

Full wwPDB X-ray Structure Validation Report (i)

Apr 11, 2022 - 10:07 am BST

PDB ID	:	7QK7
Title	:	Crystal structure of the APO form of ALDH1A3
Authors	:	Castellvi, A.; Farres, J.
Deposited on	:	2021-12-17
Resolution	:	2.29 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 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	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.29 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}	130704	6980 (2.30-2.26)	
Clashscore	141614	7711 (2.30-2.26)	
Ramachandran outliers	138981	7597 (2.30-2.26)	
Sidechain outliers	138945	7598 (2.30-2.26)	
RSRZ outliers	127900	6849 (2.30-2.26)	

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		
			22%		
1	А	529	86%	6%	8%
			23%		
1	В	529	85%	7%	8%

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	PEG	А	603	-	-	Х	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7811 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	А	489	Total 3711	C 2369	N 635	O 686	S 21	0	2	0
1	В	489	Total 3688	C 2358	N 621	O 687	S 22	0	3	0

• Molecule 1 is a protein called Aldehyde dehydrogenase family 1 member A3.

Residue	Modelled	Actual	Comment	Reference
-16	HIS	-	expression tag	UNP P47895
-15	HIS	-	expression tag	UNP P47895
-14	HIS	-	expression tag	UNP P47895
-13	HIS	-	expression tag	UNP P47895
-12	HIS	-	expression tag	UNP P47895
-11	HIS	-	expression tag	UNP P47895
-10	LEU	-	expression tag	UNP P47895
-9	GLU	-	expression tag	UNP P47895
-8	SER	-	expression tag	UNP P47895
-7	THR	-	expression tag	UNP P47895
-6	SER	-	expression tag	UNP P47895
-5	LEU	-	expression tag	UNP P47895
-4	TYR	-	expression tag	UNP P47895
-3	LYS	-	expression tag	UNP P47895
-2	LYS	-	expression tag	UNP P47895
-1	ALA	-	expression tag	UNP P47895
0	GLY	-	expression tag	UNP P47895
-16	HIS	-	expression tag	UNP P47895
-15	HIS	-	expression tag	UNP P47895
-14	HIS	-	expression tag	UNP P47895
-13	HIS	-	expression tag	UNP P47895
-12	HIS	-	expression tag	UNP P47895
-11	HIS	-	expression tag	UNP P47895
-10	LEU	-	expression tag	UNP P47895
-9	GLU	-	expression tag	UNP P47895
	Residue -16 -15 -14 -13 -12 -11 -10 -9 -8 -7 -6 -5 -4 -3 -2 -1 0 -16 -15 -14 -13 -12 -11 0 -15 -14 -13 -12 -11 -10 -9	Residue Modelled -16 HIS -15 HIS -14 HIS -13 HIS -12 HIS -11 HIS -10 LEU -9 GLU -9 GLU -8 SER -7 THR -6 SER -5 LEU -4 TYR -3 LYS -2 LYS -1 ALA 0 GLY -16 HIS -15 HIS -15 HIS -14 HIS -13 HIS -13 HIS -14 HIS -13 HIS -11 HIS -11 HIS -10 LEU -9 GLU	Residue Modelled Actual -16 HIS - -15 HIS - -14 HIS - -13 HIS - -13 HIS - -13 HIS - -11 HIS - -11 HIS - -11 HIS - -10 LEU - -9 GLU - -9 GLU - -8 SER - -7 THR - -6 SER - -5 LEU - -4 TYR - -3 LYS - -1 ALA - 0 GLY - -16 HIS - -15 HIS - -13 HIS - -13 HIS - -11 <td< td=""><td>ResidueModelledActualComment-16HIS-expression tag-15HIS-expression tag-14HIS-expression tag-13HIS-expression tag-13HIS-expression tag-11HIS-expression tag-11HIS-expression tag-11HIS-expression tag-10LEU-expression tag-9GLU-expression tag-9GLU-expression tag-9GLU-expression tag-9GLU-expression tag-9GLU-expression tag-7THR-expression tag-6SER-expression tag-5LEU-expression tag-4TYR-expression tag-3LYS-expression tag-1ALA-expression tag-1ALA-expression tag-16HIS-expression tag-15HIS-expression tag-14HIS-expression tag-13HIS-expression tag-14HIS-expression tag-13HIS-expression tag-14HIS-expression tag-13HIS-expression tag</td></td<>	ResidueModelledActualComment -16 HIS-expression tag -15 HIS-expression tag -14 HIS-expression tag -13 HIS-expression tag -13 HIS-expression tag -11 HIS-expression tag -11 HIS-expression tag -11 HIS-expression tag -10 LEU-expression tag -9 GLU-expression tag -7 THR-expression tag -6 SER-expression tag -5 LEU-expression tag -4 TYR-expression tag -3 LYS-expression tag -1 ALA-expression tag -1 ALA-expression tag -16 HIS-expression tag -15 HIS-expression tag -14 HIS-expression tag -13 HIS-expression tag -14 HIS-expression tag -13 HIS-expression tag -14 HIS-expression tag -13 HIS-expression tag

There are 34 discrepancies between the modelled and reference sequences:



Contentia	ca from pre	erous page			
Chain	Residue	Modelled	Actual	Comment	Reference
В	-8	SER	-	expression tag	UNP P47895
В	-7	THR	-	expression tag	UNP P47895
В	-6	SER	-	expression tag	UNP P47895
В	-5	LEU	-	expression tag	UNP P47895
В	-4	TYR	-	expression tag	UNP P47895
В	-3	LYS	-	expression tag	UNP P47895
В	-2	LYS	-	expression tag	UNP P47895
В	-1	ALA	-	expression tag	UNP P47895
В	0	GLY	-	expression tag	UNP P47895

• Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





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

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	175	Total O 175 175	0	0
4	В	182	Total O 183 183	0	1



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: Aldehyde dehydrogenase family 1 member A3









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants	82.96Å 90.13Å 159.19Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	48.44 - 2.29	Depositor
Resolution (A)	48.44 - 2.29	EDS
% Data completeness	98.7 (48.44-2.29)	Depositor
(in resolution range)	98.7 (48.44 - 2.29)	EDS
R_{merge}	0.12	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.87 (at 2.29 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.10.3 (18-SEP-2020)	Depositor
B B.	0.190 , 0.227	Depositor
n, n_{free}	0.194 , 0.231	DCC
R_{free} test set	2559 reflections $(4.75%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	44.0	Xtriage
Anisotropy	0.799	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for $twinning^2$	$ L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7811	wwPDB-VP
Average B, all atoms $(Å^2)$	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.71% 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, PEG

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	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.40	0/3789	0.57	0/5145	
1	В	0.43	0/3765	0.59	0/5113	
All	All	0.42	0/7554	0.58	0/10258	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3711	0	3659	18	0
1	В	3688	0	3624	19	0
2	А	21	0	30	7	0
2	В	21	0	30	2	0
3	А	12	0	16	1	0
4	А	175	0	0	0	0
4	В	183	0	0	0	0
All	All	7811	0	7359	36	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 2.



A + 1	A 4 a ma 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:A:603:PEG:H21	1:B:266:LYS:HZ3	1.34	0.92
2:A:603:PEG:H21	1:B:266:LYS:NZ	1.89	0.88
1:B:377:ALA:HB2	1:B:405:MET:HE1	1.66	0.76
1:B:371:SER:HA	1:B:374:LYS:HE2	1.67	0.75
1:B:377:ALA:HB2	1:B:405:MET:CE	2.31	0.59
1:B:29:VAL:HG21	1:B:61:CYS:SG	2.45	0.57
1:B:371:SER:HA	1:B:374:LYS:CE	2.33	0.57
1:A:377:ALA:HB2	1:A:405:MET:HE1	1.87	0.56
1:B:269:ALA:HB1	1:B:275:LYS:HG3	1.87	0.56
1:B:373:LYS:HE2	1:B:379:LEU:HD22	1.88	0.56
1:A:136:GLY:HA2	2:A:601:PEG:H22	1.87	0.55
1:A:481:LYS:H	2:B:603:PEG:H31	1.71	0.55
1:A:325:GLN:NE2	1:A:325:GLN:H	2.05	0.55
1:A:277:VAL:H	2:A:603:PEG:H31	1.73	0.53
1:A:259:THR:HA	1:A:281:LEU:HD13	1.90	0.53
1:A:377:ALA:HB2	1:A:405:MET:CE	2.41	0.51
1:B:251:ASN:HB3	2:B:603:PEG:H41	1.91	0.51
1:A:276:ARG:HA	2:A:603:PEG:H31	1.91	0.50
1:B:33:LYS:NZ	1:B:42:GLU:HG3	2.26	0.50
1:A:382:GLY:H	3:A:604:GOL:H2	1.77	0.48
1:A:263:LYS:O	1:A:267:GLU:HG3	2.14	0.47
1:B:50:ALA:HB1	1:B:59:GLN:HG3	1.98	0.45
1:A:155:THR:HB	2:A:605:PEG:H32	2.00	0.44
1:B:179:PRO:HD3	1:B:256:THR:HB	2.00	0.44
1:A:214:LEU:HD21	1:A:234:PRO:HG3	1.99	0.43
1:A:179:PRO:HD3	1:A:256:THR:HB	2.00	0.43
1:A:465:ILE:HD12	1:B:505:ILE:HG12	1.99	0.43
2:A:603:PEG:H21	1:B:266:LYS:HZ1	1.78	0.43
1:B:214:LEU:HD21	1:B:234:PRO:HG3	2.01	0.43
1:B:461:GLY:HA3	1:B:478:GLY:O	2.19	0.42
1:B:253:ILE:HG23	1:B:277:VAL:HG13	2.01	0.42
1:A:29:VAL:HG21	1:A:61:CYS:SG	2.60	0.41
1:A:310:GLN:HG3	1:A:353:GLN:HG3	2.01	0.41
1:B:259:THR:HA	1:B:281:LEU:HD13	2.01	0.41
1:A:329:GLU:HG3	1:A:333:ARG:HE	1.85	0.41
1:A:276:ARG:N	1:A:276:ARG:HD2	2.35	0.41

All (36) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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		Allowed	Outliers	Percentiles
1	А	489/529~(92%)	467 (96%)	22~(4%)	0	100 100
1	В	490/529~(93%)	466 (95%)	21 (4%)	3~(1%)	25 29
All	All	979/1058~(92%)	933~(95%)	43 (4%)	3 (0%)	41 49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	388	ASP
1	В	389	LYS
1	В	438	GLY

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	383/437~(88%)	375~(98%)	8 (2%)	53 68
1	В	379/437~(87%)	371 (98%)	8 (2%)	53 68
All	All	762/874~(87%)	746~(98%)	16 (2%)	53 68

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	26	ASN
1	А	98	ARG
1	А	118	GLU



Mol	Chain	Res	Type
1	А	121	ASP
1	А	196	CYS
1	А	324	GLU
1	А	404	ASN
1	А	413	PHE
1	В	26	ASN
1	В	28	GLU
1	В	121	ASP
1	В	133	ASP
1	В	196	CYS
1	В	203	LEU
1	В	360	LYS
1	В	413	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	325	GLN
1	В	83	GLN
1	В	152	GLN
1	В	304	GLN
1	В	325	GLN

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)

8 ligands are modelled in this entry.



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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	Turne	Chain	Dec	Dec Link		ond leng	gths	E	Bond ang	gles
	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	PEG	A	603	-	6,6,6	0.30	0	$5,\!5,\!5$	0.19	0
2	PEG	В	603	-	6,6,6	0.10	0	$5,\!5,\!5$	0.12	0
2	PEG	A	601	-	$6,\!6,\!6$	0.17	0	$5,\!5,\!5$	0.13	0
3	GOL	А	602	-	$5,\!5,\!5$	0.09	0	$5,\!5,\!5$	0.30	0
2	PEG	A	605	-	6,6,6	0.18	0	$5,\!5,\!5$	0.16	0
2	PEG	В	602	-	6,6,6	0.16	0	$5,\!5,\!5$	0.18	0
3	GOL	А	604	-	$5,\!5,\!5$	0.09	0	$5,\!5,\!5$	0.22	0
2	PEG	В	601	-	6,6,6	0.19	0	$5,\!5,\!5$	0.08	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	PEG	А	603	-	-	2/4/4/4	-
2	PEG	В	603	-	-	0/4/4/4	-
2	PEG	А	601	-	-	1/4/4/4	-
3	GOL	А	602	-	-	0/4/4/4	-
2	PEG	А	605	-	-	0/4/4/4	-
2	PEG	В	602	-	-	2/4/4/4	-
3	GOL	А	604	-	-	0/4/4/4	-
2	PEG	В	601	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	603	PEG	O2-C3-C4-O4
2	В	602	PEG	O1-C1-C2-O2
2	А	603	PEG	O1-C1-C2-O2



Mal	Chain	Dec	Trong	A
Conti	nued from	n previe	ous page	

Mol	Chain	\mathbf{Res}	Type	Atoms
2	В	601	PEG	C1-C2-O2-C3
2	А	601	PEG	C4-C3-O2-C2
2	В	602	PEG	C4-C3-O2-C2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	603	PEG	5	0
2	В	603	PEG	2	0
2	А	601	PEG	1	0
2	А	605	PEG	1	0
3	А	604	GOL	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		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9	
1	А	489/529~(92%)	1.61	118 (24%)	0	0	34, 54, 81, 108	0
1	В	489/529~(92%)	1.58	123~(25%)	0	0	35, 53, 93, 108	0
All	All	978/1058~(92%)	1.59	241 (24%)	0	0	34, 53, 90, 108	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	344	GLY	13.7
1	В	346	PRO	13.0
1	А	23	PRO	10.2
1	А	22	ARG	10.1
1	А	377	ALA	9.9
1	В	21	PRO	9.9
1	А	376	GLY	9.1
1	В	341	ARG	8.4
1	А	372	GLY	8.4
1	В	388	ASP	8.2
1	В	383	GLY	8.0
1	А	20	LEU	7.9
1	В	348	ASP	7.5
1	В	349	VAL	7.4
1	В	389	LYS	7.1
1	А	371	SER	7.0
1	А	389	LYS	6.9
1	А	386	MET	6.8
1	В	382	GLY	6.8
1	В	42	GLU	6.6
1	А	385	ALA	6.5
1	А	379	LEU	6.4
1	А	21	PRO	6.3
1	А	409	LYS	6.3



Mol	Chain	Res	Type	RSRZ
1	В	374	LYS	6.0
1	А	384	SER	5.9
1	А	383	GLY	5.8
1	В	24	ILE	5.6
1	В	343	VAL	5.4
1	А	90	ARG	5.4
1	А	27	LEU	5.3
1	В	386	MET	5.3
1	А	388	ASP	5.2
1	В	113	THR	5.2
1	В	353	GLN	5.1
1	А	348	ASP	5.1
1	В	112	ALA	4.9
1	A	351	THR	4.9
1	В	351	THR	4.8
1	В	352	GLU	4.8
1	А	31	PHE	4.7
1	А	28	GLU	4.7
1	В	376	GLY	4.7
1	А	397	VAL	4.6
1	В	69	PRO	4.6
1	А	406	ARG	4.6
1	В	25	ARG	4.6
1	В	336	GLU	4.6
1	А	343	VAL	4.6
1	В	209	THR	4.5
1	В	31	PHE	4.4
1	А	32	THR	4.4
1	В	39	GLU	4.4
1	А	112	ALA	4.4
1	А	346	PRO	4.4
1	А	299	VAL	4.3
1	А	24	ILE	4.3
1	A	279	LEU	4.3
1	В	327	TYR	4.2
1	A	156	ILE	4.2
1	В	58	GLU	4.1
1	А	349	VAL	4.1
1	В	22	ARG	4.1
1	В	364	LYS	4.1
1	А	209	THR	4.0
1	В	403	ASP	4.0



Mol	Chain	Res	Type	RSRZ
1	В	357	ILE	4.0
1	А	313[A]	CYS	4.0
1	А	368	LEU	4.0
1	В	335	VAL	4.0
1	А	436	ASP	3.9
1	А	387	GLU	3.9
1	А	407	ILE	3.9
1	В	345	ASP	3.8
1	В	377	ALA	3.8
1	В	158	THR	3.8
1	А	345	ASP	3.8
1	А	58	GLU	3.7
1	В	114	LEU	3.7
1	A	403	ASP	3.7
1	А	374	LYS	3.6
1	В	63	VAL	3.6
1	В	414	GLY	3.6
1	В	40	TRP	3.5
1	В	27	LEU	3.5
1	В	82	PHE	3.5
1	А	390	GLY	3.5
1	В	371	SER	3.5
1	А	335	VAL	3.4
1	В	370	GLU	3.4
1	В	380	GLU	3.4
1	А	427	GLU	3.3
1	А	227	PRO	3.3
1	А	418	PRO	3.3
1	А	203	LEU	3.3
1	А	329	GLU	3.3
1	А	507	LEU	3.3
1	A	421	LYS	3.2
1	В	219	LEU	3.2
1	A	357	ILE	3.2
1	А	122	THR	3.2
1	В	368	LEU	3.2
1	В	358	ASP	3.2
1	A	185	LEU	3.2
1	В	413	PHE	3.1
1	А	93	ALA	3.1
1	А	369	ILE	3.1
1	А	475	ALA	3.1



Mol	Chain	Res	Type	RSRZ
1	В	338	ALA	3.1
1	А	498	THR	3.1
1	А	29	VAL	3.0
1	В	350	LYS	3.0
1	В	61	CYS	3.0
1	А	471	LEU	3.0
1	В	116	ALA	3.0
1	В	372	GLY	3.0
1	А	365	ILE	2.9
1	А	333	ARG	2.9
1	В	384	SER	2.9
1	В	60	ILE	2.9
1	А	114	LEU	2.9
1	В	385	ALA	2.9
1	В	295	LEU	2.9
1	А	347	PHE	2.8
1	В	404	ASN	2.8
1	А	147	TRP	2.8
1	А	144	PHE	2.8
1	В	300	GLU	2.8
1	А	352	GLU	2.8
1	А	338	ALA	2.7
1	В	57	ARG	2.8
1	В	362	PHE	2.7
1	В	44	LYS	2.7
1	А	381	CYS	2.7
1	А	321	PHE	2.7
1	A	291	ALA	2.7
1	В	52	CYS	2.7
1	В	333	ARG	2.7
1	В	133	ASP	2.7
1	В	132	ILE	2.7
1	В	307	PHE	2.7
1	А	490	GLY	2.7
1	В	20	LEU	2.7
1	В	405	MET	2.7
1	В	426	GLU	2.7
1	A	176	ALA	2.7
1	В	397	VAL	2.7
1	А	61	CYS	2.6
1	В	156	ILE	2.6
1	В	492	TYR	2.6



Mol	Chain	Res	Type	RSRZ
1	В	416	VAL	2.6
1	В	392	PHE	2.6
1	А	288	ILE	2.6
1	В	478	GLY	2.6
1	В	365	ILE	2.6
1	А	380	GLU	2.6
1	А	437	TYR	2.6
1	В	339	LYS	2.6
1	А	391	LEU	2.5
1	А	337	TYR	2.5
1	А	493	ALA	2.5
1	В	375	GLU	2.5
1	В	214	LEU	2.5
1	В	279	LEU	2.5
1	А	492	TYR	2.5
1	А	294	ASP	2.5
1	А	278	THR	2.5
1	В	90	ARG	2.5
1	А	140	THR	2.5
1	В	73	LYS	2.5
1	В	67	ASP	2.5
1	В	277	VAL	2.4
1	В	500	VAL	2.4
1	В	38	ASN	2.4
1	А	339	LYS	2.4
1	А	255	PHE	2.4
1	В	470	ALA	2.4
1	А	129	ALA	2.4
1	В	110	ASP	2.4
1	В	439	LEU	2.4
1	A	422	PHE	2.4
1	А	223	ALA	2.4
1	В	391	LEU	2.3
1	В	30	LYS	2.3
1	A	39	GLU	2.3
1	А	370	GLU	2.3
1	В	86	SER	2.3
1	В	332	ARG	2.3
1	В	147	TRP	2.3
1	А	190	LYS	2.3
1	А	425	ILE	2.3
1	А	206	ALA	2.3



Mol	Chain	Res	Type	RSRZ
1	А	260	GLU	2.3
1	В	154	LYS	2.3
1	В	103	LEU	2.3
1	В	507	LEU	2.3
1	В	153	GLY	2.3
1	А	161	ASN	2.3
1	В	393	ILE	2.3
1	В	108	GLU	2.2
1	В	337	TYR	2.2
1	В	118	GLU	2.2
1	А	442	ALA	2.2
1	А	455	ALA	2.2
1	В	315	THR	2.2
1	В	423	LYS	2.2
1	А	26	ASN	2.2
1	А	179	PRO	2.2
1	А	500	VAL	2.2
1	В	126	PHE	2.2
1	А	148	ALA	2.2
1	В	291	ALA	2.2
1	А	253	ILE	2.2
1	В	356	GLN	2.2
1	А	175	GLY	2.2
1	А	487	ARG	2.1
1	В	308	PHE	2.1
1	А	448	LEU	2.1
1	А	143	TYR	2.1
1	А	168	HIS	2.1
1	В	233	VAL	2.1
1	В	320	VAL	2.1
1	В	479	GLY	2.1
1	В	278	THR	2.1
1	A	336	GLU	2.1
1	A	155	THR	2.1
1	A	153	GLY	2.1
1	A	238	PRO	2.1
1	А	281	LEU	2.1
1	В	29	VAL	2.1
1	В	468	TYR	2.1
1	В	274	LEU	2.1
1	A	405	MET	2.1
1	В	77	ALA	2.1



Mol	Chain	hain Res '		RSRZ
1	А	162	VAL	2.1
1	А	491	GLU	2.0
1	В	422	PHE	2.0
1	В	191	LEU	2.0
1	В	127	LEU	2.0
1	В	369	ILE	2.0
1	А	92	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no 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	PEG	А	605	7/7	0.57	0.38	$69,\!69,\!69,\!69$	0
2	PEG	В	603	7/7	0.60	0.39	86,87,87,87	0
3	GOL	А	604	6/6	0.70	0.17	88,88,88,88	0
2	PEG	В	601	7/7	0.74	0.25	71,72,73,73	0
2	PEG	В	602	7/7	0.79	0.26	68,69,70,70	0
2	PEG	А	603	7/7	0.82	0.43	58,59,61,62	0
3	GOL	А	602	6/6	0.85	0.40	68,69,69,69	0
2	PEG	А	601	7/7	0.88	0.39	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.

