

Full wwPDB X-ray Structure Validation Report (i)

Jun 5, 2023 – 04:31 pm BST

PDB ID	:	8ADK
Title	:	Poly(ADP-ribose) glycohydrolase (PARG) from Drosophila melanogaster
Authors	:	Ariza, A.; Fontana, P.
Deposited on	:	2022-07-08
Resolution	:	2.47 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
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)	:	2.33

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 2.47 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	5857 (2.50-2.46)		
Clashscore	141614	6594 (2.50-2.46)		
Ramachandran outliers	138981	6469 (2.50-2.46)		
Sidechain outliers	138945	6471 (2.50-2.46)		
RSRZ outliers	127900	5738 (2.50-2.46)		

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	578	72%	14%		11%
1	В	578	<mark>6%</mark> 71%	14%	•••	11%
1	С	578	8%	14%	••	11%



8ADK

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12923 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	1 A	517	Total	С	Ν	0	\mathbf{S}	0	1	0
		517	4192	2671	738	763	20	0		
1	D	\sim 17	Total	С	Ν	0	S	0	1	0
	517	4192	2671	738	763	20	0		0	
1	C	517	Total	С	Ν	0	S	0	1	0
	517	4192	2671	738	763	20	0		U	

• Molecule 1 is a protein called Poly(ADP-ribose) glycohydrolase.

Chain	Residue	Modelled	Actual Comment		Reference
А	-19	MET	-	initiating methionine	UNP O46043
А	-18	GLY	-	expression tag	UNP O46043
А	-17	SER	-	expression tag	UNP O46043
А	-16	SER	-	expression tag	UNP O46043
А	-15	HIS	-	expression tag	UNP O46043
А	-14	HIS	-	expression tag	UNP O46043
А	-13	HIS	-	expression tag	UNP O46043
А	-12	HIS	-	expression tag	UNP O46043
A	-11	HIS	-	expression tag	UNP O46043
А	-10	HIS	-	expression tag	UNP O46043
А	-9	SER	-	expression tag	UNP O46043
А	-8	SER	-	expression tag	UNP O46043
А	-7	GLY	-	expression tag	UNP O46043
А	-6	LEU	-	expression tag	UNP O46043
А	-5	VAL	-	expression tag	UNP O46043
А	-4	PRO	-	expression tag	UNP O46043
A	-3	ARG	-	expression tag	UNP O46043
А	-2	GLY	-	expression tag	UNP O46043
А	-1	SER	-	expression tag	UNP O46043
A	0	HIS	-	expression tag	UNP O46043
В	-19	MET	-	initiating methionine	UNP O46043
В	-18	GLY	-	expression tag	UNP O46043
В	-17	SER	-	expression tag	UNP 046043

There are 60 discrepancies between the modelled and reference sequences:



8A	D	K

Chain	Residue	Modelled	Actual	Actual Comment	
В	-16	SER	-	expression tag	UNP O46043
В	-15	HIS	-	expression tag	UNP O46043
В	-14	HIS	-	expression tag	UNP O46043
В	-13	HIS	-	expression tag	UNP O46043
В	-12	HIS	-	expression tag	UNP O46043
В	-11	HIS	-	expression tag	UNP O46043
В	-10	HIS	-	expression tag	UNP O46043
В	-9	SER	-	expression tag	UNP O46043
В	-8	SER	-	expression tag	UNP O46043
В	-7	GLY	-	expression tag	UNP O46043
В	-6	LEU	-	expression tag	UNP O46043
В	-5	VAL	-	expression tag	UNP O46043
В	-4	PRO	-	expression tag	UNP O46043
В	-3	ARG	-	expression tag	UNP O46043
В	-2	GLY	-	expression tag	UNP O46043
В	-1	SER	-	expression tag	UNP O46043
В	0	HIS	-	expression tag	UNP O46043
С	-19	MET	-	initiating methionine	UNP O46043
С	-18	GLY	-	expression tag	UNP O46043
С	-17	SER	-	expression tag	UNP O46043
С	-16	SER	-	expression tag	UNP O46043
C	-15	HIS	-	expression tag	UNP O46043
С	-14	HIS	-	expression tag	UNP O46043
С	-13	HIS	-	expression tag	UNP O46043
С	-12	HIS	-	expression tag	UNP O46043
С	-11	HIS	-	expression tag	UNP O46043
C	-10	HIS	-	expression tag	UNP O46043
С	-9	SER	-	expression tag	UNP O46043
C	-8	SER	-	expression tag	UNP O46043
С	-7	GLY	-	expression tag	UNP O46043
С	-6	LEU	-	expression tag	UNP O46043
C	-5	VAL	-	expression tag	UNP 046043
C	-4	PRO	-	expression tag	UNP 046043
C	-3	ARG	-	expression tag	UNP 046043
C	-2	GLY	-	expression tag	UNP 046043
С	-1	SER	-	expression tag	UNP 046043
С	0	HIS	-	expression tag	UNP O46043

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





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	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	1	Total Cl 1 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	108	Total O 108 108	0	0
5	В	89	Total O 89 89	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	80	Total O 80 80	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.

- Chain A: 72% 14% 11% MET MET SER SER HIIS SER TEU VAL SER LYS LYS 3LU 3LU RG PRO GLY GLU GLV • Molecule 1: Poly(ADP-ribose) glycohydrolase Chain B: 71% 14% 11% MET MET SSER HIISSER HIISSER HIISSER HIISSER HIISSER HIISSER HIISSER HIISSER HIISSER SER HIISSER SER HIISE SER HIISE SER HIISE SER HIISE SER HIISSER MET HIISE SER HIISSER SER HIISSER SER SER LYS JLU RG RG
- Molecule 1: Poly(ADP-ribose) glycohydrolase





• Molecule 1: Poly(ADP-ribose) glycohydrolase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	93.43Å 115.62Å 122.91Å	Deperitor
a, b, c, α , β , γ	90.00° 112.21° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	59.02 - 2.47	Depositor
Resolution (A)	58.96 - 2.47	EDS
% Data completeness	99.2 (59.02-2.47)	Depositor
(in resolution range)	99.3(58.96-2.47)	EDS
R _{merge}	0.11	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.77 (at 2.48 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
D D.	0.177 , 0.228	Depositor
Π, Π_{free}	0.183 , 0.231	DCC
R_{free} test set	4166 reflections $(4.86%)$	wwPDB-VP
Wilson B-factor ($Å^2$)	57.5	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.33 , 37.2	EDS
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12923	wwPDB-VP
Average B, all atoms $(Å^2)$	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.02% 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: GOL, CL, SO4 $\,$

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).

Mal Chain		Bo	ond lengths	Bond angles		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.68	5/4305~(0.1%)	1.04	13/5837~(0.2%)	
1	В	0.66	3/4305~(0.1%)	1.04	13/5837~(0.2%)	
1	С	0.67	6/4305~(0.1%)	1.03	15/5837~(0.3%)	
All	All	0.67	14/12915~(0.1%)	1.04	$41/17511 \ (0.2\%)$	

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	15
1	В	0	21
1	С	0	17
All	All	0	53

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	А	340	GLU	CD-OE2	8.26	1.34	1.25
1	С	340	GLU	CD-OE2	6.98	1.33	1.25
1	А	340	GLU	CD-OE1	6.90	1.33	1.25
1	А	385	GLU	CD-OE2	-6.77	1.18	1.25
1	С	227	GLU	CD-OE1	6.43	1.32	1.25
1	С	227	GLU	CD-OE2	6.40	1.32	1.25
1	С	154	GLU	CD-OE1	6.21	1.32	1.25
1	В	546	GLU	CD-OE2	5.97	1.32	1.25
1	В	340	GLU	CD-OE2	5.83	1.32	1.25
1	А	154	GLU	CD-OE1	5.56	1.31	1.25
1	С	314	GLU	CD-OE1	5.40	1.31	1.25
1	В	47	GLU	CD-OE2	5.23	1.31	1.25



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	С	546	GLU	CD-OE2	5.12	1.31	1.25
1	А	349	GLU	CD-OE1	5.11	1.31	1.25

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	281[A]	ARG	NE-CZ-NH1	-10.71	114.94	120.30
1	В	281[B]	ARG	NE-CZ-NH1	-10.71	114.94	120.30
1	А	343	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	С	86	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	А	343	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	А	86	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	В	478	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	А	260	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	А	219	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	А	478	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	С	260	ARG	NE-CZ-NH2	7.57	124.09	120.30
1	С	280	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	С	343	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	С	343	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	В	343	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	В	219	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	С	39	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	В	396	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	А	86	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	А	280	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	В	396	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	С	402	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	С	177	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	А	396	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	В	478	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	С	373	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	С	396	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	А	72	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	С	422	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	С	218	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	В	173	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	30	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	В	35	GLU	CB-CA-C	-5.33	99.75	110.40
1	A	491	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	С	491	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	С	86	ARG	NE-CZ-NH1	5.11	122.86	120.30



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	В	281[A]	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	В	281[B]	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	В	221	THR	CA-CB-CG2	5.05	119.48	112.40
1	С	219	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	А	173	ARG	NE-CZ-NH1	-5.05	117.78	120.30

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There are no chirality outliers.

All (53) planarity outliers are listed	below:
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Mol	Chain	Res	Type	Group
1	А	161	ARG	Sidechain
1	А	173	ARG	Sidechain
1	А	238	ARG	Sidechain
1	А	259	ARG	Sidechain
1	А	281[A]	ARG	Sidechain
1	А	281[B]	ARG	Sidechain
1	А	343	ARG	Sidechain
1	А	39	ARG	Sidechain
1	А	402	ARG	Sidechain
1	А	422	ARG	Sidechain
1	А	491	ARG	Sidechain
1	А	502	ARG	Sidechain
1	А	516	ARG	Sidechain
1	А	72	ARG	Sidechain
1	А	97	ARG	Sidechain
1	В	145	ARG	Sidechain
1	В	161	ARG	Sidechain
1	В	173	ARG	Sidechain
1	В	218	ARG	Sidechain
1	В	224	ARG	Sidechain
1	В	226	SER	Peptide
1	В	238	ARG	Sidechain
1	В	259	ARG	Sidechain
1	В	260	ARG	Sidechain
1	В	281[A]	ARG	Sidechain
1	В	281[B]	ARG	Sidechain
1	В	343	ARG	Sidechain
1	В	361	ARG	Sidechain
1	В	402	ARG	Sidechain
1	В	41	ARG	Sidechain
1	В	491	ARG	Sidechain
1	В	516	ARG	Sidechain



Mol	Chain	Res	Type	Group
1	В	548	LEU	Peptide
1	В	67	ARG	Sidechain
1	В	72	ARG	Sidechain
1	В	86	ARG	Sidechain
1	С	139	ARG	Sidechain
1	С	161	ARG	Sidechain
1	С	173	ARG	Sidechain
1	С	218	ARG	Sidechain
1	С	266	ARG	Sidechain
1	С	281[A]	ARG	Sidechain
1	С	281[B]	ARG	Sidechain
1	С	343	ARG	Sidechain
1	С	402	ARG	Sidechain
1	С	41	ARG	Sidechain
1	С	422	ARG	Sidechain
1	С	491	ARG	Sidechain
1	С	502	ARG	Sidechain
1	С	516	ARG	Sidechain
1	С	520	ARG	Sidechain
1	С	67	ARG	Sidechain
1	С	72	ARG	Sidechain

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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	4192	0	4121	52	0
1	В	4192	0	4121	51	0
1	С	4192	0	4121	52	0
2	А	18	0	24	3	0
2	В	12	0	16	2	0
2	С	12	0	16	1	0
3	А	10	0	0	0	0
3	В	5	0	0	0	0
3	С	10	0	0	1	0
4	А	2	0	0	1	0
4	В	1	0	0	1	0
5	А	108	0	0	2	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 6.

All (155) 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:A:266:ARG:HB3	1:A:266:ARG:HH11	1.10	1.10
1:A:266:ARG:HH11	1:A:266:ARG:CB	1.72	1.03
1:B:227:GLU:HG2	5:B:708:HOH:O	1.62	0.98
1:B:539:LYS:HE2	1:B:543:PHE:CD1	2.05	0.92
1:C:539:LYS:HE3	1:C:543:PHE:CD1	2.04	0.92
1:C:266:ARG:HA	5:C:712:HOH:O	1.70	0.91
1:A:539:LYS:HE2	1:A:543:PHE:CD1	2.09	0.87
1:A:266:ARG:HB3	1:A:266:ARG:NH1	1.93	0.84
1:C:539:LYS:HE3	1:C:543:PHE:CE1	2.16	0.81
1:C:32:VAL:HG13	1:C:36:ALA:HB3	1.67	0.77
1:A:32:VAL:HG13	1:A:36:ALA:HB3	1.67	0.77
1:B:32:VAL:HG13	1:B:36:ALA:HB3	1.68	0.76
1:C:540:LEU:O	1:C:544:ILE:HB	1.87	0.73
1:B:138:TYR:HA	1:B:141:GLN:HE21	1.54	0.72
1:B:540:LEU:O	1:B:544:ILE:HB	1.88	0.72
1:A:540:LEU:O	1:A:544:ILE:HB	1.89	0.72
1:A:41:ARG:CB	1:A:41:ARG:HH11	2.03	0.72
1:C:281[B]:ARG:HH21	1:C:281[B]:ARG:CG	2.05	0.70
1:A:545:LYS:HA	1:A:548:LEU:HD12	1.75	0.69
1:C:545:LYS:HA	1:C:548:LEU:HD12	1.76	0.68
1:B:545:LYS:HA	1:B:548:LEU:HD12	1.75	0.68
1:C:281[A]:ARG:HD3	1:C:435:ILE:O	1.95	0.66
1:B:549:LYS:O	1:B:549:LYS:HG2	1.95	0.66
1:B:539:LYS:CE	1:B:543:PHE:CD1	2.79	0.65
1:A:41:ARG:HH11	1:A:41:ARG:HB3	1.63	0.64
1:A:265:GLU:HG2	1:A:266:ARG:N	2.11	0.64
1:A:86:ARG:HH12	2:A:601:GOL:H31	1.62	0.64
1:A:539:LYS:CE	1:A:543:PHE:CD1	2.80	0.64
1:A:542:ASP:O	1:A:546:GLU:HG3	1.98	0.63
1:B:500:LEU:HD23	1:B:544:ILE:HG21	1.80	0.63
1:B:223:LYS:HD3	1:B:225:LYS:H	1.64	0.63



Chain Non-H H(added) Clashes Symm-Clashes Mol H(model) В 589 3 0 0 0 5 С 80 0 0 1 0 All All 12923 0 0 12419 155

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OADR	8A	DK
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Atom-1	Atom-2	Interatomic	Clash overlap (Å)	
	1100m 2	distance $(Å)$		
1:A:97:ARG:NE	4:A:606:CL:CL	2.69	0.62	
1:B:143:HIS:HB3	5:B:722:HOH:O	1.99	0.62	
1:A:281[A]:ARG:HD3	1:A:435:ILE:O	1.99	0.62	
1:A:41:ARG:HB3	1:A:45:GLU:OE1	1.99	0.62	
1:C:86:ARG:HH22	2:C:601:GOL:H11	1.64	0.62	
1:B:281[A]:ARG:HD3	1:B:435:ILE:O	2.00	0.61	
1:C:265:GLU:HG3	1:C:266:ARG:N	2.15	0.60	
1:C:539:LYS:CE	1:C:543:PHE:CD1	2.82	0.60	
1:C:525:LYS:HE3	1:C:525:LYS:C	2.22	0.59	
1:B:68:GLU:OE1	1:B:72:ARG:HD2	2.02	0.58	
1:A:463:TYR:CD2	1:A:537:LYS:HD2	2.38	0.58	
1:C:542:ASP:O	1:C:546:GLU:HG3	2.04	0.57	
1:A:463:TYR:HD2	1:A:537:LYS:HD2	1.69	0.57	
1:B:463:TYR:HD2	1:B:537:LYS:HD2	1.69	0.57	
1:C:463:TYR:CD2	1:C:537:LYS:HD2	2.40	0.57	
1:A:266:ARG:CB	1:A:266:ARG:NH1	2.56	0.56	
1:B:538:LYS:O	1:B:541:TYR:HB2	2.06	0.56	
1:C:538:LYS:O	1:C:541:TYR:HB2	2.06	0.56	
1:C:421:TYR:OH	1:C:461:ASP:OD2	2.19	0.56	
1:A:86:ARG:NH1	2:A:601:GOL:H31	2.21	0.55	
1:A:538:LYS:O	1:A:541:TYR:HB2	2.06	0.55	
1:B:463:TYR:CD2	1:B:537:LYS:HD2	2.42	0.54	
1:B:421:TYR:OH	1:B:461:ASP:OD2	2.22	0.54	
1:C:463:TYR:HD2	1:C:537:LYS:HD2	1.73	0.54	
1:B:423:GLU:OE1	1:B:516:ARG:HG2	2.09	0.53	
1:B:542:ASP:O	1:B:546:GLU:HG3	2.08	0.53	
1:C:297:PRO:HG2	1:C:300:ASP:OD2	2.09	0.53	
1:A:320:GLN:OE1	1:A:343:ARG:NH2	2.39	0.52	
1:A:290:ASP:HA	5:A:704:HOH:O	2.08	0.52	
1:C:281[B]:ARG:HH21	1:C:281[B]:ARG:HG3	1.73	0.52	
1:B:497:MET:HE3	1:B:537:LYS:HG2	1.92	0.52	
1:B:281[B]:ARG:HH21	1:B:281[B]:ARG:HG3	1.75	0.52	
1:B:257:TYR:HB2	1:B:348:PRO:HG2	1.93	0.51	
1:C:168:LEU:HB3	1:C:169:PRO:HD3	1.91	0.51	
1:A:421:TYR:OH	1:A:461:ASP:OD2	2.24	0.51	
1:A:266:ARG:HH11	1:A:266:ARG:CG	2.22	0.51	
1:A:423:GLU:OE1	1:A:516:ARG:HG2	2.11	0.50	
1:A:428:ARG:NH1	1:A:429:GLU:OE1	2.44	0.50	
1:B:320:GLN:OE1	1:B:343:ARG:NH2	2.44	0.49	
1:B:428:ARG:NH1	1:B:429:GLU:OE1	2.45	0.49	
1:A:257:TYR:HB2	1:A:348:PRO:HG2	1.95	0.48	



8ADK	
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		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1.B.168.LEU.HB3	1.B.169.PRO.HD3	1.95	0.48	
1:C:138:TYB:HA	1:C:141:GLN:HE21	1.77	0.48	
1:B:468:LEU:O	1:B:472:VAL:HG23	2.14	0.48	
1:C:98:GLU:OE2	1:C:102:GLY:HA2	2.13	0.48	
1:C:265:GLU:HG3	1:C:266:ARG:H	1.78	0.48	
1:C:539:LYS:O	1:C:539:LYS:HD3	2.13	0.48	
1:C:257:TYR:HB2	1:C:348:PRO:HG2	1.96	0.48	
1:A:259:ARG:HD2	5:A:742:HOH:O	2.14	0.48	
1:C:428:ARG:NH1	1:C:429:GLU:OE1	2.46	0.47	
1:A:138:TYR:HA	1:A:141:GLN:HE21	1.79	0.47	
1:C:320:GLN:OE1	1:C:343:ARG:NH2	2.44	0.46	
1:A:311:ILE:CG2	1:A:320:GLN:HB3	2.46	0.46	
1:A:41:ARG:CB	1:A:41:ARG:NH1	2.77	0.46	
1:A:38:HIS:C	1:A:39:ARG:HG2	2.36	0.46	
1:A:94:LYS:HE2	1:A:108:PHE:CE1	2.51	0.46	
1:B:137:THR:HB	1:B:138:TYR:CD2	2.50	0.46	
1:A:86:ARG:HH12	2:A:601:GOL:C3	2.27	0.46	
1:C:310:THR:OG1	1:C:313:ASP:HB2	2.15	0.46	
1:A:468:LEU:O	1:A:472:VAL:HG23	2.16	0.46	
1:C:320:GLN:O	1:C:406:ILE:HA	2.15	0.46	
1:B:497:MET:HE3	1:B:537:LYS:CG	2.46	0.46	
1:B:32:VAL:HG13	1:B:36:ALA:CB	2.43	0.45	
1:C:139:ARG:HG3	1:C:139:ARG:HH11	1.81	0.45	
1:C:423:GLU:OE1	1:C:516:ARG:HG2	2.15	0.45	
1:A:320:GLN:O	1:A:406:ILE:HA	2.16	0.45	
1:A:497:MET:HE3	1:A:497:MET:HB2	1.83	0.45	
1:B:465:LYS:O	1:B:469:GLN:HG3	2.16	0.45	
1:C:281[B]:ARG:HH21	1:C:281[B]:ARG:HG2	1.81	0.45	
1:C:228:TYR:O	3:C:604:SO4:O3	2.33	0.45	
1:C:147:LEU:HD12	1:C:147:LEU:HA	1.84	0.45	
1:B:549:LYS:O	1:B:549:LYS:CG	2.62	0.45	
1:B:320:GLN:O	1:B:406:ILE:HA	2.17	0.45	
1:C:539:LYS:O	1:C:539:LYS:CD	2.64	0.45	
1:B:297:PRO:HG2	1:B:300:ASP:OD2	2.17	0.44	
1:A:465:LYS:O	1:A:469:GLN:HG3	2.17	0.44	
1:B:372:GLU:HB3	1:B:374:TYR:CE2	2.52	0.44	
1:B:274:GLY:HA3	1:B:396:ARG:NH1	2.32	0.44	
1:C:547:GLU:OE1	1:C:547:GLU:HA	2.15	0.44	
1:A:513:SER:HA	1:A:516:ARG:HH11	1.83	0.44	
1:C:524:GLU:HA	1:C:524:GLU:OE1	2.17	0.44	
1:C:468:LEU:O	1:C:472:VAL:HG23	2.17	0.44	



8A	DK

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:507:THR:HG22	1:B:510:GLN:CG	2.48	0.43
1:A:168:LEU:HB3	1:A:169:PRO:HD3	2.01	0.43
1:C:491:ARG:NH1	1:C:492:ASP:OD1	2.51	0.43
1:B:218:ARG:HH22	2:B:601:GOL:C3	2.30	0.43
1:B:434:TYR:CE1	1:B:476:LEU:HD21	2.53	0.43
1:C:465:LYS:O	1:C:469:GLN:HG3	2.19	0.43
1:C:507:THR:HG22	1:C:510:GLN:CG	2.49	0.43
1:A:147:LEU:HD12	1:A:147:LEU:HA	1.82	0.42
1:B:514:ILE:CG2	1:B:540:LEU:HD22	2.49	0.42
1:C:69:THR:HA	1:C:70:PRO:C	2.40	0.42
1:C:497:MET:HE3	1:C:537:LYS:CG	2.50	0.42
1:C:497:MET:HE3	1:C:537:LYS:HG2	2.02	0.42
1:B:143:HIS:O	1:B:241:GLN:HG3	2.20	0.42
1:B:514:ILE:HG22	1:B:540:LEU:HD22	2.02	0.42
1:A:507:THR:HG22	1:A:510:GLN:CG	2.49	0.42
1:B:178:LEU:N	1:B:179:PRO:HD2	2.34	0.42
1:A:372:GLU:HB3	1:A:374:TYR:CE2	2.55	0.42
1:B:89:CYS:HA	1:B:110:TRP:CG	2.55	0.41
1:B:97:ARG:HD3	4:B:604:CL:CL	2.57	0.41
1:B:491:ARG:NH1	1:B:492:ASP:OD1	2.53	0.41
1:C:301:VAL:CG2	1:C:474:ALA:HA	2.51	0.41
1:C:311:ILE:CG2	1:C:320:GLN:HB3	2.50	0.41
1:B:97:ARG:HH21	1:B:97:ARG:CB	2.33	0.41
1:B:218:ARG:HH22	2:B:601:GOL:H31	1.85	0.41
1:A:539:LYS:HE3	1:A:543:PHE:CE1	2.56	0.41
1:C:178:LEU:N	1:C:179:PRO:HD2	2.35	0.41
1:A:29:TRP:O	1:A:30:ARG:HD3	2.20	0.41
1:B:513:SER:HA	1:B:516:ARG:HH11	1.85	0.41
1:A:434:TYR:CE1	1:A:476:LEU:HD21	2.56	0.41
1:A:491:ARG:NH1	1:A:492:ASP:OD1	2.54	0.41
1:B:307:ALA:HA	1:B:484:THR:OG1	2.19	0.41
1:C:32:VAL:HG13	1:C:36:ALA:CB	2.45	0.41
1:C:372:GLU:HB3	1:C:374:TYR:CE2	2.56	0.41
1:C:524:GLU:OE1	1:C:524:GLU:CA	2.69	0.41
1:C:513:SER:HA	1:C:516:ARG:HH11	1.85	0.41
1:A:274:GLY:HA3	1:A:396:ARG:NH1	2.36	0.40
1:B:147:LEU:HD12	1:B:147:LEU:HA	1.89	0.40
1:C:29:TRP:O	1:C:30:ARG:HD3	2.21	0.40
1:A:58:HIS:CG	1:A:196:SER:HB2	2.57	0.40
1:A:450:THR:HG22	1:A:480:LEU:HD11	2.04	0.40
1:B:55:GLY:HA3	5:B:766:HOH:O	2.21	0.40



α \cdot \cdot \cdot	C		
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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:HIS:CE1	1:A:361:ARG:HH21	2.40	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	Perce	entiles
1	А	514/578~(89%)	495 (96%)	17 (3%)	2(0%)	34	52
1	В	514/578~(89%)	493 (96%)	19 (4%)	2~(0%)	34	52
1	С	514/578~(89%)	495 (96%)	17 (3%)	2(0%)	34	52
All	All	1542/1734~(89%)	1483 (96%)	53 (3%)	6 (0%)	34	52

All (6) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	В	548	LEU
1	С	100	PRO
1	А	100	PRO
1	В	338	VAL
1	А	338	VAL
1	С	338	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	ntiles
1	А	455/507~(90%)	427 (94%)	28~(6%)	18	33
1	В	455/507~(90%)	429 (94%)	26~(6%)	20	37
1	С	455/507~(90%)	427 (94%)	28~(6%)	18	33
All	All	1365/1521~(90%)	1283 (94%)	82 (6%)	19	34

All (82) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	А	32	VAL
1	А	41	ARG
1	А	59	ARG
1	А	97	ARG
1	А	101	ASP
1	А	122	LYS
1	А	158	SER
1	А	199	LEU
1	А	241	GLN
1	А	265	GLU
1	А	266	ARG
1	А	326	LYS
1	А	337	CYS
1	А	343	ARG
1	А	363	PHE
1	А	417	SER
1	А	462	SER
1	А	500	LEU
1	А	507	THR
1	А	525	LYS
1	А	533	ASN
1	А	534	LYS
1	А	537	LYS
1	А	544	ILE
1	А	545	LYS
1	А	547	GLU
1	А	549	LYS
1	В	30	ARG
1	В	32	VAL
1	В	35	GLU
1	В	59	ARG
1	В	67	ARG
1	В	101	ASP



Mol	Chain	Res	Type
1	В	143	HIS
1	В	158	SER
1	В	199	LEU
1	В	221	THR
1	В	223	LYS
1	В	241	GLN
1	В	286	GLU
1	В	326	LYS
1	В	343	ARG
1	В	363	PHE
1	В	417	SER
1	В	462	SER
1	В	496	GLU
1	В	500	LEU
1	В	507	THR
1	В	524	GLU
1	В	525	LYS
1	В	534	LYS
1	В	544	ILE
1	В	549	LYS
1	С	30	ARG
1	С	49	LEU
1	С	59	ARG
1	С	68	GLU
1	С	101	ASP
1	С	158	SER
1	С	161	ARG
1	С	238	ARG
1	С	241	GLN
1	С	265	GLU
1	С	266	ARG
1	С	337	CYS
1	С	343	ARG
1	С	363	PHE
1	С	376	ASN
1	С	417	SER
1	С	496	GLU
1	С	500	LEU
1	С	507	THR
1	С	520	ARG
1	С	524	GLU
1	С	525	LYS



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Mol	Chain	Res	Type
1	С	533	ASN
1	С	539	LYS
1	С	544	ILE
1	С	545	LYS
1	С	547	GLU
1	С	549	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such side chains are listed below:

Mol	Chain	Res	Type
1	А	141	GLN
1	А	533	ASN
1	В	141	GLN
1	В	191	HIS
1	В	533	ASN
1	С	141	GLN
1	С	533	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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



Mal	Tuno	Chain	Dec	Tiple	B	ond leng	$_{\rm gths}$	E	Bond ang	gles
	vior Type Cham	Chain Res Link			Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	В	602	-	5,5,5	0.38	0	$5,\!5,\!5$	0.66	0
2	GOL	А	602	-	5,5,5	0.20	0	$5,\!5,\!5$	0.38	0
3	SO4	С	603	-	4,4,4	0.19	0	$6,\!6,\!6$	1.24	0
2	GOL	В	601	-	5,5,5	0.16	0	$5,\!5,\!5$	0.66	0
3	SO4	A	604	-	4,4,4	0.35	0	$6,\!6,\!6$	0.77	0
2	GOL	A	601	-	5,5,5	0.37	0	$5,\!5,\!5$	1.06	0
3	SO4	А	605	-	4,4,4	1.42	1 (25%)	$6,\!6,\!6$	0.93	0
3	SO4	В	603	-	4,4,4	0.36	0	6,6,6	0.70	0
2	GOL	С	602	-	5,5,5	0.54	0	$5,\!5,\!5$	0.93	0
2	GOL	С	601	-	5,5,5	0.18	0	$5,\!5,\!5$	0.36	0
2	GOL	А	603	-	5,5,5	0.60	0	$5,\!5,\!5$	1.23	0
3	SO4	С	604	-	4,4,4	0.82	0	$6,\!6,\!6$	0.59	0

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).

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	В	602	-	-	4/4/4/4	-
2	GOL	А	602	-	-	1/4/4/4	-
2	GOL	В	601	-	-	2/4/4/4	-
2	GOL	А	601	-	-	3/4/4/4	-
2	GOL	С	602	-	-	4/4/4/4	-
2	GOL	С	601	-	-	3/4/4/4	-
2	GOL	А	603	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	А	605	SO4	O2-S	2.22	1.58	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	А	601	GOL	C1-C2-C3-O3
2	А	603	GOL	C1-C2-C3-O3
2	А	603	GOL	O2-C2-C3-O3
2	В	602	GOL	C1-C2-C3-O3
2	С	602	GOL	O1-C1-C2-O2
2	С	602	GOL	O1-C1-C2-C3
2	С	602	GOL	C1-C2-C3-O3
2	С	602	GOL	O2-C2-C3-O3
2	В	601	GOL	O2-C2-C3-O3
2	А	601	GOL	O1-C1-C2-C3
2	А	603	GOL	O1-C1-C2-C3
2	В	601	GOL	C1-C2-C3-O3
2	С	601	GOL	O1-C1-C2-C3
2	В	602	GOL	O2-C2-C3-O3
2	В	602	GOL	O1-C1-C2-O2
2	С	601	GOL	O2-C2-C3-O3
2	А	602	GOL	C1-C2-C3-O3
2	В	602	GOL	O1-C1-C2-C3
2	A	601	GOL	O2-C2-C3-O3
2	А	603	GOL	O1-C1-C2-O2
2	С	601	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	601	GOL	2	0
2	А	601	GOL	3	0
2	С	601	GOL	1	0
3	С	604	SO4	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, 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	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	517/578~(89%)	0.05	16 (3%) 49 51	37, 60, 111, 158	0
1	В	517/578~(89%)	0.25	35 (6%) 17 17	39, 67, 113, 158	0
1	С	517/578~(89%)	0.50	45 (8%) 10 9	38, 64, 118, 152	0
All	All	1551/1734~(89%)	0.27	96 (6%) 20 21	37, 64, 113, 158	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	541	TYR	8.1
1	С	500	LEU	6.6
1	В	533	ASN	6.2
1	А	525	LYS	6.1
1	С	540	LEU	5.6
1	С	544	ILE	5.3
1	С	467	LEU	5.1
1	С	548	LEU	5.0
1	С	514	ILE	4.9
1	С	545	LYS	4.4
1	С	542	ASP	4.4
1	В	494	PHE	4.4
1	С	518	TYR	4.3
1	С	515	LEU	4.3
1	С	499	LEU	4.3
1	В	225	LYS	4.3
1	С	511	LEU	4.3
1	В	541	TYR	4.2
1	В	540	LEU	4.2
1	С	543	PHE	4.2
1	В	525	LYS	4.0
1	В	536	SER	4.0
1	С	503	ASN	3.9



Mol	Chain	Res	Type	RSRZ	
1	С	501	PHE	3.9	
1	А	522	ILE	3.9	
1	С	496	GLU	3.8	
1	А	548	LEU	3.8	
1	В	535	ALA	3.8	
1	С	534	LYS	3.8	
1	С	549	LYS	3.7	
1	В	544	ILE	3.6	
1	С	494	PHE	3.5	
1	В	518	TYR	3.5	
1	А	533	ASN	3.5	
1	С	522	ILE	3.5	
1	В	547	GLU	3.5	
1	А	541	TYR	3.4	
1	В	543	PHE	3.4	
1	В	26	ASP	3.4	
1	С	538	LYS	3.3	
1	А	515	LEU	3.3	
1	С	298	LEU	3.2	
1	В	224	ARG	3.2	
1	С	547	GLU	3.2	
1	С	521	LEU	3.2	
1	С	470	LEU	3.1	
1	В	500	LEU	3.1	
1	В	545	LYS	3.0	
1	В	520	ARG	3.0	
1	С	513	SER	2.9	
1	С	505	GLY	2.8	
1	В	522	ILE	2.8	
1	С	517	SER	2.8	
1	В	542	ASP	2.8	
1	С	525	LYS	2.8	
1	С	490	PHE	2.8	
1	В	459	GLY	2.7	
1	С	536	SER	2.7	
1	С	463	TYR	2.7	
1	А	545	LYS	2.7	
1	В	534	LYS	2.7	
1	В	222	LEU	2.6	
1	В	490	PHE	2.6	
1	В	458	PHE	2.6	
1	С	100	PRO	2.6	



Mol	Chain	Res	Type	RSRZ
1	В	549	LYS	2.6
1	C	510	GLN	2.6
1	С	101	ASP	2.6
1	А	543	PHE	2.5
1	А	540	LEU	2.5
1	С	520	ARG	2.5
1	В	467	LEU	2.5
1	С	102	GLY	2.5
1	В	519	SER	2.5
1	В	521	LEU	2.4
1	С	486	GLY	2.4
1	А	520	ARG	2.4
1	В	415	ALA	2.4
1	В	548	LEU	2.4
1	А	518	TYR	2.3
1	А	500	LEU	2.3
1	С	546	GLU	2.3
1	С	498	TRP	2.3
1	В	501	PHE	2.3
1	В	463	TYR	2.3
1	А	501	PHE	2.3
1	С	502	ARG	2.2
1	В	488	VAL	2.2
1	А	544	ILE	2.2
1	С	497	MET	2.2
1	В	223	LYS	2.2
1	А	490	PHE	2.1
1	С	506	THR	2.1
1	С	29	TRP	2.0
1	А	521	LEU	2.0
1	В	524	GLU	2.0

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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	$B-factors(A^2)$	Q<0.9
2	GOL	В	602	6/6	0.73	0.27	96,104,106,122	0
2	GOL	А	602	6/6	0.78	0.25	77,101,109,111	0
3	SO4	А	605	5/5	0.85	0.18	56,60,61,160	0
3	SO4	С	604	5/5	0.85	0.18	65,72,160,165	0
2	GOL	С	602	6/6	0.86	0.21	57,79,89,96	0
2	GOL	С	601	6/6	0.87	0.16	83,91,95,98	0
2	GOL	В	601	6/6	0.89	0.12	88,94,98,100	0
2	GOL	А	603	6/6	0.89	0.18	48,76,80,82	0
4	CL	А	607	1/1	0.91	0.22	75, 75, 75, 75, 75	0
2	GOL	А	601	6/6	0.93	0.10	60,69,78,82	0
3	SO4	В	603	5/5	0.96	0.17	46,68,121,141	0
4	CL	В	604	1/1	0.97	0.14	85,85,85,85	0
4	CL	А	606	1/1	0.99	0.16	$65,\!65,\!65,\!65$	0
3	SO4	С	603	5/5	0.99	0.12	58,65,74,83	0
3	SO4	А	604	5/5	0.99	0.14	45,45,55,66	0

6.5 Other polymers (i)

There are no such residues in this entry.

