

Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 - 02:00 PM JST

PDB ID	:	8H2K
Title	:	Cellodextrin phosphorylase from Clostridium thermocellum mutant - all cys-
		teine residues were substituted with serines
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Deposited on	:	2022-10-06
Resolution	:	1.37 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.37 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2907 (1.40-1.36)
Clashscore	141614	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)
RSRZ outliers	127900	2846 (1.40-1.36)

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 <=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	А	993	2% 9 1%	8% ••
1	В	993	2% 8 9%	9% •

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
5	ACT	В	1002	-	-	Х	-
5	ACT	В	1005	-	-	Х	-



8H2K

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 33276 atoms, of which 14447 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 Cellodextrin phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	А	984	Total 15293	C 5184	Н 7176	N 1353	O 1556	S 24	177	31	0
1	В	984	Total 15357	C 5194	Н 7220	N 1362	O 1560	S 21	171	33	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MET	-	initiating methionine	UNP Q93HT8
А	2	GLY	-	expression tag	UNP Q93HT8
А	65	SER	CYS	engineered mutation	UNP Q93HT8
А	81	SER	CYS	engineered mutation	UNP Q93HT8
А	226	SER	CYS	engineered mutation	UNP Q93HT8
А	230	SER	CYS	engineered mutation	UNP Q93HT8
А	241	SER	CYS	engineered mutation	UNP Q93HT8
А	354	SER	CYS	engineered mutation	UNP Q93HT8
А	373	SER	CYS	engineered mutation	UNP Q93HT8
А	607	SER	CYS	engineered mutation	UNP Q93HT8
А	626	SER	CYS	engineered mutation	UNP Q93HT8
А	630	ASP	ALA	engineered mutation	UNP Q93HT8
А	873	SER	CYS	engineered mutation	UNP Q93HT8
А	935	SER	CYS	engineered mutation	UNP Q93HT8
А	986	LEU	-	expression tag	UNP Q93HT8
А	987	GLU	-	expression tag	UNP Q93HT8
А	988	HIS	-	expression tag	UNP Q93HT8
А	989	HIS	-	expression tag	UNP Q93HT8
А	990	HIS	-	expression tag	UNP Q93HT8
А	991	HIS	-	expression tag	UNP Q93HT8
А	992	HIS	-	expression tag	UNP Q93HT8
А	993	HIS	-	expression tag	UNP Q93HT8
В	1	MET	-	initiating methionine	UNP Q93HT8
В	2	GLY	-	expression tag	UNP Q93HT8
В	65	SER	CYS	engineered mutation	UNP Q93HT8
-	•				

There are 44 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
В	81	SER	CYS	engineered mutation	UNP Q93HT8
В	226	SER	CYS	engineered mutation	UNP Q93HT8
В	230	SER	CYS	engineered mutation	UNP Q93HT8
В	241	SER	CYS	engineered mutation	UNP Q93HT8
В	354	SER	CYS	engineered mutation	UNP Q93HT8
В	373	SER	CYS	engineered mutation	UNP Q93HT8
В	607	SER	CYS	engineered mutation	UNP Q93HT8
В	626	SER	CYS	engineered mutation	UNP Q93HT8
В	630	ASP	ALA	engineered mutation	UNP Q93HT8
В	873	SER	CYS	engineered mutation	UNP Q93HT8
В	935	SER	CYS	engineered mutation	UNP Q93HT8
В	986	LEU	-	expression tag	UNP Q93HT8
В	987	GLU	-	expression tag	UNP Q93HT8
В	988	HIS	-	expression tag	UNP Q93HT8
В	989	HIS	-	expression tag	UNP Q93HT8
В	990	HIS	-	expression tag	UNP Q93HT8
В	991	HIS	-	expression tag	UNP Q93HT8
В	992	HIS	-	expression tag	UNP Q93HT8
В	993	HIS	-	expression tag	UNP Q93HT8

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total C H O 14 3 8 3	0	0
2	А	1	Total C H O 14 3 8 3	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total C H O 14 3 8 3	0	0
2	В	1	Total C H O 14 3 8 3	0	0

• Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	А	1	Total 17	$\begin{array}{c} \mathrm{C} \\ 4 \end{array}$	H 10	O 3	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	2	Total Cl 2 2	0	0
4	В	2	Total Cl 2 2	0	0

• Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{H} & \text{O} \\ 7 & 2 & 3 & 2 \end{array}$	0	0
5	В	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{H} & \text{O} \\ 7 & 2 & 3 & 2 \end{array}$	0	0
5	В	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{H} & \text{O} \\ 7 & 2 & 3 & 2 \end{array}$	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1277	Total O 1277 1277	0	0
6	В	1251	Total O 1251 1251	0	0



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: Cellodextrin phosphorylase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	83.44Å 89.05 Å 88.99 Å	Deperitor
a, b, c, α , β , γ	98.88° 110.55° 110.67°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	43.76 - 1.37	Depositor
Resolution (A)	43.78 - 1.37	EDS
% Data completeness	93.5 (43.76-1.37)	Depositor
(in resolution range)	93.1 (43.78-1.37)	EDS
R _{merge}	0.05	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.15 (at 1.37 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
B B.	0.174 , 0.200	Depositor
Π, Π_{free}	0.175 , 0.199	DCC
R_{free} test set	21009 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor ($Å^2$)	16.3	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35 , 47.0	EDS
L-test for $twinning^2$	$< L > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.449 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33276	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PEG, GOL, ACT

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	А	0.46	0/8294	0.68	2/11217~(0.0%)
1	В	0.47	0/8313	0.69	2/11239~(0.0%)
All	All	0.47	0/16607	0.69	4/22456~(0.0%)

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	А	0	1
1	В	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	798	ASN	CB-CA-C	6.75	123.91	110.40
1	В	189	MET	CA-CB-CG	-5.73	103.56	113.30
1	В	950	MET	CG-SD-CE	5.59	109.14	100.20
1	А	378	LYS	CD-CE-NZ	5.17	123.59	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	801	ALA	Peptide
1	В	799	ASP	Peptide



5.2 Too-close contacts (i)

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	А	8117	7176	7950	81	0
1	В	8137	7220	7984	90	0
2	А	12	16	16	2	0
2	В	12	16	15	2	0
3	А	7	10	10	0	0
4	А	2	0	0	0	0
4	В	2	0	0	0	0
5	В	12	9	9	6	0
6	А	1277	0	0	43	2
6	В	1251	0	0	47	2
All	All	18829	14447	15984	174	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 (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:63[B]:GLU:OE1	6:B:1101:HOH:O	1.86	0.93
1:B:63[B]:GLU:OE2	6:B:1102:HOH:O	1.88	0.90
1:A:12:LYS:H	1:A:12:LYS:HD2	1.42	0.85
1:A:346:GLU:OE2	6:A:1101:HOH:O	1.95	0.84
1:A:644:TYR:O	1:A:648[B]:LYS:HE2	1.76	0.83
1:A:644:TYR:O	1:A:648[A]:LYS:HE2	1.76	0.83
1:A:625[C]:ASP:OD1	6:A:1102:HOH:O	1.96	0.82
1:A:794:ASN:OD1	1:A:800:THR:HG21	1.78	0.82
1:A:256:LYS:HE3	2:A:1002:GOL:H2	1.62	0.80
1:B:155[B]:LYS:HE2	6:B:2148:HOH:O	1.78	0.80
1:A:798:ASN:O	1:A:799:ASP:HB3	1.83	0.77
1:B:295:ILE:HG22	6:B:1196:HOH:O	1.84	0.77
1:B:87:GLN:HG2	6:B:1965:HOH:O	1.83	0.77
1:B:817[A]:LYS:HD2	1:B:854:VAL:HG12	1.69	0.74
1:A:441:GLU:HB2	6:A:1598:HOH:O	1.86	0.74
1:A:954:GLU:HB3	1:A:985:LYS:HD2	1.68	0.74
1:A:187:PHE:HB3	6:B:1196:HOH:O	1.88	0.73



8H2K

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:888:LEU:O	6:A:1103:HOH:O	2.07	0.72
1:A:155:LYS:HB2	6:A:1114:HOH:O	1.89	0.72
1:B:441:GLU:HG3	6:B:2166:HOH:O	1.90	0.71
1:A:704[B]:ASP:OD1	6:A:1104:HOH:O	2.08	0.71
1:B:18:LEU:HD21	1:B:22:LYS:HE2	1.71	0.71
1:B:786[B]:ARG:NH1	6:B:1111:HOH:O	2.23	0.71
1:B:925:GLN:HG2	6:B:2096:HOH:O	1.91	0.70
1:A:925[A]:GLN:OE1	1:A:942:THR:HG22	1.91	0.70
1:B:110:LYS:HG3	6:B:1113:HOH:O	1.91	0.70
1:B:12:LYS:N	1:B:12:LYS:HD3	2.04	0.69
1:A:645:GLU:O	1:A:649:LYS:HG3	1.92	0.69
1:A:525[B]:GLU:HG3	6:A:1442:HOH:O	1.92	0.68
1:B:938:LYS:HE3	1:B:977:GLU:OE1	1.92	0.68
1:B:155[A]:LYS:HE2	6:B:1390:HOH:O	1.92	0.68
1:B:12:LYS:HE3	6:B:2086:HOH:O	1.94	0.68
1:B:925:GLN:OE1	1:B:942:THR:HG22	1.95	0.67
1:B:106:ASN:ND2	6:B:1113:HOH:O	2.25	0.66
1:B:12:LYS:HE2	6:B:2023:HOH:O	1.95	0.66
1:B:219:ASP:HB2	6:B:2000:HOH:O	1.94	0.66
1:A:983:LYS:NZ	6:A:1112:HOH:O	2.28	0.66
1:B:155[A]:LYS:HE3	6:B:1355:HOH:O	1.95	0.65
1:B:110:LYS:HE3	6:B:1602:HOH:O	1.95	0.65
1:A:255:LYS:HG3	1:A:258:PHE:CE2	2.32	0.64
1:A:479:VAL:HG13	6:A:1123:HOH:O	1.98	0.63
1:B:890[A]:SER:OG	5:B:1005:ACT:H2	1.98	0.63
1:A:165[B]:VAL:HG23	1:A:489:PHE:CZ	2.34	0.62
1:B:155[B]:LYS:NZ	6:B:1117:HOH:O	2.32	0.62
1:A:319:ILE:O	1:A:338[A]:THR:HG23	2.00	0.62
1:B:792:ASP:OD1	1:B:794:ASN:ND2	2.33	0.62
1:B:155[B]:LYS:N	1:B:155[B]:LYS:HD2	2.15	0.61
1:B:428:ASP:OD2	1:B:432:ARG:NH2	2.31	0.61
1:A:238:LYS:HD3	6:A:1141:HOH:O	2.00	0.61
1:B:521:ASP:O	1:B:525[A]:GLU:HG3	1.99	0.61
1:B:874[B]:THR:HG23	1:B:885[B]:ILE:O	2.00	0.61
1:B:964:ILE:HD12	1:B:966:ASN:O	2.00	0.61
1:B:125[B]:GLU:OE1	1:B:465:LYS:HG3	2.01	0.61
1:A:12:LYS:HD2	1:A:12:LYS:N	2.15	0.61
1:B:319:ILE:O	1:B:338[A]:THR:HG23	2.01	0.60
1:B:704:ASP:HB3	6:B:1981:HOH:O	2.00	0.60
1:B:338[A]:THR:HG22	6:B:2057:HOH:O	2.02	0.60
1:A:255:LYS:HD2	6:A:2036:HOH:O	2.01	0.60



8H2K	

Atom 1 Atom 2		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:465[A]:LYS:HD3	6:A:1307:HOH:O	2.01	0.60
1:B:117:LYS:O	1:B:117:LYS:HE3	2.01	0.60
1:A:106:ASN:O	1:A:110:LYS:HG3	2.02	0.59
1:A:359:ASP:OD2	1:A:378:LYS:HE2	2.02	0.59
1:A:151:ARG:NH2	6:A:1114:HOH:O	2.31	0.59
1:A:165[B]:VAL:HG23	1:A:489:PHE:CE2	2.37	0.59
1:A:853:LEU:HD23	2:A:1001:GOL:H11	1.84	0.59
1:A:297:GLU:HG3	6:A:1977:HOH:O	2.02	0.59
1:B:296[B]:PHE:CG	6:B:1196:HOH:O	2.52	0.58
1:A:798:ASN:O	1:A:799:ASP:CB	2.51	0.58
1:A:338[A]:THR:HG22	6:A:2041:HOH:O	2.04	0.58
1:B:223:GLU:OE2	6:B:1107:HOH:O	2.17	0.58
1:A:432:ARG:HA	1:A:435[A]:GLU:HG3	1.85	0.58
1:B:938:LYS:HE3	1:B:977:GLU:CD	2.24	0.57
5:B:1005:ACT:H1	6:B:1147:HOH:O	2.04	0.57
1:B:960:ASP:OD2	6:B:1106:HOH:O	2.17	0.57
1:B:400:THR:O	5:B:1002:ACT:H1	2.04	0.57
1:B:730[B]:THR:HG22	6:B:1330:HOH:O	2.05	0.57
5:B:1005:ACT:H1	6:B:1466:HOH:O	2.05	0.56
1:A:641:LYS:HB3	6:A:1943:HOH:O	2.06	0.56
1:B:628:LYS:HG3	1:B:800:THR:HG23	1.86	0.56
1:A:18:LEU:HD23	1:A:45:VAL:HG13	1.89	0.55
1:A:465[B]:LYS:N	1:A:465[B]:LYS:HD2	2.22	0.55
1:B:90:TYR:HB3	6:B:1207:HOH:O	2.06	0.54
1:A:801:ALA:C	1:A:802:THR:O	2.45	0.54
1:B:735:LYS:HE3	2:B:1003:GOL:O3	2.07	0.54
1:A:700:LYS:HD2	6:A:1420:HOH:O	2.07	0.53
1:B:631:SER:HB3	6:B:1939:HOH:O	2.09	0.53
1:A:297:GLU:HB2	6:A:1977:HOH:O	2.08	0.53
1:A:12:LYS:H	1:A:12:LYS:CD	2.18	0.53
1:A:890:SER:HB3	6:A:1103:HOH:O	2.09	0.53
1:B:873[A]:SER:OG	6:B:1104:HOH:O	2.08	0.53
1:A:256:LYS:HE2	6:A:1992:HOH:O	2.08	0.52
1:B:885[B]:ILE:CD1	6:B:1332:HOH:O	2.57	0.52
1:A:641:LYS:NZ	1:A:645:GLU:OE2	2.38	0.52
1:B:238:LYS:HE3	6:B:1604:HOH:O	2.09	0.52
1:B:296[B]:PHE:CD2	6:B:1196:HOH:O	2.62	0.52
1:B:890[B]:SER:HB3	5:B:1005:ACT:H2	1.91	0.52
1:B:659:MET:HE3	6:B:1458:HOH:O	2.09	0.51
1:B:708:LYS:HG2	1:B:709:HIS:CE1	2.45	0.51
1:B:648:LYS:HG3	$1:B:\overline{649:LYS:N}$	2.26	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:18:LEU:O	1:B:18:LEU:HD23	2.11	0.50
1:A:589:ASN:ND2	6:A:1128:HOH:O	2.39	0.50
1:A:255:LYS:CD	6:A:2036:HOH:O	2.57	0.50
1:A:910:ARG:HB2	6:A:1802:HOH:O	2.12	0.50
1:B:63[B]:GLU:OE1	1:B:63[B]:GLU:N	2.44	0.50
1:A:347:LYS:HE3	1:A:435[B]:GLU:OE1	2.11	0.50
1:B:90:TYR:HD1	1:B:100:GLU:HA	1.76	0.49
1:A:931:LYS:HE2	6:A:1370:HOH:O	2.11	0.49
1:B:10[B]:ASN:ND2	6:B:1108:HOH:O	2.20	0.48
1:A:964:ILE:HD12	1:A:966:ASN:O	2.14	0.48
1:B:704:ASP:CB	6:B:1981:HOH:O	2.58	0.48
1:A:255:LYS:HE3	6:A:1127:HOH:O	2.13	0.48
1:A:275:LYS:NZ	6:A:1131:HOH:O	2.42	0.47
1:A:52:PRO:HG3	1:A:117:LYS:HE3	1.97	0.47
1:A:885:ILE:CD1	6:A:1589:HOH:O	2.62	0.47
1:A:521:ASP:O	1:A:525[A]:GLU:HG3	2.15	0.47
1:A:631:SER:HB3	6:A:1922:HOH:O	2.15	0.47
1:B:402:ILE:HG13	5:B:1002:ACT:H2	1.96	0.47
1:B:628:LYS:HG3	1:B:800:THR:CG2	2.45	0.47
1:B:94:GLU:HG2	6:B:1850:HOH:O	2.14	0.47
1:B:817[B]:LYS:HZ3	1:B:874[B]:THR:HG22	1.80	0.47
1:B:890[A]:SER:HB3	6:B:1104:HOH:O	2.14	0.47
1:A:151:ARG:HB2	1:A:157[A]:THR:HG23	1.97	0.47
1:A:885:ILE:HD11	6:A:1589:HOH:O	2.16	0.46
1:B:873[B]:SER:O	1:B:888:LEU:O	2.33	0.46
1:B:776:LYS:HD3	1:B:846:ILE:HD11	1.98	0.46
1:A:107:LYS:CE	6:A:2063:HOH:O	2.63	0.46
1:A:800:THR:O	1:A:801:ALA:HB2	2.17	0.46
1:A:890:SER:CB	6:A:1103:HOH:O	2.64	0.45
1:A:962:GLN:HB3	6:A:1772:HOH:O	2.16	0.45
1:B:22:LYS:HG2	6:B:1850:HOH:O	2.15	0.45
1:A:797:ALA:O	1:A:800:THR:HG23	2.16	0.45
1:B:786[B]:ARG:NH2	6:B:1121:HOH:O	2.35	0.45
1:A:938:LYS:HE2	1:A:977:GLU:OE1	2.16	0.44
1:B:155[A]:LYS:HG3	6:B:1355:HOH:O	2.16	0.44
1:B:255[A]:LYS:HE2	1:B:255[A]:LYS:HB2	1.33	0.44
1:B:461:ASN:ND2	6:B:1155:HOH:O	2.49	0.44
1:B:645:GLU:O	1:B:648:LYS:HG2	2.17	0.44
1:A:832:LYS:HE2	1:A:916:ASN:O	2.16	0.44
1:B:985:LYS:NZ	6:B:1159:HOH:O	2.50	0.44
1:B:18:LEU:HD22	1:B:45:VAL:HG22	1.99	0.44



8H2K

A + a == 1	A + a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:26:LYS:HD2	1:A:96:GLY:HA2	2.00	0.43
1:A:107:LYS:HE2	6:A:2063:HOH:O	2.18	0.43
1:B:133:LEU:HD12	1:B:224:ALA:HB1	2.00	0.43
1:B:155[A]:LYS:HD2	6:B:2165:HOH:O	2.17	0.43
1:B:39:ASP:CB	6:B:2009:HOH:O	2.67	0.43
1:B:728:SER:O	1:B:738:LYS:HE3	2.17	0.43
1:A:938:LYS:CE	1:A:977:GLU:OE1	2.67	0.43
1:B:730[B]:THR:HG23	1:B:731:TYR:HD1	1.84	0.43
1:A:117:LYS:HD2	6:A:1279:HOH:O	2.18	0.42
1:A:694[B]:GLN:HG2	1:A:695:MET:CE	2.48	0.42
1:A:347:LYS:HG3	6:A:1861:HOH:O	2.20	0.42
1:A:766:GLU:CG	6:A:1105:HOH:O	2.66	0.42
1:B:799:ASP:HA	1:B:801:ALA:H	1.84	0.42
1:A:465[B]:LYS:HD2	1:A:465[B]:LYS:H	1.81	0.42
2:B:1003:GOL:H2	6:B:1667:HOH:O	2.18	0.42
1:A:766:GLU:OE2	6:A:1105:HOH:O	2.22	0.42
1:A:641:LYS:HD3	6:A:1943:HOH:O	2.20	0.42
1:B:85:GLU:OE1	1:B:98:LYS:NZ	2.47	0.42
1:B:766:GLU:CG	6:B:1120:HOH:O	2.67	0.42
1:B:925:GLN:HG3	1:B:926:LEU:N	2.35	0.41
1:B:80:VAL:HG12	1:B:93:LEU:HD23	2.02	0.41
1:B:209:LYS:HE2	6:B:2091:HOH:O	2.21	0.41
1:B:874[B]:THR:HG21	1:B:884:ASN:HB3	2.03	0.41
1:B:90:TYR:CD1	1:B:100:GLU:HA	2.55	0.41
6:A:2027:HOH:O	1:B:296[A]:PHE:CE1	2.68	0.41
1:A:297:GLU:CB	6:A:1977:HOH:O	2.68	0.41
1:A:338[A]:THR:CG2	6:A:2041:HOH:O	2.66	0.41
1:B:794:ASN:HA	1:B:797:ALA:O	2.21	0.41
1:A:659:MET:HG3	6:A:2179:HOH:O	2.21	0.40
1:B:434:PHE:HA	1:B:439:SER:OG	2.21	0.40
1:B:856:PRO:O	1:B:870:PRO:HA	2.22	0.40
1:A:479:VAL:HG12	1:A:510:SER:HB3	2.03	0.40
1:A:985:LYS:HG2	6:A:1991:HOH:O	2.22	0.40
1:B:839:LEU:O	1:B:843:MET:HG3	2.21	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)
6:A:1999:HOH:O	6:B:1434:HOH:O[1_454]	2.14	0.06
6:A:2082:HOH:O	6:B:2058:HOH:O[1_454]	2.19	0.01



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	Percer	ntiles
1	А	1013/993~(102%)	978~(96%)	33~(3%)	2(0%)	47	21
1	В	1016/993~(102%)	985~(97%)	30~(3%)	1 (0%)	51	23
All	All	2029/1986~(102%)	1963 (97%)	63 (3%)	3 (0%)	47	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	801	ALA
1	А	802	THR
1	В	802	THR

5.3.2 Protein sidechains (i)

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	А	881/859~(103%)	868~(98%)	13 (2%)	65 36
1	В	883/859~(103%)	868~(98%)	15 (2%)	60 30
All	All	1764/1718~(103%)	1736~(98%)	28 (2%)	71 33

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	117	LYS
1	А	163	LYS
1	А	174	PHE



Mol	Chain	Res	Type
1	А	219	ASP
1	А	232	ARG
1	А	465[A]	LYS
1	А	465[B]	LYS
1	А	586	ASP
1	А	648[A]	LYS
1	А	648[B]	LYS
1	А	715	PHE
1	А	804[A]	HIS
1	А	804[B]	HIS
1	В	103	GLU
1	В	117	LYS
1	В	156[A]	ARG
1	В	156[B]	ARG
1	В	163	LYS
1	В	174	PHE
1	В	232	ARG
1	В	255[A]	LYS
1	В	255[B]	LYS
1	В	373[A]	SER
1	В	373[B]	SER
1	В	378[A]	LYS
1	В	378[B]	LYS
1	В	715	PHE
1	В	794	ASN

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

Mol	Chain	Res	Type
1	В	368	HIS
1	В	459	GLN
1	В	687	ASN
1	В	818	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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).

Mal	Tune Chain Peg Link		Tink	В	ond leng	gths	Bond angles			
	туре	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	GOL	А	1001	-	$5,\!5,\!5$	0.92	0	$5,\!5,\!5$	0.98	0
5	ACT	В	1002	-	3,3,3	1.10	0	$3,\!3,\!3$	1.62	0
3	PEG	A	1003	-	$6,\!6,\!6$	0.07	0	$5,\!5,\!5$	0.21	0
5	ACT	В	1004	-	3,3,3	1.31	0	3, 3, 3	1.38	0
2	GOL	В	1001	-	$5,\!5,\!5$	0.87	0	$5,\!5,\!5$	1.00	0
2	GOL	В	1003	-	$5,\!5,\!5$	1.58	1 (20%)	$5,\!5,\!5$	0.77	0
2	GOL	А	1002	-	$5,\!5,\!5$	0.89	0	$5,\!5,\!5$	0.77	0
5	ACT	В	1005	-	3,3,3	0.84	0	3,3,3	1.57	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	GOL	А	1001	-	-	1/4/4/4	-
3	PEG	А	1003	-	-	1/4/4/4	-
2	GOL	В	1001	-	-	2/4/4/4	-
2	GOL	В	1003	-	-	4/4/4/4	-
2	GOL	А	1002	-	-	0/4/4/4	-



All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	1003	GOL	O2-C2	-2.28	1.36	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	1001	GOL	O1-C1-C2-C3
2	В	1003	GOL	O1-C1-C2-C3
2	В	1001	GOL	O1-C1-C2-O2
2	В	1003	GOL	O1-C1-C2-O2
2	В	1003	GOL	O2-C2-C3-O3
2	А	1001	GOL	C1-C2-C3-O3
2	В	1003	GOL	C1-C2-C3-O3
3	А	1003	PEG	O2-C3-C4-O4

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	1001	GOL	1	0
5	В	1002	ACT	2	0
2	В	1003	GOL	2	0
2	А	1002	GOL	1	0
5	В	1005	ACT	4	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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	984/993~(99%)	0.16	18 (1%) 68 71	11, 17, 41, 86	8 (0%)
1	В	984/993~(99%)	0.17	21 (2%) 63 65	11, 17, 41, 88	7 (0%)
All	All	1968/1986~(99%)	0.16	39 (1%) 65 68	11, 17, 41, 88	15 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	801	ALA	17.1
1	В	800	THR	12.4
1	В	799	ASP	9.5
1	В	801	ALA	7.5
1	А	798	ASN	6.1
1	А	799	ASP	5.7
1	В	798	ASN	5.5
1	В	802	THR	4.3
1	В	90	TYR	4.0
1	А	800	THR	3.9
1	В	24	GLY	3.8
1	А	13	ILE	3.6
1	А	802	THR	3.5
1	А	27	ILE	3.3
1	В	27	ILE	3.3
1	В	86	GLY	3.1
1	А	99	ILE	2.8
1	А	92	VAL	2.8
1	В	463	GLY	2.8
1	В	12	LYS	2.6
1	А	90	TYR	2.4
1	В	296[A]	PHE	2.4
1	В	13	ILE	2.4
1	A	2	GLY	2.4



Mol	Chain	Res	Type	RSRZ
1	В	19	LEU	2.4
1	В	25	ASN	2.4
1	В	93	LEU	2.4
1	А	650	THR	2.4
1	А	651	ASN	2.3
1	В	28	ASN	2.3
1	В	797	ALA	2.3
1	А	25	ASN	2.3
1	В	70	TYR	2.3
1	А	83	VAL	2.2
1	А	296[A]	PHE	2.2
1	А	340	ILE	2.2
1	А	93	LEU	2.1
1	B	349	PHE	2.1
1	B	111	ALA	2.1

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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 monosaccharides 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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	GOL	А	1001	6/6	0.58	0.21	33,43,52,53	0
5	ACT	В	1004	4/4	0.74	0.23	34,47,47,51	0
2	GOL	А	1002	6/6	0.79	0.21	30,50,67,75	0
5	ACT	В	1002	4/4	0.81	0.17	37,40,46,46	0
3	PEG	А	1003	7/7	0.81	0.12	37,45,53,53	0
2	GOL	В	1001	6/6	0.86	0.13	$30,\!45,\!54,\!54$	0
2	GOL	В	1003	6/6	0.89	0.15	20,28,37,44	0
5	ACT	В	1005	4/4	0.96	0.09	16,20,29,48	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	CL	В	1006	1/1	0.99	0.07	14,14,14,14	0
4	CL	А	1005	1/1	0.99	0.04	13,13,13,13	0
4	CL	В	1007	1/1	1.00	0.08	14,14,14,14	0
4	CL	А	1004	1/1	1.00	0.07	12,12,12,12	0

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6.5 Other polymers (i)

There are no such residues in this entry.

