



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:16 PM GMT

PDB ID : 3WN6
Title : Crystal structure of alpha-amylase AmyI-1 from *Oryza sativa*
Authors : Ochiai, A.; Sugai, H.; Harada, K.; Tanaka, S.; Ishiyama, Y.; Ito, K.; Tanaka, T.; Uchiumi, T.; Taniguchi, M.; Mitsui, T.
Deposited on : 2013-12-05
Resolution : 2.16 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

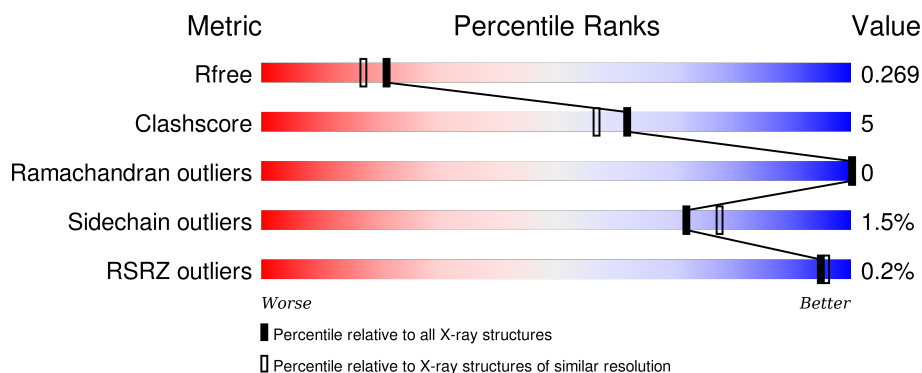
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	404	<div> <div>90%</div> <div>10%</div> </div>
1	B	404	<div> <div>91%</div> <div>9%</div> </div>
1	C	404	<div> <div>91%</div> <div>9%</div> </div>
1	D	404	<div> <div>88%</div> <div>12%</div> </div>

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
3	GOL	A	504	-	-	-	X
3	GOL	B	506	-	-	-	X
4	TAR	C	506	-	-	X	-
4	TAR	C	507	-	-	X	-
5	PEG	A	509	-	-	-	X
5	PEG	D	508	-	-	X	X
5	PEG	D	510	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14765 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 Alpha-amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	3	0
			3222	2058	552	598	14			
1	B	404	Total	C	N	O	S	0	10	0
			3280	2087	564	616	13			
1	C	404	Total	C	N	O	S	0	1	0
			3209	2047	550	599	13			
1	D	404	Total	C	N	O	S	0	6	0
			3249	2071	559	606	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	GLY	ENGINEERED MUTATION	UNP P17654
B	25	MET	GLY	ENGINEERED MUTATION	UNP P17654
C	25	MET	GLY	ENGINEERED MUTATION	UNP P17654
D	25	MET	GLY	ENGINEERED MUTATION	UNP P17654

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

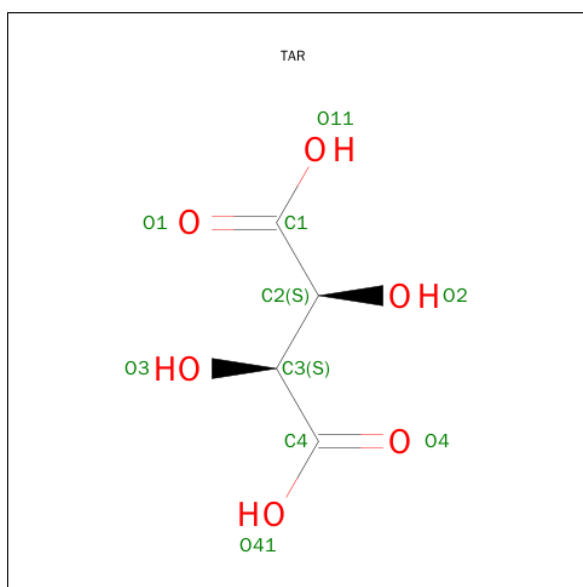
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		
2	A	3	Total	Ca	0	0
			3	3		
2	D	3	Total	Ca	0	0
			3	3		
2	C	3	Total	Ca	0	0
			3	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	4	6		
4	A	1	Total	C	O	0	0
			10	4	6		
4	B	1	Total	C	O	0	0
			10	4	6		
4	C	1	Total	C	O	0	0
			10	4	6		
4	C	1	Total	C	O	0	0
			10	4	6		
4	D	1	Total	C	O	0	0
			10	4	6		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

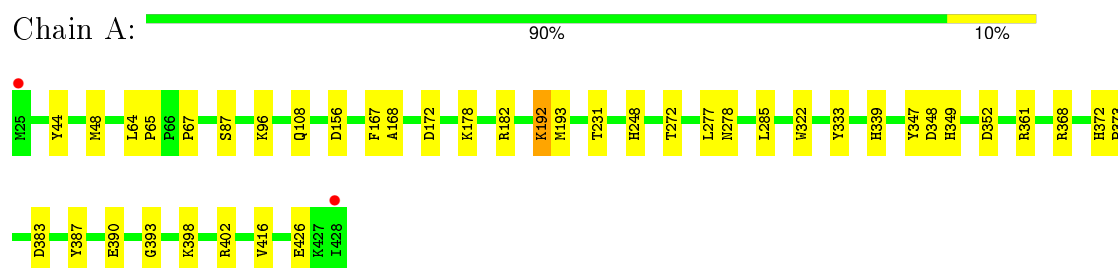
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	405	Total	O	0	0
			405	405		
6	B	420	Total	O	0	0
			420	420		
6	C	393	Total	O	0	0
			393	393		
6	D	412	Total	O	0	0
			412	412		

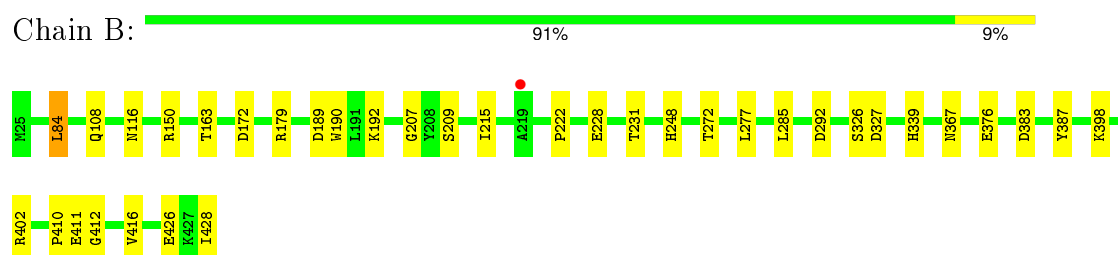
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

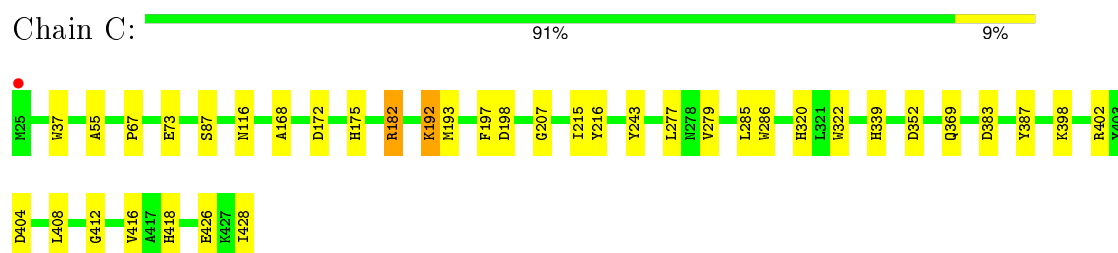
• Molecule 1: Alpha-amylase



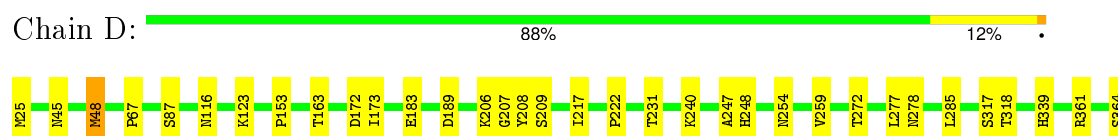
• Molecule 1: Alpha-amylase



• Molecule 1: Alpha-amylase



• Molecule 1: Alpha-amylase



R369	I371 H372 P373	E376	D383	Y387	K398	R402	P410 E411 G412	V416 A417 H418	E426	K427 I428
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.92Å 125.28Å 96.64Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	48.32 – 2.16 48.32 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.32-2.16) 98.7 (48.32-2.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.199 , 0.243 0.226 , 0.269	Depositor DCC
R_{free} test set	4462 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.2	EDS
Estimated twinning fraction	0.551 for H, K, L 0.449 for H, -K, -L 0.288 for h,-k,-l	Xtriage
Reported twinning fraction	0.551 for H, K, L 0.449 for H, -K, -L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	18 of 88953 reflections (0.020%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14765	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.61 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2758e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: GOL, CA, PEG, TAR

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	0/3326	0.73	2/4520 (0.0%)
1	B	0.68	0/3378	0.74	4/4592 (0.1%)
1	C	0.69	0/3307	0.75	2/4496 (0.0%)
1	D	0.69	0/3347	0.74	5/4548 (0.1%)
All	All	0.68	0/13358	0.74	13/18156 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	182	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	A	277	LEU	CA-CB-CG	6.28	129.73	115.30
1	B	277	LEU	CA-CB-CG	6.25	129.67	115.30
1	D	277	LEU	CA-CB-CG	6.24	129.65	115.30
1	C	402	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	D	368	ARG	CB-CA-C	-5.80	98.80	110.40
1	D	402	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	48	MET	CG-SD-CE	-5.55	91.32	100.20
1	D	368	ARG	CG-CD-NE	5.46	123.25	111.80
1	B	189[A]	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	B	189[B]	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	B	402	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	402	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	3222	0	3045	32	0
1	B	3280	0	3081	23	0
1	C	3209	0	3020	31	0
1	D	3249	0	3064	39	2
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	12	0	16	1	0
3	B	18	0	24	2	0
3	C	12	0	16	5	0
3	D	12	0	16	4	0
4	A	20	0	8	1	0
4	B	10	0	4	0	0
4	C	20	0	8	5	0
4	D	10	0	4	1	0
5	A	14	0	20	3	0
5	B	7	0	10	0	0
5	D	28	0	40	5	0
6	A	405	0	0	21	2
6	B	420	0	0	10	0
6	C	393	0	0	19	0
6	D	412	0	0	20	0
All	All	14765	0	12376	137	2

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 5.

All (137) 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:348:ASP:HA	6:A:946:HOH:O	1.41	1.15
1:B:150[B]:ARG:HG2	1:B:150[B]:ARG:HH11	0.96	1.08
1:D:217:ILE:HA	6:D:827:HOH:O	1.62	0.96
1:D:418:HIS:CG	6:D:856:HOH:O	2.18	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150[B]:ARG:CG	1:B:150[B]:ARG:HH11	1.80	0.93
1:B:150[B]:ARG:HG2	1:B:150[B]:ARG:NH1	1.76	0.92
1:D:318:THR:HG23	6:D:875:HOH:O	1.74	0.87
4:C:506:TAR:O4	4:C:507:TAR:O1	1.93	0.86
4:C:506:TAR:H2	6:C:603:HOH:O	1.75	0.85
1:C:73:GLU:HB2	6:C:869:HOH:O	1.81	0.81
3:D:505:GOL:H32	6:D:602:HOH:O	1.82	0.79
1:C:37:TRP:CE2	6:C:869:HOH:O	2.37	0.77
1:D:418:HIS:CD2	6:D:856:HOH:O	2.37	0.75
1:D:418:HIS:CE1	6:D:856:HOH:O	2.41	0.74
1:A:96[B]:LYS:NZ	6:A:809:HOH:O	2.17	0.74
1:A:352:ASP:OD2	6:A:946:HOH:O	2.06	0.73
1:A:361:ARG:HD3	6:A:850:HOH:O	1.87	0.73
1:D:418:HIS:ND1	6:D:856:HOH:O	2.22	0.70
1:C:418:HIS:CE1	3:C:505:GOL:H2	2.26	0.69
1:A:368:ARG:HD3	6:A:848:HOH:O	1.91	0.69
1:C:192:LYS:HD2	1:C:197:PHE:O	1.93	0.69
1:A:178:LYS:NZ	6:A:974:HOH:O	2.26	0.68
1:B:327:ASP:OD2	6:B:755:HOH:O	2.12	0.68
1:A:182:ARG:NH2	6:A:997:HOH:O	2.27	0.66
1:A:156:ASP:OD2	6:A:936:HOH:O	2.13	0.66
3:D:504:GOL:H2	6:D:604:HOH:O	1.97	0.65
1:C:404:ASP:OD2	6:C:716:HOH:O	2.15	0.65
4:C:506:TAR:C4	4:C:507:TAR:O1	2.46	0.64
1:C:55:ALA:O	6:C:671:HOH:O	2.15	0.63
1:C:418:HIS:CD2	6:C:923:HOH:O	2.51	0.63
1:C:37:TRP:NE1	6:C:869:HOH:O	2.32	0.62
1:C:175:HIS:HD2	1:C:216:TYR:OH	1.81	0.62
1:B:410:PRO:HB3	6:B:1015:HOH:O	1.99	0.62
1:A:182:ARG:NE	6:A:955:HOH:O	2.34	0.61
1:C:192:LYS:HG3	1:C:193:MET:N	2.12	0.61
1:C:182:ARG:HB2	6:C:760:HOH:O	2.01	0.60
1:B:179:ARG:HH12	3:B:506:GOL:H31	1.66	0.60
1:D:364[B]:SER:O	1:D:368:ARG:HG3	2.02	0.60
4:D:506:TAR:C1	6:D:948:HOH:O	2.50	0.60
1:D:318:THR:N	6:D:875:HOH:O	2.35	0.60
4:C:506:TAR:O41	4:C:507:TAR:C1	2.50	0.59
1:D:25:MET:HG3	1:D:371:ILE:O	2.01	0.59
3:D:504:GOL:C2	6:D:604:HOH:O	2.49	0.59
1:A:108:GLN:NE2	6:A:719:HOH:O	2.37	0.58
1:C:198:ASP:O	6:C:724:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:HIS:HD2	1:B:272:THR:OG1	1.87	0.57
1:B:192:LYS:HD3	6:B:987:HOH:O	2.06	0.56
1:A:248:HIS:HD2	1:A:272:THR:OG1	1.87	0.56
1:D:248:HIS:HD2	1:D:272:THR:OG1	1.88	0.55
1:C:182:ARG:NE	6:C:873:HOH:O	2.28	0.54
1:C:352:ASP:OD2	6:C:749:HOH:O	2.18	0.54
1:D:317:SER:C	6:D:875:HOH:O	2.46	0.53
4:C:506:TAR:C4	4:C:507:TAR:C1	2.87	0.53
3:D:505:GOL:C3	6:D:602:HOH:O	2.48	0.53
1:D:45:ASN:O	1:D:48:MET:HB2	2.09	0.53
1:A:352:ASP:CG	6:A:946:HOH:O	2.47	0.52
1:B:231:THR:O	1:B:248:HIS:HE1	1.93	0.52
1:C:37:TRP:CZ2	6:C:869:HOH:O	2.61	0.52
1:B:222:PRO:HA	6:B:987:HOH:O	2.09	0.52
1:D:206:LYS:HA	5:D:508:PEG:C1	2.40	0.52
1:D:116:ASN:ND2	1:D:207:GLY:HA3	2.25	0.52
1:C:286:TRP:HB2	1:D:247:ALA:HB2	1.92	0.51
1:D:412:GLY:O	1:D:428:ILE:N	2.35	0.51
1:B:367[B]:ASN:ND2	6:B:802:HOH:O	2.43	0.50
1:B:411:GLU:CD	1:B:411:GLU:H	2.14	0.50
1:C:243:TYR:H	1:D:254:ASN:HD21	1.58	0.50
1:A:231:THR:O	1:A:248:HIS:HE1	1.95	0.49
1:D:231:THR:O	1:D:248:HIS:HE1	1.95	0.49
1:B:163:THR:HB	1:B:209[A]:SER:OG	2.13	0.49
1:D:411:GLU:CD	1:D:411:GLU:H	2.16	0.49
1:C:412:GLY:O	1:C:428:ILE:N	2.35	0.49
1:D:410:PRO:HB3	6:D:959:HOH:O	2.12	0.48
1:A:339:HIS:HE1	1:A:387:TYR:OH	1.95	0.48
1:A:48:MET:CE	6:A:834:HOH:O	2.61	0.48
1:C:416:VAL:HG21	1:C:426:GLU:HG3	1.96	0.48
1:A:193[A]:MET:HG2	6:A:878:HOH:O	2.13	0.48
1:D:416:VAL:HG21	1:D:426:GLU:HG3	1.96	0.48
1:B:339:HIS:HE1	1:B:387:TYR:OH	1.96	0.48
1:A:416:VAL:HG21	1:A:426:GLU:HG3	1.96	0.48
1:B:412:GLY:O	1:B:428:ILE:N	2.34	0.48
1:C:168:ALA:HB1	6:C:802:HOH:O	2.13	0.47
1:D:163:THR:O	5:D:508:PEG:H41	2.15	0.47
1:B:326:SER:N	6:B:716:HOH:O	2.22	0.47
1:B:416:VAL:HG21	1:B:426:GLU:HG3	1.96	0.47
1:D:361:ARG:NH2	6:D:977:HOH:O	2.37	0.47
1:C:243:TYR:H	1:D:254:ASN:ND2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:HIS:HE1	1:D:387:TYR:OH	1.97	0.47
1:A:278:ASN:HB3	5:A:509:PEG:C4	2.44	0.47
1:C:339:HIS:HE1	1:C:387:TYR:OH	1.97	0.47
1:C:116:ASN:ND2	1:C:207:GLY:HA3	2.30	0.47
3:C:504:GOL:C1	6:C:602:HOH:O	2.62	0.47
1:A:347:TYR:HD1	6:A:946:HOH:O	1.98	0.46
1:C:320:HIS:CG	6:C:658:HOH:O	2.67	0.46
1:B:228:GLU:HG3	6:B:635:HOH:O	2.16	0.46
3:B:506:GOL:H2	6:B:771:HOH:O	2.14	0.46
1:A:278:ASN:HB3	5:A:509:PEG:H41	1.98	0.45
1:B:116:ASN:ND2	1:B:207:GLY:HA3	2.31	0.45
1:D:163:THR:HB	1:D:209[B]:SER:OG	2.16	0.45
3:C:504:GOL:H11	6:C:602:HOH:O	2.16	0.45
4:A:506:TAR:O11	4:A:506:TAR:C4	2.65	0.45
1:A:333:TYR:OH	1:A:349:HIS:HD2	1.99	0.44
6:A:713:HOH:O	1:D:240:LYS:HD3	2.17	0.44
1:B:108:GLN:OE1	6:B:950:HOH:O	2.21	0.44
3:A:505:GOL:H2	6:A:603:HOH:O	2.18	0.43
1:A:192:LYS:CG	1:A:193[B]:MET:N	2.80	0.43
1:D:372:HIS:HB2	1:D:373:PRO:CD	2.49	0.43
1:D:123:LYS:HE2	6:D:794:HOH:O	2.18	0.43
1:D:163:THR:O	5:D:508:PEG:C4	2.67	0.43
1:C:408:LEU:HD21	6:C:824:HOH:O	2.18	0.42
1:C:418:HIS:HE1	3:C:505:GOL:H2	1.77	0.42
1:A:168:ALA:HB1	6:A:779:HOH:O	2.18	0.42
1:D:217:ILE:HG12	6:D:827:HOH:O	2.18	0.42
1:C:285:LEU:HB2	1:C:383:ASP:O	2.20	0.42
1:C:67:PRO:O	1:C:87:SER:HB2	2.20	0.41
1:C:418:HIS:CE1	3:C:505:GOL:H12	2.56	0.41
1:A:167:PHE:CD1	6:A:798:HOH:O	2.72	0.41
1:B:285:LEU:HB2	1:B:383:ASP:O	2.20	0.41
1:A:372:HIS:HB2	1:A:373:PRO:CD	2.50	0.41
1:C:279:VAL:CG2	6:C:781:HOH:O	2.69	0.41
1:D:153:PRO:HA	5:D:510:PEG:H21	2.02	0.41
1:D:173:ILE:HG13	6:D:611:HOH:O	2.21	0.41
1:D:278:ASN:HB3	6:D:885:HOH:O	2.21	0.41
1:D:285:LEU:HB2	1:D:383:ASP:O	2.20	0.41
1:A:67:PRO:O	1:A:87:SER:HB2	2.21	0.41
1:A:44:TYR:OH	6:A:610:HOH:O	2.22	0.41
1:A:285:LEU:HB2	1:A:383:ASP:O	2.20	0.41
1:A:390:GLU:OE2	1:A:393:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:GLN:NE2	6:C:971:HOH:O	2.54	0.41
6:A:713:HOH:O	1:D:240:LYS:HE2	2.20	0.40
1:D:208:TYR:O	5:D:508:PEG:H11	2.21	0.40
1:D:67:PRO:O	1:D:87:SER:HB2	2.21	0.40
1:B:84:LEU:HD22	1:B:190:TRP:CH2	2.56	0.40
1:B:292:ASP:OD2	6:B:966:HOH:O	2.21	0.40
1:D:222:PRO:HG3	6:D:827:HOH:O	2.22	0.40
1:A:278:ASN:HB3	5:A:509:PEG:H32	2.04	0.40
1:A:168:ALA:HB2	6:A:771:HOH:O	2.21	0.40
1:A:64:LEU:HB3	1:A:65:PRO:HD2	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ASP:OD2	6:A:955:HOH:O[2_645]	2.14	0.06
1:D:183:GLU:OE2	6:A:884:HOH:O[2_645]	2.16	0.04

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	405/404 (100%)	388 (96%)	17 (4%)	0	100	100
1	B	412/404 (102%)	395 (96%)	17 (4%)	0	100	100
1	C	403/404 (100%)	387 (96%)	16 (4%)	0	100	100
1	D	408/404 (101%)	386 (95%)	22 (5%)	0	100	100
All	All	1628/1616 (101%)	1556 (96%)	72 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/326 (101%)	325 (99%)	4 (1%)	78	83
1	B	336/326 (103%)	330 (98%)	6 (2%)	66	71
1	C	327/326 (100%)	321 (98%)	6 (2%)	66	71
1	D	332/326 (102%)	327 (98%)	5 (2%)	72	78
All	All	1324/1304 (102%)	1303 (98%)	21 (2%)	72	76

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	ASP
1	A	192	LYS
1	A	322	TRP
1	A	398	LYS
1	B	84	LEU
1	B	172	ASP
1	B	215[A]	ILE
1	B	215[B]	ILE
1	B	376	GLU
1	B	398	LYS
1	C	172	ASP
1	C	192	LYS
1	C	215	ILE
1	C	277	LEU
1	C	322	TRP
1	C	398	LYS
1	D	172	ASP
1	D	259	VAL
1	D	376	GLU
1	D	398	LYS
1	D	428	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	235	ASN
1	A	248	HIS
1	A	278	ASN
1	A	339	HIS
1	A	349	HIS
1	B	235	ASN
1	B	246	ASN
1	B	248	HIS
1	B	250	GLN
1	B	278	ASN
1	B	339	HIS
1	B	372	HIS
1	C	26	GLN
1	C	175	HIS
1	C	235	ASN
1	C	278	ASN
1	C	339	HIS
1	C	369	GLN
1	C	418	HIS
1	D	26	GLN
1	D	45	ASN
1	D	108	GLN
1	D	116	ASN
1	D	242	ASN
1	D	248	HIS
1	D	250	GLN
1	D	254	ASN
1	D	278	ASN
1	D	339	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 34 ligands modelled in this entry, 12 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GOL	A	504	-	5,5,5	0.84	0	5,5,5	1.37	0
3	GOL	A	505	-	5,5,5	0.59	0	5,5,5	0.55	0
4	TAR	A	506	-	3,9,9	0.58	0	6,12,12	1.35	0
4	TAR	A	507	-	3,9,9	0.11	0	6,12,12	0.57	0
5	PEG	A	508	-	6,6,6	0.57	0	5,5,5	0.66	0
5	PEG	A	509	-	6,6,6	0.74	0	5,5,5	0.15	0
3	GOL	B	504	-	5,5,5	0.48	0	5,5,5	0.56	0
3	GOL	B	505	-	5,5,5	0.67	0	5,5,5	0.38	0
3	GOL	B	506	-	5,5,5	0.43	0	5,5,5	0.93	0
4	TAR	B	507	-	3,9,9	0.61	0	6,12,12	0.73	0
5	PEG	B	508	-	6,6,6	0.46	0	5,5,5	0.46	0
3	GOL	C	504	-	5,5,5	0.48	0	5,5,5	0.47	0
3	GOL	C	505	-	5,5,5	0.70	0	5,5,5	0.89	0
4	TAR	C	506	-	3,9,9	0.55	0	6,12,12	2.72	2 (33%)
4	TAR	C	507	-	3,9,9	0.32	0	6,12,12	2.44	2 (33%)
3	GOL	D	504	-	5,5,5	0.38	0	5,5,5	0.50	0
3	GOL	D	505	-	5,5,5	0.25	0	5,5,5	0.60	0
4	TAR	D	506	-	3,9,9	0.31	0	6,12,12	0.96	0
5	PEG	D	507	-	6,6,6	0.61	0	5,5,5	0.43	0
5	PEG	D	508	-	6,6,6	0.52	0	5,5,5	0.32	0
5	PEG	D	509	-	6,6,6	0.52	0	5,5,5	0.42	0
5	PEG	D	510	-	6,6,6	0.60	0	5,5,5	0.41	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	A	504	-	-	0/4/4/4	0/0/0/0
3	GOL	A	505	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TAR	A	506	-	-	0/4/12/12	0/0/0/0
4	TAR	A	507	-	-	0/4/12/12	0/0/0/0
5	PEG	A	508	-	-	0/4/4/4	0/0/0/0
5	PEG	A	509	-	-	0/4/4/4	0/0/0/0
3	GOL	B	504	-	-	0/4/4/4	0/0/0/0
3	GOL	B	505	-	-	0/4/4/4	0/0/0/0
3	GOL	B	506	-	-	0/4/4/4	0/0/0/0
4	TAR	B	507	-	-	0/4/12/12	0/0/0/0
5	PEG	B	508	-	-	0/4/4/4	0/0/0/0
3	GOL	C	504	-	-	0/4/4/4	0/0/0/0
3	GOL	C	505	-	-	0/4/4/4	0/0/0/0
4	TAR	C	506	-	-	0/4/12/12	0/0/0/0
4	TAR	C	507	-	-	0/4/12/12	0/0/0/0
3	GOL	D	504	-	-	0/4/4/4	0/0/0/0
3	GOL	D	505	-	-	0/4/4/4	0/0/0/0
4	TAR	D	506	-	-	0/4/12/12	0/0/0/0
5	PEG	D	507	-	-	0/4/4/4	0/0/0/0
5	PEG	D	508	-	-	0/4/4/4	0/0/0/0
5	PEG	D	509	-	-	0/4/4/4	0/0/0/0
5	PEG	D	510	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	506	TAR	C4-C3-C2	-5.98	101.09	113.35
4	C	507	TAR	C4-C3-C2	-4.14	104.86	113.35
4	C	507	TAR	O2-C2-C1	-2.96	103.74	111.21
4	C	506	TAR	O3-C3-C2	2.08	114.48	108.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	505	GOL	1	0
4	A	506	TAR	1	0
5	A	509	PEG	3	0
3	B	506	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	504	GOL	2	0
3	C	505	GOL	3	0
4	C	506	TAR	5	0
4	C	507	TAR	4	0
3	D	504	GOL	2	0
3	D	505	GOL	2	0
4	D	506	TAR	1	0
5	D	508	PEG	4	0
5	D	510	PEG	1	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	404/404 (100%)	-0.09	2 (0%) 91 93	14, 22, 34, 49	0
1	B	404/404 (100%)	-0.13	1 (0%) 95 96	14, 20, 32, 49	0
1	C	404/404 (100%)	-0.10	1 (0%) 95 96	11, 20, 33, 54	0
1	D	404/404 (100%)	-0.19	0 100 100	11, 20, 31, 46	0
All	All	1616/1616 (100%)	-0.13	4 (0%) 95 96	11, 21, 33, 54	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	219	ALA	2.8
1	C	25	MET	2.8
1	A	428	ILE	2.4
1	A	25	MET	2.1

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 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(Å ²)	Q<0.9
3	GOL	A	504	6/6	0.76	0.26	7.72	31,37,38,40	0
5	PEG	D	508	7/7	0.84	0.19	3.32	33,38,40,43	0
5	PEG	A	509	7/7	0.84	0.18	2.96	27,33,36,37	0
5	PEG	D	510	7/7	0.78	0.18	2.42	43,44,47,50	0
3	GOL	B	506	6/6	0.84	0.18	2.16	32,35,37,41	0
3	GOL	D	505	6/6	0.82	0.13	1.48	32,35,36,37	0
3	GOL	B	505	6/6	0.82	0.15	1.45	36,37,40,42	0
3	GOL	A	505	6/6	0.79	0.15	1.39	33,38,39,39	0
3	GOL	B	504	6/6	0.83	0.12	0.81	37,41,41,43	0
3	GOL	C	504	6/6	0.84	0.12	0.73	36,41,42,44	0
5	PEG	A	508	7/7	0.91	0.13	0.32	30,34,35,37	0
2	CA	A	503	1/1	0.99	0.05	-1.95	26,26,26,26	0
2	CA	B	503	1/1	0.98	0.04	-3.16	21,21,21,21	0
2	CA	B	501	1/1	0.97	0.05	-3.26	21,21,21,21	0
2	CA	A	501	1/1	1.00	0.05	-3.35	14,14,14,14	0
2	CA	C	503	1/1	0.99	0.05	-3.57	28,28,28,28	0
2	CA	B	502	1/1	0.99	0.05	-3.68	16,16,16,16	0
2	CA	D	503	1/1	0.99	0.06	-3.80	26,26,26,26	0
2	CA	D	501	1/1	0.97	0.05	-3.82	18,18,18,18	0
2	CA	C	501	1/1	0.99	0.04	-3.97	16,16,16,16	0
2	CA	C	502	1/1	0.99	0.05	-4.05	24,24,24,24	0
2	CA	A	502	1/1	0.99	0.03	-4.25	24,24,24,24	0
2	CA	D	502	1/1	0.99	0.03	-5.80	23,23,23,23	0
5	PEG	D	507	7/7	0.64	0.29	-	47,54,59,62	0
4	TAR	B	507	10/10	0.65	0.14	-	49,53,56,56	0
4	TAR	C	506	10/10	0.82	0.14	-	49,54,55,59	0
4	TAR	A	506	10/10	0.64	0.24	-	57,65,72,76	0
4	TAR	C	507	10/10	0.84	0.14	-	39,46,47,50	0
5	PEG	B	508	7/7	0.73	0.18	-	41,44,47,47	0
3	GOL	D	504	6/6	0.85	0.16	-	38,43,44,45	0
4	TAR	D	506	10/10	0.82	0.13	-	38,45,48,51	0
3	GOL	C	505	6/6	0.83	0.29	-	30,30,32,32	0
5	PEG	D	509	7/7	0.76	0.17	-	46,48,49,50	0
4	TAR	A	507	10/10	0.75	0.17	-	48,54,56,66	0

6.5 Other polymers ⓘ

There are no such residues in this entry.