546	GLN
1	A	666	ASN
2	B	180	ASN
2	B	194	HIS
2	B	208	HIS
1	C	546	GLN
1	C	666	ASN
2	D	20	HIS
2	D	180	ASN
2	D	194	HIS
2	D	208	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\# Z > 2$
3	GOL	B	301	-	5,5,5	0.44	0	5,5,5	0.56	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
3	GOL	B	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	GOL	O1-C1-C2-C3
3	B	301	GOL	C1-C2-C3-O3
3	B	301	GOL	O1-C1-C2-O2
3	B	301	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	GOL	2	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](#)

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	408/427 (95%)	-0.36	5 (1%) 76 73	21, 43, 75, 141	0
1	C	408/427 (95%)	-0.35	5 (1%) 76 73	23, 43, 75, 141	0
2	B	206/230 (89%)	-0.12	2 (0%) 79 76	25, 46, 89, 137	0
2	D	206/230 (89%)	-0.12	2 (0%) 79 76	26, 48, 89, 137	0
All	All	1228/1314 (93%)	-0.28	14 (1%) 78 74	21, 44, 79, 141	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	452	LEU	5.0
1	A	452	LEU	3.9
2	D	61	LEU	3.1
1	C	482	PHE	3.1
1	A	482	PHE	2.8
2	B	61	LEU	2.7
2	D	206	PHE	2.4
1	C	691	TRP	2.3
2	B	206	PHE	2.2
1	C	642	LYS	2.1
1	C	480	SER	2.0
1	A	642	LYS	2.0
1	A	691	TRP	2.0
1	A	849	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
3	GOL	B	301	6/6	0.83	0.12	48,62,80,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.