



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:37 PM GMT

PDB ID : 4TWK
Title : Crystal structure of human two pore domain potassium ion channel TREK1 (K2P2.1)
Authors : Pike, A.C.W.; Dong, Y.Y.; Tessitore, A.; Goubin, S.; Strain-Damerell, C.; Mukhopadhyay, S.; Kupinska, K.; Wang, D.; Chalk, R.; Berridge, G.; Grieben, M.; Shrestha, L.; Ang, J.H.; Mackenzie, A.; Quigley, A.; Bushell, S.R.; Shintre, C.A.; Faust, B.; Chu, A.; Dong, L.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Burgess-Brown, N.A.; Carpenter, E.P.
Deposited on : 2014-06-30
Resolution : 2.60 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

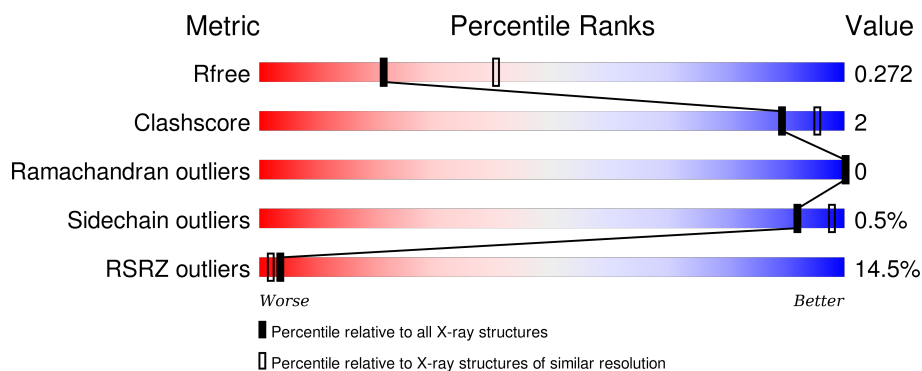
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	283	<div> <div>14%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>10%</div> </div> </div>
1	B	283	<div> <div>12%</div> <div> <div></div> <div>81%</div> <div>•</div> <div>15%</div> </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	37X	A	405	-	-	-	X
4	MG	A	407	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3941 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 Potassium channel subfamily K member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1908	1271	301	331	5			
1	B	241	Total	C	N	O	S	0	0	0
			1838	1232	285	316	5			

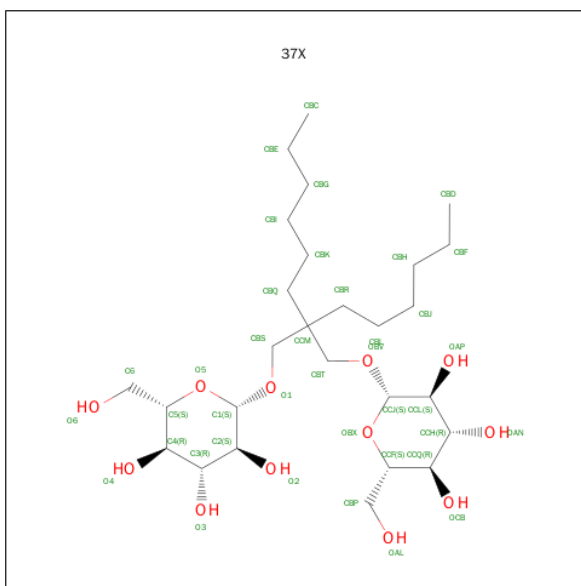
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP O95069
A	301	ALA	-	expression tag	UNP O95069
A	302	GLU	-	expression tag	UNP O95069
A	303	ASN	-	expression tag	UNP O95069
A	304	LEU	-	expression tag	UNP O95069
A	305	TYR	-	expression tag	UNP O95069
A	306	PHE	-	expression tag	UNP O95069
A	307	GLN	-	expression tag	UNP O95069
B	25	MET	-	initiating methionine	UNP O95069
B	301	ALA	-	expression tag	UNP O95069
B	302	GLU	-	expression tag	UNP O95069
B	303	ASN	-	expression tag	UNP O95069
B	304	LEU	-	expression tag	UNP O95069
B	305	TYR	-	expression tag	UNP O95069
B	306	PHE	-	expression tag	UNP O95069
B	307	GLN	-	expression tag	UNP O95069

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	2	Total	K	0	0
			2	2		

- Molecule 3 is Octyl Glucose Neopentyl Glycol (three-letter code: 37X) (formula: $C_{27}H_{52}O_{12}$).

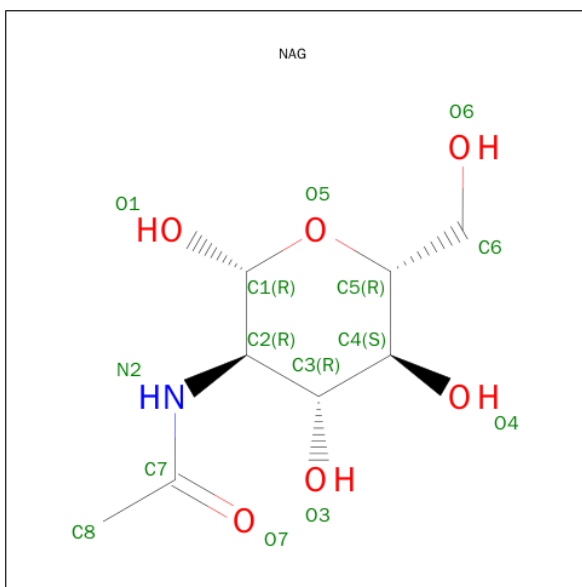


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 18	C 12	O 6	0	0
3	A	1	Total 25	C 19	O 6	0	0
3	A	1	Total 39	C 27	O 12	0	0
3	A	1	Total 29	C 22	O 7	0	0
3	B	1	Total 39	C 27	O 12	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

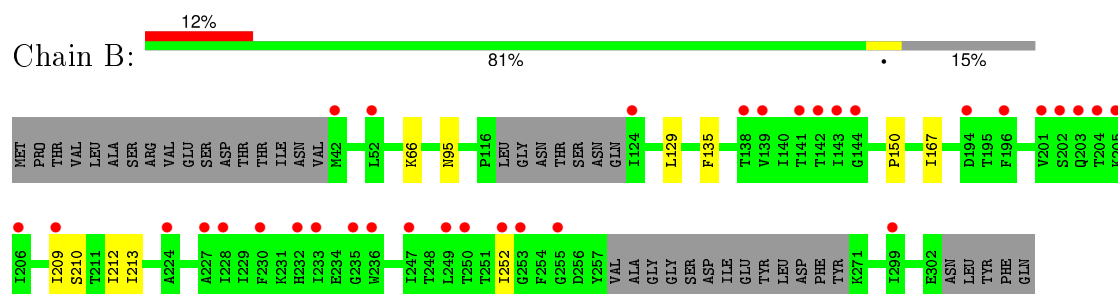


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	14	Total	O	0	0
			14	14		

- Molecule 1: Potassium channel subfamily K member 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.47Å 105.97Å 128.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.94 – 2.60 33.88 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.94-2.60) 99.7 (33.88-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.87 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.231 , 0.258 0.246 , 0.272	Depositor DCC
R_{free} test set	1607 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 89.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 31710 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3941	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 37X, MG, K, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.47	0/1953	0.58	0/2667
1	B	0.48	0/1884	0.58	1/2573 (0.0%)
All	All	0.48	0/3837	0.58	1/5240 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	ASN	CA-CB-CG	5.06	124.54	113.40

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	A	1908	0	1893	15	0
1	B	1838	0	1834	7	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	111	0	140	2	0
3	B	39	0	52	1	0
4	A	1	0	0	0	0
5	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	13	0	0	0	0
6	B	14	0	0	0	0
All	All	3941	0	3932	19	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.

All (19) 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:105:GLN:HB3	3:B:402:37X:H32	1.76	0.68
1:A:143:ILE:HG23	1:A:253:GLY:HA2	1.88	0.54
1:A:129:LEU:HG	1:B:66:LYS:HD2	1.91	0.53
1:A:66:LYS:HD2	1:B:129:LEU:HG	1.93	0.51
1:A:78:THR:O	1:A:82:ILE:HG12	2.11	0.51
1:A:252:ILE:HD11	1:B:167:ILE:HD11	1.94	0.49
1:A:209:ILE:HA	1:A:212:ILE:HD12	1.95	0.48
1:B:209:ILE:HA	1:B:212:ILE:HD12	1.95	0.48
3:A:406:37X:H36	3:A:406:37X:H34	1.98	0.46
1:A:298:VAL:HG21	3:A:406:37X:H22	1.99	0.45
1:A:145:PHE:HD1	1:A:254:PHE:HE1	1.66	0.44
1:B:135:PHE:CZ	1:B:150:PRO:HD3	2.53	0.44
1:A:196:PHE:HD1	1:A:201:VAL:HG21	1.82	0.43
1:A:43:LYS:O	1:A:47:VAL:HG23	2.19	0.42
1:A:219:CYS:O	1:A:223:VAL:HB	2.20	0.42
1:A:117:LEU:HA	1:A:118:GLY:HA2	1.93	0.42
1:A:167:ILE:HD11	1:B:252:ILE:HD11	2.02	0.41
1:A:110:ILE:HG12	1:A:115:ILE:HG12	2.03	0.41
1:B:210:SER:HA	1:B:213:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	249/283 (88%)	246 (99%)	3 (1%)	0	100	100
1	B	235/283 (83%)	229 (97%)	6 (3%)	0	100	100
All	All	484/566 (86%)	475 (98%)	9 (2%)	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	194/240 (81%)	192 (99%)	2 (1%)	82	94
1	B	189/240 (79%)	189 (100%)	0	100	100
All	All	383/480 (80%)	381 (100%)	2 (0%)	92	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	PHE
1	A	306	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	105	GLN

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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	37X	A	403	-	18,18,40	0.31	0	21,26,54	1.75	1 (4%)
3	37X	A	404	-	25,25,40	0.35	0	29,33,54	0.87	2 (6%)
3	37X	A	405	-	40,40,40	0.31	0	48,54,54	1.24	3 (6%)
3	37X	A	406	-	29,29,40	0.41	0	32,37,54	1.31	2 (6%)
5	NAG	B	401	1	14,14,15	0.30	0	15,19,21	0.55	0
3	37X	B	402	-	40,40,40	0.28	0	48,54,54	0.62	2 (4%)

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	37X	A	403	-	-	0/11/31/70	0/1/1/2
3	37X	A	404	-	-	0/20/40/70	0/1/1/2
3	37X	A	405	-	-	0/30/70/70	0/2/2/2
3	37X	A	406	-	-	0/26/46/70	0/1/1/2
5	NAG	B	401	1	-	0/6/23/26	0/1/1/1
3	37X	B	402	-	-	0/30/70/70	0/2/2/2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	37X	CBS-CCM-CBT	-6.94	95.34	109.06
3	A	405	37X	CBT-CCM-CBS	-4.83	81.43	109.63
3	A	404	37X	CBT-CCM-CBS	-3.27	102.62	109.70
3	B	402	37X	CBT-OBV-CCJ	2.13	119.29	113.17
3	A	405	37X	CBT-OBV-CCJ	2.53	120.43	113.17
3	B	402	37X	CBR-CCM-CBQ	2.61	114.70	109.73
3	A	404	37X	CBS-O1-C1	2.74	121.03	113.17
3	A	406	37X	CBR-CCM-CBQ	3.89	117.13	109.73
3	A	406	37X	OBV-CBT-CCM	5.51	113.18	109.29
3	A	405	37X	CBR-CCM-CBQ	6.11	121.36	109.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	406	37X	2	0
3	B	402	37X	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	255/283 (90%)	0.69	39 (15%)	3 1	63, 106, 164, 194	0
1	B	241/283 (85%)	0.59	33 (13%)	4 2	60, 106, 191, 207	0
All	All	496/566 (87%)	0.64	72 (14%)	3 2	60, 106, 172, 207	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	THR	7.0
1	B	196	PHE	6.3
1	A	259	ALA	4.9
1	B	209	ILE	4.3
1	B	42	MET	4.2
1	A	255	GLY	4.1
1	A	186	GLY	4.1
1	B	202	SER	4.1
1	A	77	ARG	4.1
1	B	232	HIS	4.0
1	A	252	ILE	4.0
1	A	204	THR	3.8
1	A	117	LEU	3.8
1	A	38	THR	3.8
1	A	189	ILE	3.7
1	A	201	VAL	3.6
1	B	143	ILE	3.5
1	B	230	PHE	3.4
1	B	253	GLY	3.3
1	A	59	ILE	3.2
1	A	256	ASP	3.2
1	B	141	THR	3.1
1	A	143	ILE	3.1
1	B	236	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	142	THR	3.0
1	B	252	ILE	3.0
1	A	42	MET	3.0
1	B	206	ILE	3.0
1	A	206	ILE	3.0
1	B	144	GLY	3.0
1	A	304	LEU	2.9
1	A	185	PHE	2.9
1	B	139	VAL	2.8
1	A	253	GLY	2.8
1	A	39	ILE	2.8
1	B	233	ILE	2.8
1	B	228	ILE	2.8
1	A	146	GLY	2.7
1	B	224	ALA	2.7
1	B	124	ILE	2.6
1	A	224	ALA	2.5
1	A	76	GLN	2.5
1	A	89	SER	2.5
1	A	188	GLY	2.5
1	B	52	LEU	2.5
1	A	144	GLY	2.5
1	A	263	ASP	2.5
1	B	205	LYS	2.4
1	A	202	SER	2.3
1	B	201	VAL	2.3
1	B	247	ILE	2.3
1	B	250	THR	2.3
1	B	138	THR	2.3
1	A	75	SER	2.3
1	A	84	LYS	2.3
1	A	52	LEU	2.2
1	B	255	GLY	2.2
1	A	50	ILE	2.2
1	B	235	GLY	2.2
1	B	227	ALA	2.2
1	A	251	THR	2.1
1	A	103	ILE	2.1
1	B	194	ASP	2.1
1	A	157	ILE	2.1
1	B	299	ILE	2.1
1	A	165	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	46	THR	2.1
1	B	203	GLN	2.1
1	A	250	THR	2.1
1	B	249	LEU	2.0
1	A	274	VAL	2.0
1	A	236	TRP	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 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
4	MG	A	407	1/1	0.99	0.32	2.19	101,101,101,101	0
3	37X	A	405	39/39	0.66	0.41	1.88	165,179,181,181	0
3	37X	A	406	29/39	0.73	0.30	1.43	133,145,155,155	0
3	37X	B	402	39/39	0.87	0.23	0.99	107,140,144,145	0
2	K	A	402	1/1	0.93	0.39	0.20	108,108,108,108	0
3	37X	A	403	18/39	0.91	0.16	-0.03	80,85,97,97	0
3	37X	A	404	25/39	0.85	0.17	-0.62	131,141,152,152	0
2	K	B	403	1/1	0.98	0.32	-0.91	61,61,61,61	0
2	K	A	401	1/1	0.94	0.22	-2.28	64,64,64,64	0
5	NAG	B	401	14/15	0.78	0.26	-	196,197,199,199	0

6.5 Other polymers [i](#)

There are no such residues in this entry.