Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:39 PM GMT

PDB ID	:	4PKC
Title	:	Benzylsuccinate alpha-gamma complex
Authors	:	Funk, M.A.; Drennan, C.L.
Deposited on	:	2014-05-14
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

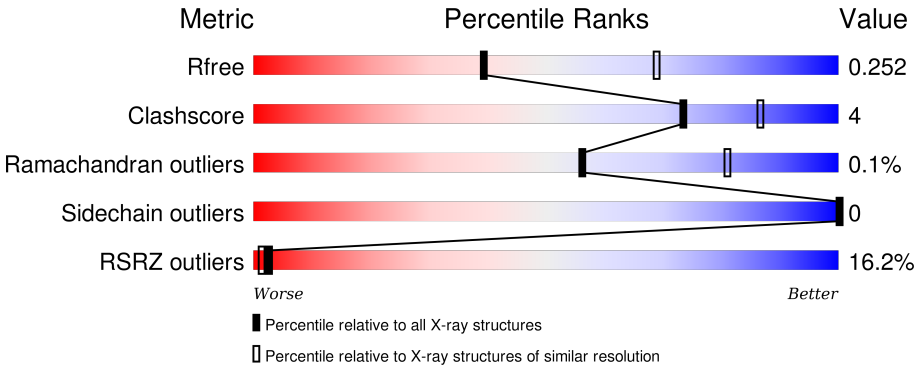
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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 <=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	878	16% 85% 11% .
2	C	60	3% 55% 13% 32%

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	CL	A	901	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7193 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 TutD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	843	Total	C	N	O	S	0	0	0
			6672	4212	1156	1266	38			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	789	ILE	MET	variant	UNP O68395
A	866	SER	-	expression tag	UNP O68395
A	867	GLY	-	expression tag	UNP O68395
A	868	THR	-	expression tag	UNP O68395
A	869	GLY	-	expression tag	UNP O68395
A	870	SER	-	expression tag	UNP O68395
A	871	GLY	-	expression tag	UNP O68395
A	872	SER	-	expression tag	UNP O68395
A	873	SER	-	expression tag	UNP O68395
A	874	HIS	-	expression tag	UNP O68395
A	875	HIS	-	expression tag	UNP O68395
A	876	HIS	-	expression tag	UNP O68395
A	877	HIS	-	expression tag	UNP O68395
A	878	HIS	-	expression tag	UNP O68395
A	879	HIS	-	expression tag	UNP O68395

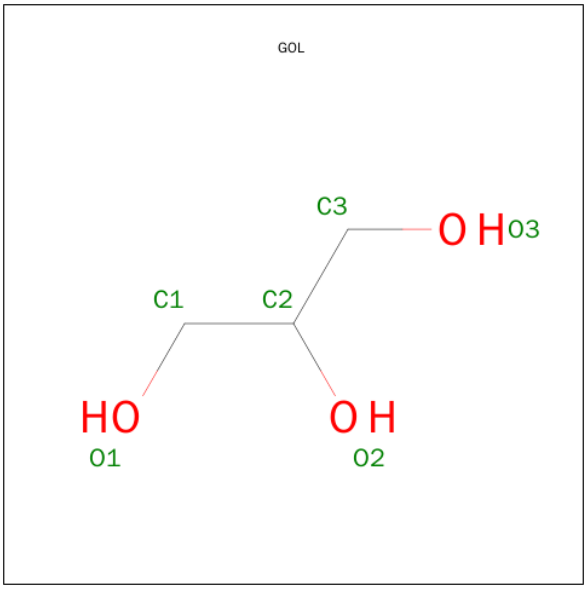
- Molecule 2 is a protein called TutF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	41	Total	C	N	O	S	0	0	0
			320	204	52	63	1			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

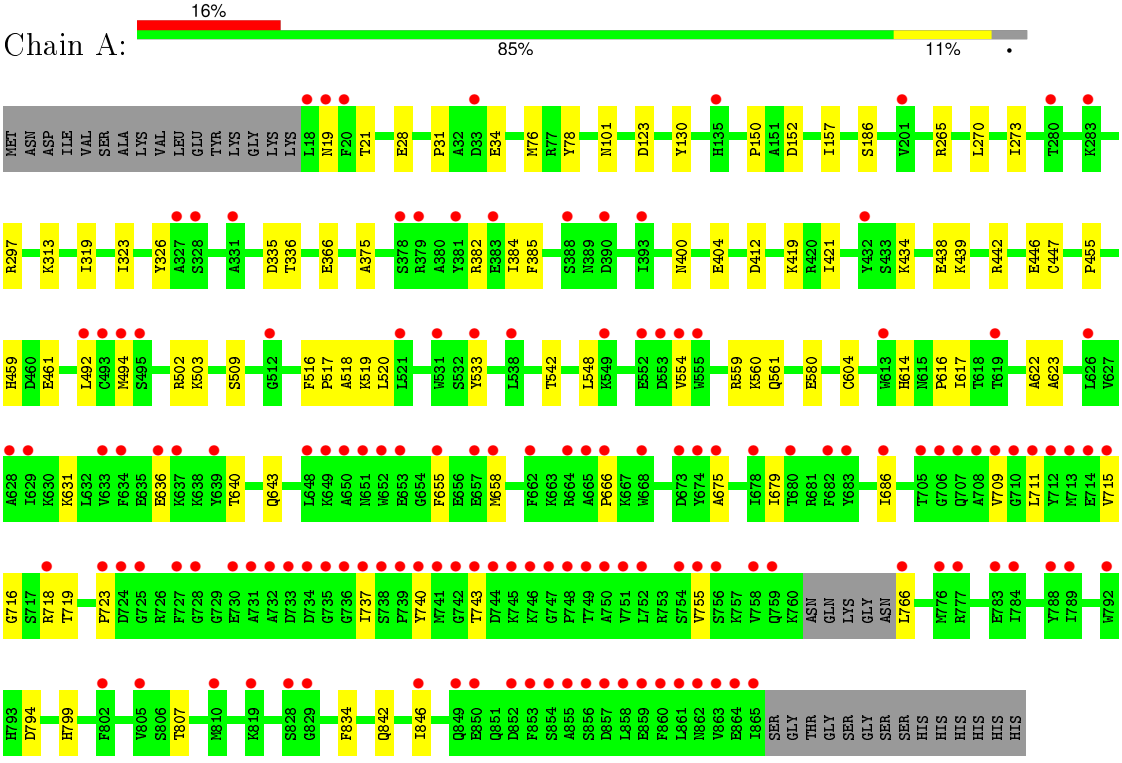
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	185	Total O 185 185	0	0
5	C	9	Total O 9 9	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

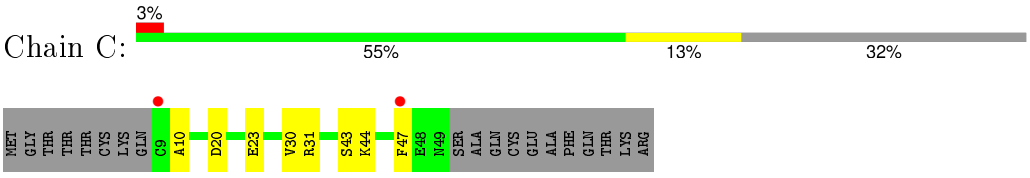
- Molecule 1: TutD

Chain A:



- Molecule 2: TutF

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	154.86Å 154.86Å 82.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 2.60 48.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.97-2.60) 85.1 (48.97-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1678)	Depositor
R, R_{free}	0.217 , 0.257 0.214 , 0.252	Depositor DCC
R_{free} test set	2676 reflections (10.06%)	DCC
Wilson B-factor (Å^2)	45.8	Xtriage
Anisotropy	0.915	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 30755 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7193	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, CL

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	0.21	0/6825	0.36	0/9224
2	C	0.20	0/328	0.33	0/442
All	All	0.21	0/7153	0.36	0/9666

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	6672	0	6508	54	0
2	C	320	0	291	6	0
3	A	1	0	0	2	0
4	A	6	0	8	0	0
5	A	185	0	0	3	0
5	C	9	0	0	1	0
All	All	7193	0	6807	57	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 4.

All (57) 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:375:ALA:O	1:A:382:ARG:NH1	2.12	0.83
2:C:44:LYS:NZ	5:C:109:HOH:O	2.10	0.79
1:A:123:ASP:OD2	5:A:1181:HOH:O	2.11	0.69
1:A:494:MET:HE1	1:A:709:VAL:HB	1.78	0.65
1:A:666:PRO:HB2	1:A:675:ALA:HB2	1.79	0.64
1:A:297:ARG:NH2	5:A:1138:HOH:O	2.28	0.64
1:A:623:ALA:HB1	1:A:679:ILE:HG13	1.79	0.64
1:A:631:LYS:NZ	1:A:636:GLU:OE1	2.27	0.64
1:A:542:THR:HG22	1:A:560:LYS:HD3	1.81	0.62
1:A:313:LYS:NZ	1:A:366:GLU:OE2	2.23	0.61
1:A:655:PHE:HB3	1:A:658:MET:HB3	1.83	0.61
1:A:709:VAL:HG13	1:A:711:LEU:HD23	1.82	0.61
1:A:270:LEU:HD13	2:C:43:SER:HB2	1.84	0.59
1:A:520:LEU:HD12	1:A:561:GLN:HB3	1.84	0.58
1:A:737:ILE:HD13	1:A:755:VAL:HG13	1.85	0.58
1:A:419:LYS:HD2	1:A:446:GLU:HB3	1.88	0.56
1:A:412:ASP:OD2	1:A:439:LYS:NZ	2.31	0.56
1:A:400:ASN:HD21	1:A:404:GLU:HB2	1.71	0.56
1:A:509:SER:OG	1:A:580:GLU:OE2	2.23	0.55
1:A:335:ASP:OD1	1:A:336:THR:N	2.38	0.55
1:A:384:ILE:HG21	1:A:711:LEU:HD22	1.88	0.54
1:A:548:LEU:HD21	1:A:554:VAL:HB	1.88	0.54
1:A:492:LEU:HB2	3:A:901:CL:CL	2.45	0.53
1:A:604:CYS:SG	5:A:1116:HOH:O	2.59	0.53
2:C:23:GLU:OE2	2:C:47:PHE:HZ	1.93	0.52
1:A:130:TYR:CE1	1:A:326:TYR:HB2	2.48	0.49
1:A:186:SER:HB2	1:A:519:LYS:HE2	1.95	0.49
1:A:518:ALA:HA	1:A:622:ALA:HB2	1.96	0.48
1:A:31:PRO:HB2	1:A:34:GLU:HG2	1.94	0.48
1:A:533:TYR:OH	1:A:718:ARG:NH2	2.47	0.47
2:C:10:ALA:HA	2:C:31:ARG:HG2	1.94	0.47
1:A:19:ASN:HD22	1:A:21:THR:HG22	1.79	0.47
1:A:319:ILE:HD13	1:A:323:ILE:HD12	1.97	0.47
1:A:614:HIS:O	1:A:616:PRO:HD3	2.16	0.46
1:A:834:PHE:O	1:A:842:GLN:NE2	2.41	0.45
1:A:21:THR:OG1	1:A:28:GLU:OE1	2.34	0.45
1:A:640:THR:HG23	1:A:643:GLN:H	1.81	0.44
1:A:76:MET:HB3	1:A:157:ILE:HG21	1.99	0.44
1:A:559:ARG:HG3	1:A:686:ILE:HD12	2.00	0.44
1:A:766:LEU:HA	1:A:799:HIS:HB3	1.99	0.44
1:A:265:ARG:NH2	2:C:20:ASP:OD2	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:PHE:HE1	1:A:709:VAL:HG22	1.84	0.43
1:A:459:HIS:HE1	1:A:461:GLU:HB2	1.83	0.43
1:A:502:ARG:HG2	1:A:503:LYS:HG3	2.00	0.42
1:A:273:ILE:HG21	2:C:30:VAL:HG21	2.02	0.42
1:A:516:PHE:CE1	1:A:715:VAL:HG21	2.54	0.42
1:A:447:CYS:HB2	1:A:455:PRO:HD3	2.01	0.41
1:A:434:LYS:NZ	1:A:794:ASP:OD1	2.40	0.41
1:A:421:ILE:HA	1:A:421:ILE:HD12	1.97	0.41
1:A:716:GLY:HA2	1:A:719:THR:HG22	2.02	0.41
1:A:517:PRO:HD2	1:A:617:ILE:O	2.20	0.41
1:A:740:TYR:HB3	1:A:743:THR:HG21	2.03	0.41
1:A:807:THR:HG23	1:A:846:ILE:HG23	2.04	0.40
1:A:494:MET:HG2	3:A:901:CL:CL	2.59	0.40
1:A:438:GLU:OE2	1:A:442:ARG:NH1	2.46	0.40
1:A:78:TYR:O	1:A:101:ASN:ND2	2.44	0.40
1:A:150:PRO:HB2	1:A:152:ASP:OD1	2.21	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	839/878 (96%)	805 (96%)	33 (4%)	1 (0%)	56 81
2	C	39/60 (65%)	37 (95%)	2 (5%)	0	100 100
All	All	878/938 (94%)	842 (96%)	35 (4%)	1 (0%)	56 81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	723	PRO

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	706/741 (95%)	706 (100%)	0	100	100
2	C	31/51 (61%)	31 (100%)	0	100	100
All	All	737/792 (93%)	737 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	643	GLN
1	A	849	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
4	GOL	A	902	-	5,5,5	0.33	0	5,5,5	0.24	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
4	GOL	A	902	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	A	843/878 (96%)	0.94	141 (16%) 2 1	45, 68, 161, 240	0
2	C	41/60 (68%)	0.34	2 (4%) 33 26	52, 69, 94, 119	0
All	All	884/938 (94%)	0.92	143 (16%) 3 1	45, 68, 161, 240	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	742	GLY	19.8
1	A	741	MET	18.4
1	A	743	THR	15.6
1	A	668	TRP	11.8
1	A	732	ALA	11.8
1	A	860	PHE	9.5
1	A	728	GLY	9.5
1	A	740	TYR	9.4
1	A	850	GLU	8.4
1	A	744	ASP	8.4
1	A	755	VAL	8.1
1	A	758	VAL	8.0
1	A	737	ILE	7.9
1	A	637	LYS	7.8
1	A	666	PRO	7.3
1	A	745	LYS	7.3
1	A	706	GLY	7.2
1	A	752	LEU	7.1
1	A	856	SER	7.0
1	A	708	ALA	6.9
1	A	712	TYR	6.8
1	A	714	GLU	6.5
1	A	858	LEU	6.4
1	A	784	ILE	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	710	GLY	6.2
1	A	747	GLY	6.1
1	A	855	ALA	6.1
1	A	678	ILE	5.8
1	A	655	PHE	5.8
1	A	861	LEU	5.7
1	A	18	LEU	5.7
1	A	674	TYR	5.7
1	A	766	LEU	5.7
1	A	739	PRO	5.5
1	A	865	ILE	5.5
1	A	675	ALA	5.5
1	A	665	ALA	5.5
1	A	686	ILE	5.5
1	A	653	GLU	5.4
1	A	754	SER	5.3
1	A	863	VAL	5.2
1	A	854	SER	5.1
1	A	664	ARG	5.1
1	A	662	PHE	4.9
1	A	715	VAL	4.8
1	A	748	PRO	4.6
1	A	724	ASP	4.6
1	A	746	LYS	4.5
1	A	862	ASN	4.5
1	A	494	MET	4.4
1	A	657	GLU	4.4
1	A	759	GLN	4.4
1	A	493	CYS	4.3
1	A	738	SER	4.3
1	A	658	MET	4.3
1	A	713	MET	4.2
1	A	857	ASP	4.2
1	A	628	ALA	4.1
1	A	723	PRO	4.0
1	A	652	TRP	4.0
1	A	749	THR	3.9
1	A	733	ASP	3.9
1	A	629	ILE	3.8
1	A	711	LEU	3.8
1	A	327	ALA	3.8
1	A	792	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	705	THR	3.8
1	A	552	GLU	3.7
1	A	634	PHE	3.7
1	A	19	ASN	3.6
1	A	734	ASP	3.6
1	A	828	SER	3.5
1	A	626	LEU	3.4
1	A	853	PHE	3.4
1	A	651	ASN	3.4
1	A	682	PHE	3.4
1	A	859	GLU	3.4
1	A	328	SER	3.4
1	A	864	GLU	3.3
1	A	725	GLY	3.3
1	A	549	LYS	3.2
1	A	756	SER	3.2
1	A	512	GLY	3.2
1	A	736	GLY	3.1
1	A	648	LEU	3.0
1	A	379	ARG	3.0
1	A	673	ASP	3.0
1	A	283	LYS	3.0
1	A	846	ILE	3.0
1	A	554	VAL	2.9
1	A	707	GLN	2.9
1	A	383	GLU	2.8
1	A	521	LEU	2.7
1	A	783	GLU	2.6
1	A	718	ARG	2.6
1	A	727	PHE	2.6
2	C	47	PHE	2.6
2	C	9	CYS	2.6
1	A	492	LEU	2.6
1	A	735	GLY	2.6
1	A	777	ARG	2.6
1	A	852	ASP	2.5
1	A	280	THR	2.5
1	A	613	TRP	2.5
1	A	731	ALA	2.5
1	A	381	TYR	2.5
1	A	331	ALA	2.5
1	A	393	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	680	THR	2.5
1	A	829	GLY	2.5
1	A	33	ASP	2.5
1	A	683	TYR	2.4
1	A	388	SER	2.4
1	A	849	GLN	2.4
1	A	201	VAL	2.4
1	A	650	ALA	2.4
1	A	805	VAL	2.4
1	A	709	VAL	2.3
1	A	789	ILE	2.3
1	A	649	LYS	2.3
1	A	788	TYR	2.3
1	A	553	ASP	2.3
1	A	538	LEU	2.3
1	A	802	PHE	2.3
1	A	390	ASP	2.3
1	A	533	TYR	2.3
1	A	819	LYS	2.2
1	A	633	VAL	2.2
1	A	639	TYR	2.2
1	A	730	GLU	2.2
1	A	810	MET	2.2
1	A	555	TRP	2.1
1	A	20	PHE	2.1
1	A	619	THR	2.1
1	A	495	SER	2.1
1	A	135	HIS	2.1
1	A	751	VAL	2.1
1	A	636	GLU	2.1
1	A	432	TYR	2.1
1	A	378	SER	2.0
1	A	750	ALA	2.0
1	A	531	TRP	2.0
1	A	776	MET	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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	A	902	6/6	0.81	0.25	-	63,72,73,90	0
3	CL	A	901	1/1	0.73	0.48	-	85,85,85,85	0

6.5 Other polymers (i)

There are no such residues in this entry.