



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:56 PM UTC

PDB ID : 2PHL / pdb_00002phl
Title : THE STRUCTURE OF PHASEOLIN AT 2.2 ANGSTROMS RESOLUTION:
IMPLICATIONS FOR A COMMON VICILIN(SLASH)LEGUMIN STRUC-
TURE AND THE GENETIC ENGINEERING OF SEED STORAGE PRO-
TEINS
Authors : Lawrence, M.C.; Izard, T.; Beuchat, M.; Blagrove, R.J.; Colman, P.M.
Deposited on : 1994-07-07
Resolution : 2.20 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

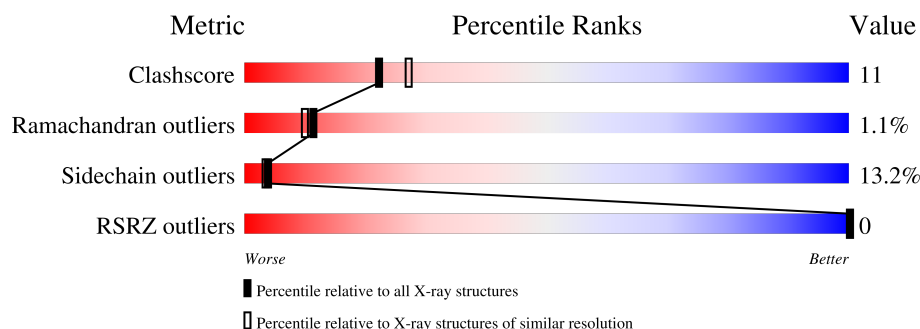
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	397	
1	B	397	
1	C	397	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	902	X	-	-	-

2 Entry composition [i](#)

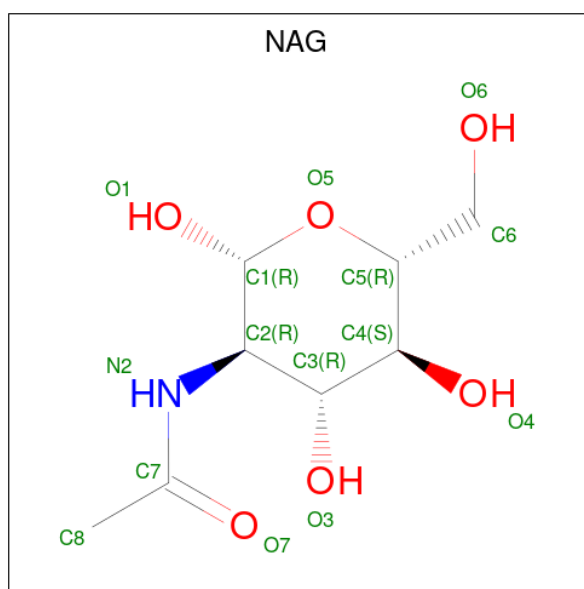
There are 4 unique types of molecules in this entry. The entry contains 8746 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHASEOLIN.

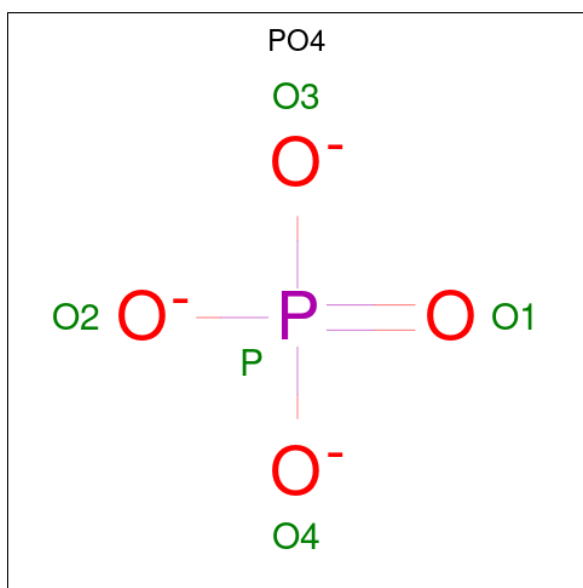
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2870	1819	484	564	3			
1	B	360	Total	C	N	O	S	0	0	0
			2870	1819	484	564	3			
1	C	361	Total	C	N	O	S	0	0	0
			2879	1824	486	566	3			

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



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

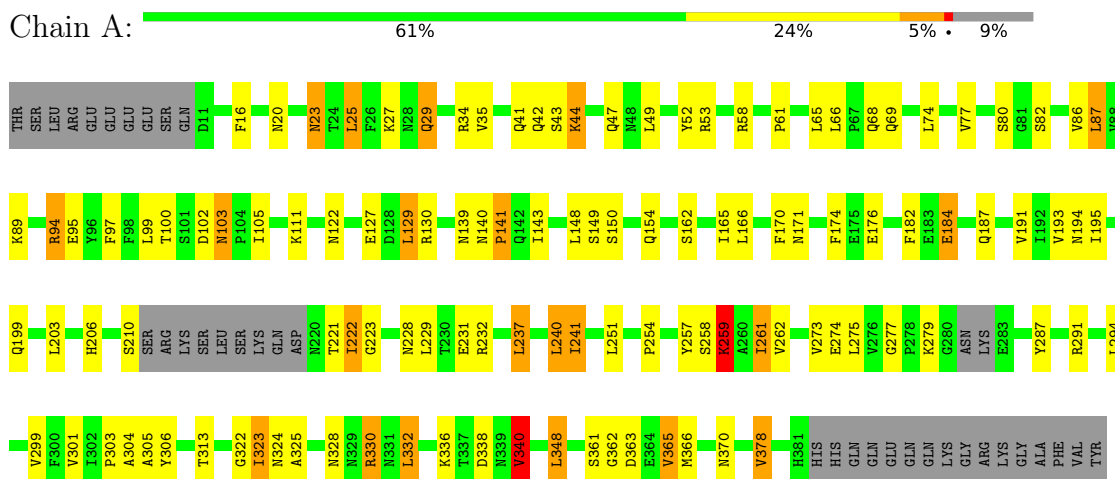
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	24	Total	O	0	0
			24	24		
4	C	22	Total	O	0	0
			22	22		

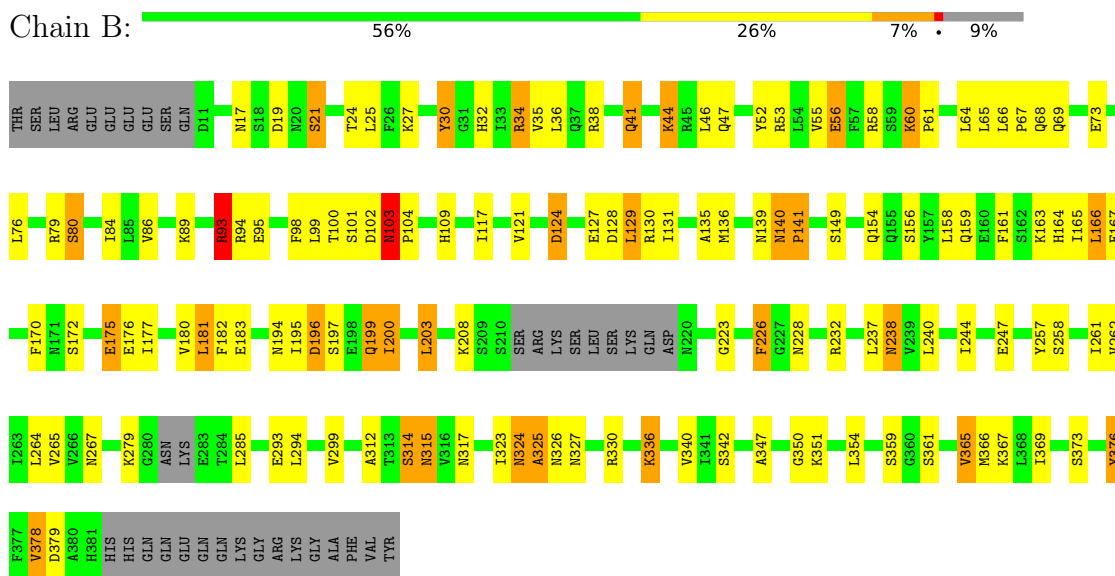
3 Residue-property plots

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: PHASEOLIN

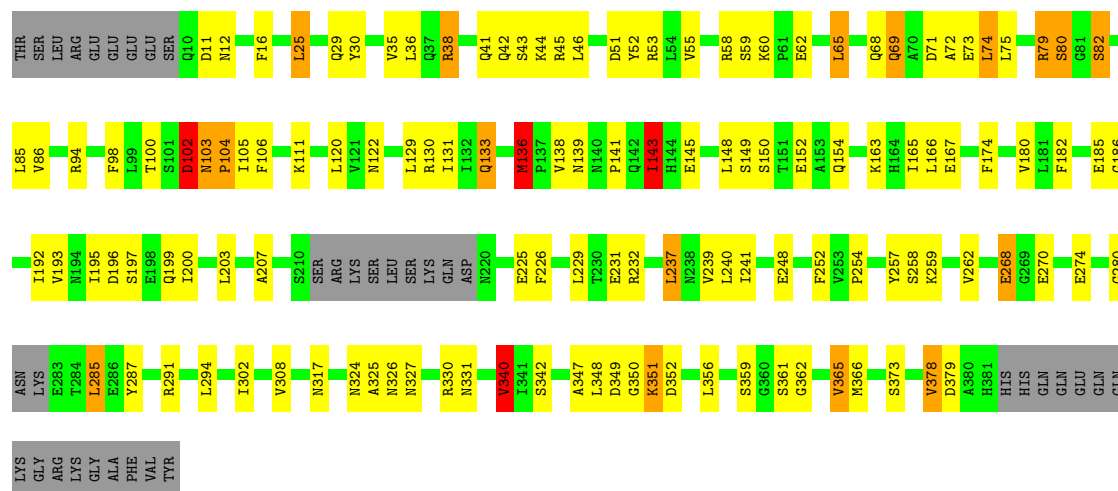


• Molecule 1: PHASEOLIN



• Molecule 1: PHASEOLIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.81Å 114.08Å 137.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20 6.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.20) 49.0 (6.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.178 , (Not available) 0.173 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 107.1	EDS
L-test for twinning ¹	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8746	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: PO4, NAG

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	0.67	0/2925	1.14	22/3958 (0.6%)
1	B	0.65	1/2925 (0.0%)	1.17	30/3958 (0.8%)
1	C	0.68	1/2934 (0.0%)	1.16	27/3970 (0.7%)
All	All	0.67	2/8784 (0.0%)	1.16	79/11886 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	143	ILE	CA-CB	5.53	1.60	1.54
1	B	93	ARG	CZ-NH1	5.38	1.40	1.32

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	SER	N-CA-C	10.47	123.75	111.71
1	A	102	ASP	N-CA-C	9.40	125.39	113.55
1	C	102	ASP	N-CA-C	8.71	124.53	113.55
1	B	258	SER	N-CA-C	8.51	120.18	111.07
1	A	262	VAL	N-CA-C	8.26	120.17	108.36
1	B	103	ASN	CA-C-N	8.16	130.04	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	ASN	C-N-CA	8.16	130.04	119.84
1	A	139	ASN	N-CA-C	8.12	121.67	111.69
1	B	182	PHE	N-CA-C	8.10	123.34	113.38
1	A	182	PHE	N-CA-C	7.42	123.47	113.97
1	C	139	ASN	N-CA-C	6.93	119.86	111.40
1	C	103	ASN	CA-C-N	6.92	128.49	119.84
1	C	103	ASN	C-N-CA	6.92	128.49	119.84
1	A	258	SER	N-CA-C	6.92	119.41	111.11
1	A	340	VAL	CB-CA-C	-6.66	103.44	111.97
1	B	102	ASP	N-CA-C	6.64	121.12	111.02
1	C	182	PHE	N-CA-C	6.64	121.39	113.28
1	C	258	SER	N-CA-C	6.61	118.48	111.28
1	C	262	VAL	N-CA-C	6.58	117.77	108.36
1	B	325	ALA	N-CA-C	6.52	120.50	112.54
1	A	89	LYS	CA-C-N	6.44	126.20	119.05
1	A	89	LYS	C-N-CA	6.44	126.20	119.05
1	B	262	VAL	N-CA-C	6.39	117.07	107.80
1	B	25	LEU	N-CA-C	-6.29	105.63	113.55
1	C	149	SER	N-CA-C	6.22	118.74	110.53
1	B	226	PHE	N-CA-C	6.20	121.13	113.50
1	A	149	SER	N-CA-C	6.16	118.50	110.43
1	A	141	PRO	N-CA-C	6.14	121.83	113.84
1	B	140	ASN	N-CA-C	-6.14	102.61	108.07
1	C	192	ILE	N-CA-C	-6.08	98.98	107.80
1	C	252	PHE	N-CA-C	-6.08	97.29	107.99
1	C	180	VAL	N-CA-C	6.04	119.51	111.17
1	C	51	ASP	N-CA-C	5.99	119.64	112.93
1	B	66	LEU	CA-C-N	5.96	125.98	119.90
1	B	66	LEU	C-N-CA	5.96	125.98	119.90
1	C	302	ILE	CA-C-N	5.80	125.75	119.78
1	C	302	ILE	C-N-CA	5.80	125.75	119.78
1	A	325	ALA	N-CA-C	5.79	120.47	113.41
1	B	196	ASP	N-CA-C	5.78	118.65	109.24
1	C	340	VAL	CB-CA-C	-5.75	103.25	112.16
1	C	141	PRO	N-CA-C	5.72	121.28	113.84
1	B	101	SER	N-CA-C	5.71	117.51	111.28
1	B	261	ILE	N-CA-C	-5.64	100.46	108.58
1	B	89	LYS	CA-C-N	5.64	125.31	119.56
1	B	89	LYS	C-N-CA	5.64	125.31	119.56
1	B	350	GLY	N-CA-C	5.63	126.52	113.18
1	A	370	ASN	N-CA-C	5.61	120.13	113.28
1	A	277	GLY	CA-C-N	5.61	125.89	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	GLY	C-N-CA	5.61	125.89	119.83
1	A	336	LYS	N-CA-C	5.58	119.26	112.23
1	C	30	TYR	N-CA-C	5.58	120.15	113.23
1	A	42	GLN	N-CA-C	-5.56	105.22	111.28
1	B	30	TYR	N-CA-C	5.54	120.03	113.28
1	B	315	ASN	N-CA-C	-5.52	102.11	110.28
1	B	139	ASN	N-CA-C	5.49	117.07	111.14
1	B	200	ILE	N-CA-C	5.49	120.53	113.07
1	C	136	MET	CA-C-N	5.45	125.39	119.78
1	C	136	MET	C-N-CA	5.45	125.39	119.78
1	C	378	VAL	N-CA-CB	-5.42	103.34	112.44
1	A	222	ILE	N-CA-C	-5.36	100.47	108.46
1	A	259	LYS	N-CA-C	5.36	121.36	114.56
1	C	133	GLN	N-CA-C	5.31	118.09	109.06
1	B	314	SER	N-CA-C	-5.28	101.26	108.38
1	A	77	VAL	N-CA-C	5.27	115.57	107.77
1	C	74	LEU	N-CA-C	5.27	118.08	109.59
1	B	149	SER	N-CA-C	5.27	117.66	110.55
1	C	324	ASN	N-CA-C	-5.25	104.17	111.52
1	B	158	LEU	N-CA-C	-5.24	106.15	112.54
1	B	238	ASN	N-CA-C	-5.22	106.21	112.58
1	C	359	SER	N-CA-C	5.20	116.95	111.28
1	A	127	GLU	N-CA-C	5.16	118.52	110.32
1	B	141	PRO	N-CA-C	5.15	123.07	112.47
1	A	176	GLU	N-CA-C	-5.14	105.57	111.07
1	C	207	ALA	N-CA-C	-5.14	105.37	110.97
1	A	47	GLN	N-CA-C	5.13	117.78	111.82
1	C	285	LEU	N-CA-C	-5.08	106.40	112.59
1	C	325	ALA	N-CA-C	5.05	119.71	113.50
1	B	199	GLN	N-CA-C	5.04	117.16	111.11
1	B	359	SER	N-CA-C	5.01	116.82	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	287	TYR	Sidechain
1	C	287	TYR	Sidechain

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	2870	0	2797	53	0
1	B	2870	0	2797	77	0
1	C	2879	0	2805	61	0
2	A	14	0	13	1	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
4	A	24	0	0	0	0
4	B	24	0	0	1	0
4	C	22	0	0	1	0
All	All	8746	0	8438	181	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 11.

All (181) 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:A:340:VAL:HG11	1:B:117:ILE:HD12	1.63	0.81
1:B:17:ASN:HD21	1:B:19:ASP:HB2	1.50	0.76
1:A:229:LEU:HD23	1:A:330:ARG:HH21	1.51	0.75
1:B:140:ASN:HB2	1:B:141:PRO:HD2	1.70	0.73
1:C:43:SER:HB3	1:C:46:LEU:HD13	1.72	0.70
1:B:257:TYR:CE1	1:B:330:ARG:HG3	2.28	0.69
1:B:17:ASN:ND2	1:B:19:ASP:HB2	2.08	0.69
1:B:361:SER:O	1:B:365:VAL:HG13	1.93	0.69
1:B:41:GLN:HE21	1:B:41:GLN:HA	1.58	0.68
1:A:111:LYS:HE2	1:A:237:LEU:HG	1.76	0.68
1:C:85:LEU:HD13	1:C:120:LEU:HD13	1.77	0.66
1:A:229:LEU:CD2	1:A:330:ARG:HH21	2.09	0.65
1:B:195:ILE:HD13	1:B:200:ILE:HG21	1.79	0.64
1:B:176:GLU:O	1:B:180:VAL:HG23	1.98	0.63
1:C:68:GLN:NE2	1:C:145:GLU:HB3	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LEU:HD21	1:C:241:ILE:HD11	1.79	0.63
1:C:103:ASN:ND2	1:C:105:ILE:HD11	2.13	0.63
1:C:226:PHE:CZ	1:C:379:ASP:HB2	2.36	0.61
1:A:257:TYR:CE1	1:A:330:ARG:HG3	2.35	0.60
1:A:193:VAL:HG11	1:C:356:LEU:HD22	1.84	0.60
1:A:87:LEU:O	1:A:94:ARG:HA	2.02	0.59
1:A:61:PRO:HA	1:A:122:ASN:OD1	2.03	0.59
1:A:361:SER:O	1:A:365:VAL:HG13	2.03	0.59
1:A:223:GLY:HA3	1:A:228:ASN:OD1	2.03	0.59
1:B:80:SER:HB3	1:B:130:ARG:HB2	1.84	0.58
1:A:162:SER:OG	1:A:165:ILE:HD13	2.04	0.58
1:A:362:GLY:O	1:A:366:MET:HB2	2.04	0.58
1:B:21:SER:HB3	1:B:36:LEU:CD1	2.33	0.58
1:C:38:ARG:HB2	1:C:41:GLN:HG2	1.85	0.58
1:B:354:LEU:CD1	1:B:366:MET:HE3	2.34	0.58
1:A:222:ILE:HD12	1:A:330:ARG:HH22	1.69	0.57
1:B:30:TYR:HA	1:B:60:LYS:HG3	1.85	0.57
1:C:103:ASN:HD22	1:C:105:ILE:HD11	1.70	0.57
1:B:44:LYS:HE3	1:B:47:GLN:HE21	1.69	0.57
1:C:36:LEU:O	1:C:53:ARG:NH1	2.38	0.56
1:C:257:TYR:CE1	1:C:330:ARG:HG2	2.40	0.56
1:B:44:LYS:HE3	1:B:47:GLN:NE2	2.19	0.56
1:B:347:ALA:HA	1:C:94:ARG:HD2	1.87	0.56
1:C:361:SER:O	1:C:365:VAL:HG13	2.05	0.56
1:B:161:PHE:HB2	1:B:166:LEU:HD21	1.88	0.56
1:B:100:THR:HG21	1:B:103:ASN:OD1	2.06	0.56
1:B:226:PHE:CE2	1:B:379:ASP:HB2	2.41	0.55
1:B:366:MET:HA	1:B:366:MET:HE2	1.88	0.55
1:A:82:SER:OG	1:A:100:THR:HG22	2.07	0.55
1:C:45:ARG:NH2	1:C:280:GLY:HA2	2.21	0.54
1:C:351:LYS:HB2	1:C:351:LYS:NZ	2.21	0.54
1:C:79:ARG:O	1:C:80:SER:HB3	2.07	0.54
1:A:44:LYS:HB2	1:A:44:LYS:NZ	2.23	0.53
1:A:206:HIS:HD2	1:C:348:LEU:HG	1.73	0.53
1:C:163:LYS:O	1:C:167:GLU:HG3	2.09	0.53
1:C:35:VAL:HG12	1:C:53:ARG:NH1	2.23	0.53
1:C:105:ILE:HG13	1:C:106:PHE:CD1	2.44	0.53
1:A:232:ARG:HB2	1:A:241:ILE:HG12	1.91	0.53
1:A:323:ILE:O	1:A:324:ASN:HB3	2.08	0.53
1:A:194:ASN:HD22	1:A:194:ASN:C	2.18	0.52
1:C:68:GLN:HE22	1:C:145:GLU:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ASN:HD22	1:C:340:VAL:CG1	2.23	0.51
1:B:354:LEU:HD13	1:B:365:VAL:CG2	2.41	0.51
1:B:163:LYS:O	1:B:167:GLU:HG3	2.11	0.51
1:B:196:ASP:HB3	1:B:199:GLN:NE2	2.25	0.51
1:B:30:TYR:CZ	1:B:194:ASN:HB2	2.45	0.51
1:B:61:PRO:HB3	1:B:124:ASP:O	2.11	0.51
1:B:326:ASN:O	1:B:327:ASN:HB2	2.11	0.50
1:A:25:LEU:HD12	1:C:285:LEU:HD21	1.94	0.50
1:B:93:ARG:HH21	1:B:95:GLU:HG3	1.77	0.50
1:A:94:ARG:HD3	1:C:347:ALA:HA	1.92	0.50
1:B:129:LEU:HD22	1:B:131:ILE:HG13	1.94	0.49
1:A:16:PHE:HB2	1:A:299:VAL:HB	1.93	0.49
1:A:103:ASN:ND2	1:A:105:ILE:HG12	2.26	0.49
1:C:274:GLU:HG2	1:C:291:ARG:HG2	1.95	0.49
1:C:231:GLU:C	1:C:232:ARG:HG3	2.38	0.49
1:C:60:LYS:HA	1:C:60:LYS:HE2	1.95	0.49
1:B:135:ALA:C	1:B:136:MET:HG3	2.36	0.49
1:C:58:ARG:NH1	3:C:952:PO4:O2	2.43	0.49
1:B:76:LEU:O	1:B:109:HIS:HA	2.13	0.49
1:C:196:ASP:HB3	1:C:199:GLN:HG3	1.94	0.48
1:B:285:LEU:HD21	1:C:25:LEU:HD13	1.96	0.48
1:B:195:ILE:HD13	1:B:200:ILE:CG2	2.44	0.48
1:C:254:PRO:HA	1:C:308:VAL:O	2.13	0.48
1:C:79:ARG:HG3	1:C:130:ARG:O	2.12	0.48
1:B:366:MET:O	1:B:369:ILE:HG22	2.13	0.48
1:A:194:ASN:HD22	1:A:195:ILE:N	2.12	0.48
1:C:351:LYS:HB2	1:C:351:LYS:HZ3	1.78	0.48
1:B:244:ILE:O	1:B:317:ASN:HA	2.14	0.47
1:C:82:SER:HB3	1:C:98:PHE:CZ	2.49	0.47
1:A:348:LEU:HD13	1:B:203:LEU:HA	1.96	0.47
1:C:62:GLU:HA	1:C:122:ASN:O	2.15	0.47
1:C:35:VAL:HG12	1:C:53:ARG:HH12	1.79	0.47
1:C:362:GLY:O	1:C:366:MET:HB2	2.15	0.47
1:B:240:LEU:HB2	1:B:325:ALA:CB	2.45	0.46
1:B:44:LYS:HD2	1:B:44:LYS:HA	1.42	0.46
1:B:98:PHE:HE1	1:B:100:THR:OG1	1.97	0.46
1:A:87:LEU:HD22	1:A:97:PHE:HE2	1.81	0.46
1:B:35:VAL:HG22	1:B:55:VAL:HG22	1.97	0.46
1:C:38:ARG:CB	1:C:41:GLN:HG2	2.46	0.46
1:B:35:VAL:HG12	1:B:53:ARG:HH12	1.81	0.46
1:A:140:ASN:HB2	1:A:141:PRO:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:GLU:H	1:B:175:GLU:CD	2.23	0.46
1:C:11:ASP:CG	1:C:12:ASN:H	2.22	0.46
1:A:275:LEU:HD11	1:A:306:TYR:HB3	1.98	0.46
1:C:163:LYS:HE2	1:C:174:PHE:CD2	2.51	0.46
1:B:36:LEU:HD22	1:B:299:VAL:HG21	1.98	0.45
1:B:172:SER:HB2	1:B:177:ILE:HG13	1.98	0.45
1:A:27:LYS:HB2	1:A:27:LYS:HE3	1.67	0.45
1:A:80:SER:HB2	1:A:130:ARG:HB2	1.99	0.45
1:C:52:TYR:HE1	1:C:136:MET:HE3	1.82	0.45
1:B:36:LEU:O	1:B:53:ARG:NH1	2.49	0.45
1:B:378:VAL:CG1	1:B:379:ASP:N	2.79	0.45
1:B:156:SER:O	1:B:159:GLN:HB2	2.17	0.45
1:B:58:ARG:NH1	1:B:130:ARG:HD2	2.32	0.45
1:A:58:ARG:HA	1:A:129:LEU:O	2.17	0.45
1:B:265:VAL:HG22	1:B:299:VAL:HG22	1.98	0.45
1:A:184:GLU:O	1:A:187:GLN:HG2	2.17	0.44
1:A:240:LEU:CD2	1:A:322:GLY:HA3	2.47	0.44
1:B:34:ARG:HD3	1:B:56:GLU:OE1	2.17	0.44
1:A:66:LEU:HD12	1:A:191:VAL:HA	2.00	0.44
1:B:177:ILE:O	1:B:181:LEU:HB2	2.17	0.44
1:B:237:LEU:O	1:B:238:ASN:HB3	2.18	0.44
1:C:331:ASN:HD22	1:C:340:VAL:HG11	1.82	0.44
1:A:241:ILE:N	1:A:241:ILE:HD13	2.33	0.44
1:B:53:ARG:HD2	1:B:141:PRO:O	2.17	0.44
1:B:61:PRO:HD3	1:B:128:ASP:OD1	2.18	0.44
1:A:199:GLN:HG3	1:C:352:ASP:OD2	2.17	0.44
1:A:221:THR:HA	1:A:229:LEU:O	2.18	0.44
1:C:71:ASP:O	1:C:138:VAL:HG23	2.17	0.44
1:B:336:LYS:O	1:B:336:LYS:HG2	2.17	0.44
1:C:55:VAL:HB	1:C:133:GLN:HG3	1.99	0.44
1:C:268:GLU:HB2	1:C:317:ASN:OD1	2.17	0.43
1:A:251:LEU:HB3	1:A:378:VAL:HG12	2.00	0.43
1:B:84:ILE:HB	1:B:121:VAL:HB	1.99	0.43
1:B:330:ARG:HD2	1:B:376:TYR:OH	2.18	0.43
1:C:349:ASP:OD1	1:C:349:ASP:N	2.51	0.43
1:A:332:LEU:HB2	1:A:338:ASP:O	2.18	0.43
1:B:238:ASN:HD21	1:B:324:ASN:HA	1.81	0.43
1:A:273:VAL:O	1:A:291:ARG:HA	2.18	0.43
1:B:73:GLU:HB3	1:B:136:MET:HE3	1.99	0.43
1:B:342:SER:HA	1:B:366:MET:HE1	1.99	0.43
1:A:170:PHE:O	1:A:171:ASN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:GLN:HE21	1:C:69:GLN:HB3	1.60	0.43
1:B:161:PHE:HB2	1:B:166:LEU:CD2	2.49	0.43
1:A:206:HIS:CD2	1:C:348:LEU:HG	2.54	0.42
1:B:52:TYR:CE1	1:B:136:MET:HG2	2.54	0.42
1:C:326:ASN:O	1:C:327:ASN:HB2	2.17	0.42
1:A:229:LEU:HD23	1:A:330:ARG:NH2	2.27	0.42
1:A:52:TYR:O	1:A:53:ARG:HD2	2.20	0.42
1:B:354:LEU:HD11	1:B:366:MET:HE3	2.02	0.42
1:C:237:LEU:O	1:C:239:VAL:HG23	2.19	0.42
1:A:301:VAL:O	1:A:303:PRO:HD3	2.19	0.42
1:B:27:LYS:HG3	1:B:32:HIS:HB3	2.01	0.42
1:B:41:GLN:HA	1:B:41:GLN:NE2	2.28	0.42
1:B:166:LEU:HD12	1:B:170:PHE:HE2	1.85	0.42
1:C:16:PHE:CZ	1:C:42:GLN:NE2	2.88	0.42
1:C:120:LEU:HD21	1:C:131:ILE:CD1	2.49	0.42
1:C:72:ALA:CB	1:C:143:ILE:HD13	2.50	0.42
1:B:264:LEU:O	1:B:299:VAL:HA	2.19	0.41
1:A:25:LEU:HD23	1:A:35:VAL:HG23	2.03	0.41
1:A:228:ASN:ND2	2:A:900:NAG:O7	2.53	0.41
1:C:111:LYS:O	1:C:111:LYS:HG3	2.20	0.41
1:B:164:HIS:HA	1:B:167:GLU:HG3	2.01	0.41
1:A:49:LEU:HD11	1:A:261:ILE:HD11	2.02	0.41
1:B:247:GLU:HA	1:B:315:ASN:ND2	2.35	0.41
1:B:366:MET:HE2	1:B:369:ILE:HG21	2.02	0.41
1:B:30:TYR:CE1	1:B:194:ASN:HB2	2.55	0.41
1:B:68:GLN:O	1:B:117:ILE:HA	2.20	0.41
1:B:223:GLY:HA3	1:B:228:ASN:HA	2.03	0.41
1:B:240:LEU:HB2	1:B:325:ALA:HB1	2.01	0.41
1:B:267:ASN:HB2	1:B:317:ASN:OD1	2.20	0.41
1:C:102:ASP:O	1:C:104:PRO:HD3	2.21	0.41
1:B:312:ALA:HB1	1:B:314:SER:O	2.20	0.41
1:B:238:ASN:OD1	1:B:326:ASN:ND2	2.53	0.41
1:C:103:ASN:O	1:C:105:ILE:N	2.53	0.41
1:A:257:TYR:CZ	1:A:330:ARG:HD2	2.56	0.41
1:A:259:LYS:HG3	1:A:328:ASN:HA	2.02	0.41
1:C:365:VAL:CG2	1:C:366:MET:N	2.83	0.41
1:C:259:LYS:HE3	1:C:259:LYS:HB3	1.62	0.41
1:A:23:ASN:O	1:A:34:ARG:HA	2.21	0.40
1:B:41:GLN:HG2	4:B:506:HOH:O	2.20	0.40
1:C:11:ASP:CG	1:C:12:ASN:N	2.80	0.40
1:A:304:ALA:O	1:A:305:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:LEU:HD13	4:C:534:HOH:O	2.22	0.40
1:A:273:VAL:HG12	1:A:294:LEU:HD13	2.03	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	354/397 (89%)	326 (92%)	27 (8%)	1 (0%)	36	42
1	B	354/397 (89%)	323 (91%)	25 (7%)	6 (2%)	7	5
1	C	355/397 (89%)	325 (92%)	25 (7%)	5 (1%)	9	7
All	All	1063/1191 (89%)	974 (92%)	77 (7%)	12 (1%)	11	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	350	GLY
1	A	29	GLN
1	C	80	SER
1	C	104	PRO
1	B	80	SER
1	B	104	PRO
1	C	186	GLY
1	B	197	SER
1	B	279	LYS
1	B	376	TYR
1	B	324	ASN
1	C	200	ILE

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	320/354 (90%)	275 (86%)	45 (14%)	3	3
1	B	320/354 (90%)	280 (88%)	40 (12%)	4	4
1	C	321/354 (91%)	279 (87%)	42 (13%)	4	3
All	All	961/1062 (90%)	834 (87%)	127 (13%)	4	3

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	23	ASN
1	A	25	LEU
1	A	29	GLN
1	A	41	GLN
1	A	43	SER
1	A	44	LYS
1	A	65	LEU
1	A	68	GLN
1	A	69	GLN
1	A	74	LEU
1	A	86	VAL
1	A	87	LEU
1	A	94	ARG
1	A	95	GLU
1	A	99	LEU
1	A	103	ASN
1	A	129	LEU
1	A	143	ILE
1	A	148	LEU
1	A	150	SER
1	A	154	GLN
1	A	166	LEU
1	A	174	PHE
1	A	184	GLU
1	A	203	LEU

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Mol	Chain	Res	Type
1	A	210	SER
1	A	231	GLU
1	A	237	LEU
1	A	240	LEU
1	A	241	ILE
1	A	254	PRO
1	A	259	LYS
1	A	261	ILE
1	A	274	GLU
1	A	279	LYS
1	A	313	THR
1	A	323	ILE
1	A	330	ARG
1	A	332	LEU
1	A	340	VAL
1	A	348	LEU
1	A	363	ASP
1	A	365	VAL
1	A	378	VAL
1	B	24	THR
1	B	34	ARG
1	B	38	ARG
1	B	41	GLN
1	B	44	LYS
1	B	46	LEU
1	B	56	GLU
1	B	60	LYS
1	B	64	LEU
1	B	65	LEU
1	B	67	PRO
1	B	69	GLN
1	B	79	ARG
1	B	86	VAL
1	B	93	ARG
1	B	94	ARG
1	B	99	LEU
1	B	103	ASN
1	B	124	ASP
1	B	127	GLU
1	B	129	LEU
1	B	154	GLN
1	B	165	ILE

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Mol	Chain	Res	Type
1	B	166	LEU
1	B	175	GLU
1	B	181	LEU
1	B	183	GLU
1	B	203	LEU
1	B	208	LYS
1	B	232	ARG
1	B	293	GLU
1	B	294	LEU
1	B	323	ILE
1	B	336	LYS
1	B	340	VAL
1	B	351	LYS
1	B	365	VAL
1	B	367	LYS
1	B	373	SER
1	B	378	VAL
1	C	25	LEU
1	C	29	GLN
1	C	38	ARG
1	C	44	LYS
1	C	59	SER
1	C	65	LEU
1	C	69	GLN
1	C	73	GLU
1	C	74	LEU
1	C	79	ARG
1	C	82	SER
1	C	86	VAL
1	C	100	THR
1	C	102	ASP
1	C	129	LEU
1	C	136	MET
1	C	143	ILE
1	C	148	LEU
1	C	150	SER
1	C	152	GLU
1	C	154	GLN
1	C	165	ILE
1	C	166	LEU
1	C	185	GLU
1	C	193	VAL

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Mol	Chain	Res	Type
1	C	195	ILE
1	C	197	SER
1	C	203	LEU
1	C	225	GLU
1	C	229	LEU
1	C	237	LEU
1	C	240	LEU
1	C	248	GLU
1	C	268	GLU
1	C	270	GLU
1	C	294	LEU
1	C	340	VAL
1	C	342	SER
1	C	351	LYS
1	C	365	VAL
1	C	373	SER
1	C	378	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	68	GLN
1	A	69	GLN
1	A	194	ASN
1	A	199	GLN
1	A	206	HIS
1	A	329	ASN
1	A	331	ASN
1	B	17	ASN
1	B	41	GLN
1	B	47	GLN
1	B	110	GLN
1	B	164	HIS
1	B	187	GLN
1	B	238	ASN
1	B	315	ASN
1	B	326	ASN
1	C	37	GLN
1	C	42	GLN
1	C	68	GLN
1	C	69	GLN

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Mol	Chain	Res	Type
1	C	110	GLN
1	C	122	ASN
1	C	154	GLN
1	C	155	GLN
1	C	159	GLN
1	C	188	GLN
1	C	194	ASN
1	C	326	ASN
1	C	329	ASN
1	C	331	ASN
1	C	381	HIS

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](#)

6 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	$\# Z > 2$
3	PO4	A	950	-	4,4,4	1.34	0	6,6,6	1.10	0
3	PO4	C	952	-	4,4,4	2.16	3 (75%)	6,6,6	1.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	902	1	14,14,15	1.46	3 (21%)	17,19,21	3.45	11 (64%)
2	NAG	A	900	1	14,14,15	1.80	2 (14%)	17,19,21	2.55	5 (29%)
2	NAG	B	901	1	14,14,15	1.09	1 (7%)	17,19,21	1.82	5 (29%)
3	PO4	B	951	-	4,4,4	2.04	2 (50%)	6,6,6	1.33	1 (16%)

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	C	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	900	1	-	1/6/23/26	0/1/1/1
2	NAG	B	901	1	-	1/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	NAG	C1-C2	4.81	1.58	1.52
2	A	900	NAG	C4-C5	-4.02	1.44	1.53
2	C	902	NAG	C4-C5	3.11	1.59	1.53
3	C	952	PO4	P-O2	-2.97	1.46	1.54
3	B	951	PO4	P-O2	-2.86	1.46	1.54
2	C	902	NAG	C4-C3	2.33	1.58	1.52
2	B	901	NAG	C1-C2	2.33	1.55	1.52
3	C	952	PO4	P-O3	-2.27	1.48	1.54
3	B	951	PO4	P-O4	-2.14	1.48	1.54
3	C	952	PO4	P-O4	-2.06	1.48	1.54
2	C	902	NAG	C3-C2	2.06	1.56	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	902	NAG	C1-C2-N2	8.70	124.15	110.43
2	A	900	NAG	C1-C2-N2	7.03	121.51	110.43
2	C	902	NAG	O5-C1-C2	6.50	121.35	111.29
2	C	902	NAG	C6-C5-C4	5.74	127.11	113.02
2	A	900	NAG	C1-O5-C5	5.37	119.38	112.19
2	B	901	NAG	C1-O5-C5	3.94	117.46	112.19
2	C	902	NAG	O5-C5-C4	-3.30	102.79	110.83
2	B	901	NAG	O7-C7-C8	-3.14	116.46	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	NAG	C2-N2-C7	2.89	126.77	122.90
2	B	901	NAG	C8-C7-N2	2.69	120.58	116.12
2	C	902	NAG	O3-C3-C2	2.60	114.80	109.40
2	A	900	NAG	C4-C3-C2	-2.54	107.29	111.02
2	C	902	NAG	C3-C4-C5	-2.52	105.66	110.23
2	C	902	NAG	O7-C7-C8	-2.50	117.60	122.05
2	C	902	NAG	C2-N2-C7	-2.35	119.76	122.90
2	C	902	NAG	C4-C3-C2	-2.26	107.71	111.02
2	B	901	NAG	C4-C3-C2	-2.23	107.74	111.02
2	C	902	NAG	C8-C7-N2	2.21	119.78	116.12
2	A	900	NAG	O5-C5-C6	2.18	111.91	107.66
3	B	951	PO4	O4-P-O1	-2.15	103.34	110.95
2	A	900	NAG	O5-C1-C2	-2.10	108.04	111.29
2	C	902	NAG	O4-C4-C5	2.03	114.31	109.32

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	902	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	NAG	C1-C2-N2-C7
2	B	901	NAG	C3-C2-N2-C7
2	C	902	NAG	C1-C2-N2-C7
2	C	902	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	952	PO4	1	0
2	A	900	NAG	1	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 [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	360/397 (90%)	-0.98	0 100 100	8, 28, 54, 84	0
1	B	360/397 (90%)	-0.90	0 100 100	13, 34, 61, 89	0
1	C	361/397 (90%)	-0.95	0 100 100	12, 29, 57, 80	0
All	All	1081/1191 (90%)	-0.95	0 100 100	8, 30, 58, 89	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	NAG	B	901	14/15	0.79	0.11	71,77,90,94	0
2	NAG	A	900	14/15	0.87	0.10	53,57,64,67	0
2	NAG	C	902	14/15	0.90	0.08	49,63,78,78	0
3	PO4	C	952	5/5	0.98	0.07	57,60,65,65	0
3	PO4	B	951	5/5	0.99	0.05	33,39,43,43	0
3	PO4	A	950	5/5	0.99	0.03	38,39,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.