



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 19, 2018 – 08:05 AM EST

PDB ID : 3QAK
Title : Agonist bound structure of the human adenosine A2a receptor
Authors : Xu, F.; Wu, H.; Katritch, V.; Han, G.W.; Cherezov, V.; Stevens, R.; GPCR Network (GPCR)
Deposited on : 2011-01-11
Resolution : 2.71 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030736

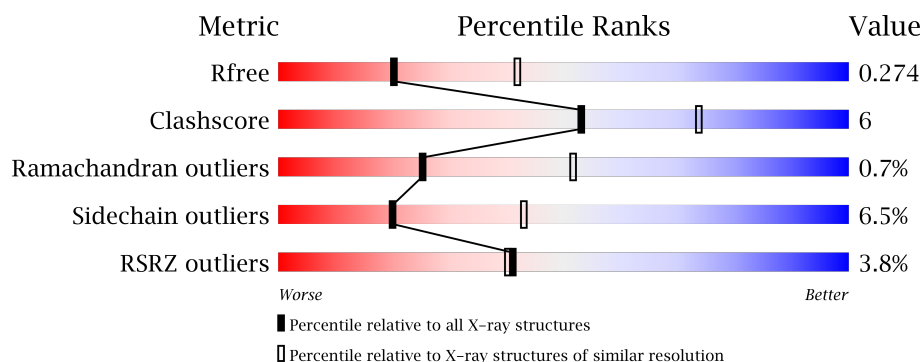
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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}	100719	2649 (2.74-2.70)
Clashscore	112137	2993 (2.74-2.70)
Ramachandran outliers	110173	2946 (2.74-2.70)
Sidechain outliers	110143	2947 (2.74-2.70)
RSRZ outliers	101464	2665 (2.74-2.70)

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	488	

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	OLC	A	1202	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3568 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 Adenosine receptor A2a, lysozyme chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3480	2268	597	591	24			

There are 28 discrepancies between the modelled and reference sequences:

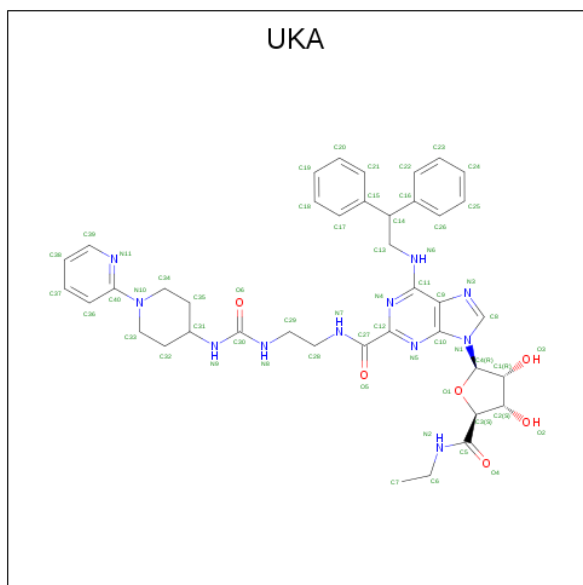
Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	ASP	-	EXPRESSION TAG	UNP P29274
A	-13	TYR	-	EXPRESSION TAG	UNP P29274
A	-12	LYS	-	EXPRESSION TAG	UNP P29274
A	-11	ASP	-	EXPRESSION TAG	UNP P29274
A	-10	ASP	-	EXPRESSION TAG	UNP P29274
A	-9	ASP	-	EXPRESSION TAG	UNP P29274
A	-8	ASP	-	EXPRESSION TAG	UNP P29274
A	-7	ALA	-	EXPRESSION TAG	UNP P29274
A	-6	MET	-	EXPRESSION TAG	UNP P29274
A	-5	GLY	-	EXPRESSION TAG	UNP P29274
A	-4	GLN	-	EXPRESSION TAG	UNP P29274
A	-3	PRO	-	EXPRESSION TAG	UNP P29274
A	-2	VAL	-	EXPRESSION TAG	UNP P29274
A	-1	GLY	-	EXPRESSION TAG	UNP P29274
A	0	ALA	-	EXPRESSION TAG	UNP P29274
A	1	PRO	-	EXPRESSION TAG	UNP P29274
A	1054	THR	CYS	engineered mutation	UNP P00720
A	1097	ALA	CYS	engineered mutation	UNP P00720
A	317	HIS	-	EXPRESSION TAG	UNP P29274
A	318	HIS	-	EXPRESSION TAG	UNP P29274
A	319	HIS	-	EXPRESSION TAG	UNP P29274
A	320	HIS	-	EXPRESSION TAG	UNP P29274
A	321	HIS	-	EXPRESSION TAG	UNP P29274
A	322	HIS	-	EXPRESSION TAG	UNP P29274
A	323	HIS	-	EXPRESSION TAG	UNP P29274
A	324	HIS	-	EXPRESSION TAG	UNP P29274
A	325	HIS	-	EXPRESSION TAG	UNP P29274

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Chain	Residue	Modelled	Actual	Comment	Reference
A	326	HIS	-	EXPRESSION TAG	UNP P29274

- Molecule 2 is 6-(2,2-diphenylethylamino)-9-[(2R,3R,4S,5S)-5-(ethylcarbamoyl)-3,4-dihydroxy-oxolan-2-yl]-N-[2-[(1-pyridin-2-yl)piperidin-4-yl]carbamoylamino]ethyl]purine-2-carboxamide (three-letter code: UKA) (formula: C₄₀H₄₇N₁₁O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			57	40	11	6		

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	8	4		
3	A	1	Total	C	O	0	0
			13	9	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		

These plots are drawn for all protein, RNA and DNA 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:
-
- 75% 14% 9%
- ASP TYR LYS ASP ASP ASP ALA MET GLY GLN PRO VAL GLY PRO PRO I3 M4 S7 E13 A20 I21 V25 V40 V46 S47 L43 A49 I60 I66 L78 A81 C82 F83 V84 L85 T88 Q89 S90 S91 I106 R107 I108 V109 L110 R111 V116 R120 V130 I135 T138 P139 M140 G147 Q148 PRO LYS GLU GLY LYS ASN HIS SER GLN G158 E161 L167 F168 F180 A184 C185 L192 M193 I200 L1007 G1012 L1013 R1014 L1015 K1016 I1017 Y1018 T1021 T1026 I1027 H1031 S1036 T1046 R1052 L1091 R1095 K1135 R222 K227 A231 A232 K233 L235 A236 I237 L238 V239 L247 P248 D261 C262 S263 H264 L272 L276 S277 S281 V282 V283 N284 P285 F286 I287 R293 R300 R304 S305 H306 V307 L308 ARG GLN GLN GLU PRO PHE IWS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.84Å 78.94Å 86.58Å 90.00° 100.54° 90.00°	Depositor
Resolution (Å)	29.61 – 2.71 29.61 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.61-2.71) 96.4 (29.61-2.71)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.217 , 0.273 0.218 , 0.274	Depositor DCC
R_{free} test set	840 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3568	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.69% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OLC, UKA

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	0.54	0/3555	0.63	0/4831

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 ⓘ

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	3480	0	3578	45	0
2	A	57	0	47	0	0
3	A	25	0	28	1	0
4	A	6	0	0	0	0
All	All	3568	0	3653	45	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 (45) 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:200:ILE:HD12	1:A:235:LEU:CD2	2.05	0.86
1:A:282:VAL:HG23	1:A:283:VAL:HG13	1.65	0.78
1:A:200:ILE:HD12	1:A:235:LEU:HD23	1.68	0.74
1:A:89:GLN:OE1	1:A:185:CYS:HB3	1.88	0.74
1:A:66:ILE:HD11	1:A:81:ALA:HA	1.76	0.68
1:A:81:ALA:O	1:A:84:VAL:HG13	1.97	0.65
1:A:1014:ARG:HG3	1:A:1018:TYR:CE2	2.33	0.63
1:A:66:ILE:CG2	1:A:66:ILE:O	2.48	0.62
1:A:66:ILE:O	1:A:66:ILE:HG22	2.00	0.61
1:A:40:VAL:HG11	1:A:116:VAL:HG12	1.80	0.61
1:A:237:ILE:HG21	1:A:287:ILE:HG21	1.83	0.60
1:A:21:ILE:O	1:A:25:VAL:HG23	2.05	0.56
1:A:46:VAL:O	1:A:49:ALA:HB3	2.05	0.55
1:A:110:LEU:HD11	1:A:1012:GLY:HA3	1.89	0.55
1:A:282:VAL:CG2	1:A:283:VAL:HG13	2.36	0.54
1:A:200:ILE:HD12	1:A:235:LEU:HD21	1.85	0.54
1:A:307:VAL:HG12	1:A:308:LEU:HD12	1.89	0.53
1:A:180:PHE:O	1:A:184:ALA:HB3	2.09	0.53
1:A:66:ILE:O	1:A:167:LEU:HA	2.10	0.52
1:A:161:GLU:HG3	1:A:161:GLU:O	2.09	0.51
1:A:282:VAL:HG23	1:A:283:VAL:CG1	2.39	0.49
1:A:284:ASN:O	1:A:285:PRO:C	2.50	0.49
1:A:135:ILE:HD13	1:A:185:CYS:SG	2.53	0.49
1:A:1026:THR:HG23	1:A:1031:HIS:C	2.35	0.47
1:A:148:GLN:HA	1:A:148:GLN:HE21	1.80	0.46
1:A:264:HIS:ND1	1:A:264:HIS:N	2.63	0.46
1:A:247:LEU:O	1:A:248:PRO:C	2.52	0.45
1:A:200:ILE:HG22	1:A:232:ALA:HB2	2.00	0.44
1:A:282:VAL:HG23	1:A:283:VAL:N	2.31	0.44
1:A:1091:LEU:HD22	1:A:1095:ARG:HB3	2.00	0.44
1:A:138:THR:HB	1:A:139:PRO:HD3	1.99	0.44
1:A:13:GLU:CG	1:A:60:ILE:HG23	2.49	0.43
1:A:85:LEU:O	1:A:89:GLN:HB2	2.17	0.43
1:A:66:ILE:CG2	1:A:168:PHE:HB2	2.48	0.43
1:A:20:ALA:CB	1:A:282:VAL:HB	2.48	0.43
1:A:66:ILE:CD1	1:A:84:VAL:HG11	2.48	0.43
1:A:111:ARG:HH22	1:A:1015:LEU:H	1.67	0.43
1:A:89:GLN:OE1	1:A:185:CYS:CB	2.63	0.43
1:A:272:LEU:HD13	3:A:1202:OLC:H5	2.01	0.42
1:A:66:ILE:HG21	1:A:168:PHE:HB2	2.00	0.42
1:A:66:ILE:HD13	1:A:66:ILE:HG21	1.81	0.41
1:A:193:MET:HB3	1:A:239:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:LEU:O	1:A:1046:LEU:HD12	2.21	0.40
1:A:106:ILE:HD11	1:A:231:ALA:CB	2.52	0.40
1:A:1017:ILE:HG12	1:A:1027: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	440/488 (90%)	414 (94%)	23 (5%)	3 (1%)	25 52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	SER
1	A	305	SER
1	A	66	ILE

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	A	369/409 (90%)	345 (94%)	24 (6%)	20 43

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	13	GLU
1	A	47	SER
1	A	78	LEU
1	A	83	PHE
1	A	84	VAL
1	A	108	ILE
1	A	120	ARG
1	A	130	VAL
1	A	140	MET
1	A	148	GLN
1	A	161	GLU
1	A	192	LEU
1	A	1007	LEU
1	A	1021	THR
1	A	1036	SER
1	A	1052	ARG
1	A	222	ARG
1	A	227	LYS
1	A	233	LYS
1	A	235	LEU
1	A	264	HIS
1	A	276	LEU
1	A	300	ARG

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	148	GLN
1	A	181	ASN

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

3 ligands are modelled in this entry.

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
2	UKA	A	1200	-	58,63,63	1.02	2 (3%)	72,87,87	1.64	11 (15%)
3	OLC	A	1201	-	11,11,24	1.49	1 (9%)	12,12,25	1.20	2 (16%)
3	OLC	A	1202	-	12,12,24	1.41	1 (8%)	13,13,25	1.16	1 (7%)

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	UKA	A	1200	-	-	0/37/69/69	0/7/7/7
3	OLC	A	1201	-	-	0/11/11/24	0/0/0/0
3	OLC	A	1202	-	-	0/12/12/24	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1200	UKA	C12-C27	-4.74	1.50	1.53
2	A	1200	UKA	C40-N10	2.55	1.42	1.37
3	A	1202	OLC	O20-C1	4.64	1.47	1.33
3	A	1201	OLC	O20-C1	4.69	1.47	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1200	UKA	N5-C12-N4	-4.15	120.05	126.00
2	A	1200	UKA	C35-C34-N10	-3.92	103.57	111.22
2	A	1200	UKA	C36-C40-N11	-2.90	117.99	123.34
2	A	1200	UKA	C12-C27-N7	-2.66	113.44	115.80
2	A	1200	UKA	C10-C9-N3	-2.32	107.17	109.41
3	A	1201	OLC	O20-C1-O19	-2.06	118.45	123.55
2	A	1200	UKA	C38-C39-N11	-2.00	120.11	123.43
2	A	1200	UKA	C3-C5-N2	2.61	118.71	115.47
3	A	1202	OLC	O20-C1-C2	2.84	120.16	111.90
3	A	1201	OLC	O20-C1-C2	2.91	120.36	111.90
2	A	1200	UKA	C11-N4-C12	3.33	122.00	115.94
2	A	1200	UKA	C27-C12-N5	3.88	121.82	117.43
2	A	1200	UKA	C12-N5-C10	4.51	120.69	115.09
2	A	1200	UKA	C39-N11-C40	4.64	123.19	116.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1202	OLC	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/488 (90%)	-0.03	17 (3%) 41 40	43, 60, 85, 126	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	LEU	5.0
1	A	261	ASP	4.0
1	A	1021	THR	3.5
1	A	306	HIS	3.2
1	A	293	ARG	3.0
1	A	305	SER	3.0
1	A	307	VAL	2.9
1	A	1135	LYS	2.9
1	A	262	CYS	2.8
1	A	304	ARG	2.6
1	A	147	GLY	2.6
1	A	4	MET	2.3
1	A	264	HIS	2.3
1	A	91	SER	2.3
1	A	111	ARG	2.1
1	A	88	THR	2.1
1	A	277	SER	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
3	OLC	A	1202	13/25	0.89	0.30	3.28	69,70,71,72	0
3	OLC	A	1201	12/25	0.85	0.30	1.24	94,95,95,96	0
2	UKA	A	1200	57/57	0.85	0.25	0.52	42,47,71,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.