



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:42 pm GMT

PDB ID : 3S8Z
Title : Crystal structure of LRP6-E3E4
Authors : Cheng, Z.; Xu, W.
Deposited on : 2011-05-31
Resolution : 2.80 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 : trunk28620
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) : recalc28949

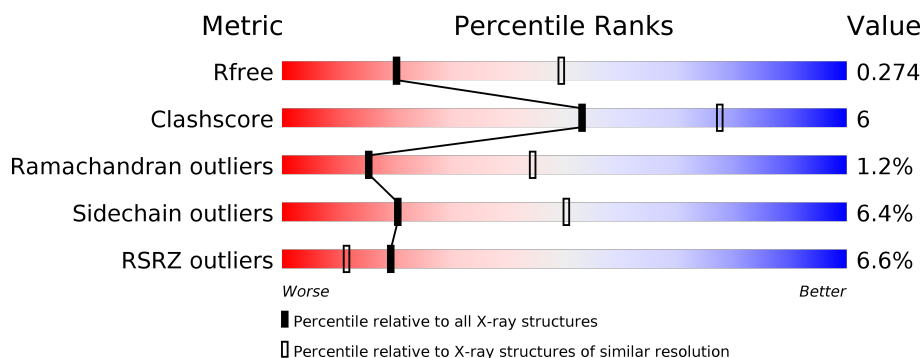
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	623	<div> <div>6%</div> <div>77%</div> <div>18%</div> <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
2	NAG	A	1244	X	-	-	-
2	NAG	A	1248	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4903 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.

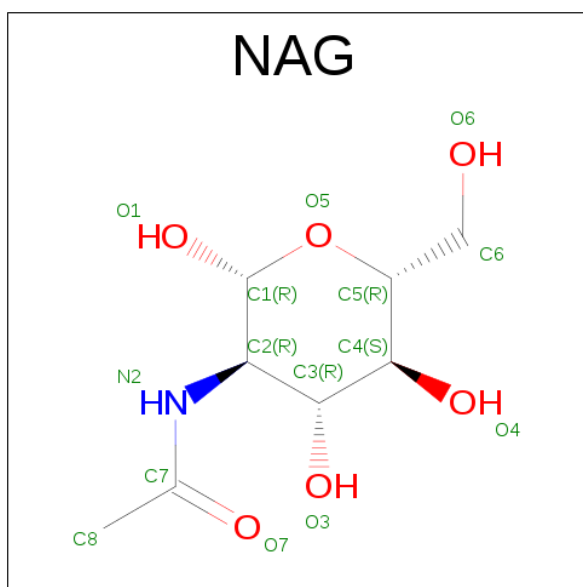
- Molecule 1 is a protein called Low-density lipoprotein receptor-related protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	606	4833	3035	856	917	25	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	621	HIS	-	EXPRESSION TAG	UNP O75581
A	622	HIS	-	EXPRESSION TAG	UNP O75581
A	623	HIS	-	EXPRESSION TAG	UNP O75581
A	624	HIS	-	EXPRESSION TAG	UNP O75581
A	625	HIS	-	EXPRESSION TAG	UNP O75581
A	626	HIS	-	EXPRESSION TAG	UNP O75581
A	627	HIS	-	EXPRESSION TAG	UNP O75581
A	628	HIS	-	EXPRESSION TAG	UNP O75581
A	1062	ILE	VAL	VARIANT	UNP O75581

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

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 ($\text{RSRZ} > 2$). 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:
-
- 6% 77% 18%

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.60Å 83.75Å 166.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 52.96 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.80) 99.9 (52.96-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.257 , 0.282 0.251 , 0.274	Depositor DCC
R_{free} test set	1225 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	69.6	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4903	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.34	0/4935	0.56	1/6696 (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	A	814	LEU	CA-CB-CG	5.10	127.03	115.30

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	4833	0	4717	60	0
2	A	42	0	39	0	0
3	A	28	0	25	1	0
All	All	4903	0	4781	60	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 (60) 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:657:PRO:HG2	1:A:693:GLY:HA2	1.43	0.98
1:A:729:ILE:HB	1:A:743:VAL:HG13	1.70	0.74
1:A:982:ILE:HG22	1:A:989:ILE:HG12	1.70	0.72
1:A:919:HIS:HD2	1:A:946:ARG:HE	1.41	0.69
1:A:1188:LEU:H	1:A:1188:LEU:HD23	1.59	0.66
1:A:812:THR:HB	1:A:814:LEU:HD22	1.80	0.62
1:A:1037:VAL:HG23	1:A:1053:LYS:HB3	1.82	0.61
1:A:1050:VAL:HG11	3:A:1245:NAG:H82	1.83	0.60
1:A:647:LEU:O	1:A:648:GLU:HG2	2.03	0.58
1:A:727:ASN:ND2	1:A:748:ASP:O	2.36	0.58
1:A:990:ARG:HG2	1:A:1001:THR:HG22	1.86	0.57
1:A:1188:LEU:CD2	1:A:1188:LEU:H	2.18	0.57
1:A:852:ARG:HH22	1:A:866:ARG:HH22	1.53	0.56
1:A:1151:THR:HG21	1:A:1192:HIS:HA	1.88	0.54
1:A:1160:ILE:HD12	1:A:1191:ILE:HB	1.88	0.54
1:A:813:ASN:HB3	1:A:832:LEU:O	2.07	0.54
1:A:747:LEU:HD22	1:A:750:PRO:HG3	1.91	0.53
1:A:833:PRO:HB2	1:A:851:SER:HB3	1.89	0.52
1:A:940:GLN:HE21	1:A:945:ASN:HD21	1.57	0.52
1:A:798:ILE:O	1:A:886:ARG:NH2	2.41	0.52
1:A:638:ARG:HD2	1:A:874:ASP:O	2.11	0.50
1:A:767:TRP:CE2	1:A:792:ARG:HB3	2.47	0.50
1:A:944:ILE:HG21	1:A:979:LEU:HD21	1.92	0.49
1:A:991:LYS:HE3	1:A:1000:PHE:HB3	1.94	0.49
1:A:703:GLY:HA2	1:A:958:ILE:HD12	1.94	0.49
1:A:819:ASN:HD22	1:A:824:ASN:HD22	1.61	0.49
1:A:715:LEU:HD12	1:A:757:PRO:HB2	1.95	0.48
1:A:1099:SER:O	1:A:1136:ARG:NH2	2.40	0.48
1:A:793:ALA:HA	1:A:808:THR:O	2.14	0.48
1:A:985:ARG:O	1:A:986:GLN:HB2	2.13	0.48
1:A:656:ILE:HG22	1:A:658:LEU:HG	1.94	0.47
1:A:841:TYR:HB2	1:A:881:VAL:HG11	1.95	0.47
1:A:981:TRP:CZ2	1:A:990:ARG:HD2	2.50	0.47
1:A:634:LEU:HD23	1:A:645:ILE:HD11	1.97	0.47
1:A:881:VAL:HG13	1:A:886:ARG:HD2	1.97	0.47
1:A:647:LEU:C	1:A:649:THR:H	2.19	0.47
1:A:1146:GLN:O	1:A:1146:GLN:HG3	2.16	0.46
1:A:644:ARG:HG3	1:A:654:VAL:HG23	1.97	0.46
1:A:1040:VAL:HG12	1:A:1049:GLY:O	2.17	0.45
1:A:1019:LEU:HB2	1:A:1028:ILE:HD11	1.99	0.44
1:A:676:ILE:HG12	1:A:677:TYR:N	2.33	0.43
1:A:669:PHE:CE2	1:A:671:VAL:HG13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:ILE:CG2	1:A:989:ILE:HG12	2.45	0.43
1:A:677:TYR:OH	1:A:734:LEU:HB3	2.19	0.43
1:A:981:TRP:CE2	1:A:990:ARG:HB3	2.54	0.42
1:A:843:ASP:HA	1:A:860:LYS:HD3	2.01	0.42
1:A:870:GLN:HB3	1:A:873:LEU:HD12	2.01	0.42
1:A:1237:LEU:O	1:A:1239:ASP:N	2.49	0.41
1:A:667:LEU:HB2	1:A:880:LEU:HD23	2.02	0.41
1:A:919:HIS:CD2	1:A:946:ARG:HE	2.28	0.41
1:A:1146:GLN:HB2	1:A:1146:GLN:HE21	1.73	0.41
1:A:699:VAL:HG12	1:A:700:VAL:HG23	2.02	0.41
1:A:636:PHE:HB3	1:A:879:ILE:HG22	2.02	0.41
1:A:669:PHE:HE2	1:A:671:VAL:HG13	1.86	0.40
1:A:809:ASP:HB3	1:A:814:LEU:HD23	2.03	0.40
1:A:765:THR:HG22	1:A:773:ILE:HG12	2.03	0.40
1:A:940:GLN:NE2	1:A:945:ASN:HD21	2.20	0.40
1:A:642:ILE:HD12	1:A:658:LEU:CD1	2.51	0.40
1:A:643:ARG:NH1	1:A:655:ALA:HB2	2.36	0.40
1:A:724:THR:O	1:A:727:ASN:ND2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	602/623 (97%)	550 (91%)	45 (8%)	7 (1%)	15	44

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	911	GLY
1	A	1186	ALA
1	A	648	GLU

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Mol	Chain	Res	Type
1	A	1153	PHE
1	A	987	ASN
1	A	1142	SER
1	A	1174	GLY

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	529/546 (97%)	495 (94%)	34 (6%)	20	50

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	631	GLU
1	A	661	VAL
1	A	671	VAL
1	A	675	ARG
1	A	683	LEU
1	A	741	VAL
1	A	743	VAL
1	A	790	VAL
1	A	812	THR
1	A	814	LEU
1	A	820	MET
1	A	881	VAL
1	A	934	THR
1	A	977	LYS
1	A	983	ASP
1	A	990	ARG
1	A	991	LYS
1	A	1004	VAL
1	A	1028	ILE
1	A	1046	ARG
1	A	1056	GLN
1	A	1109	LEU

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Mol	Chain	Res	Type
1	A	1115	LYS
1	A	1125	ARG
1	A	1130	ASP
1	A	1139	LEU
1	A	1146	GLN
1	A	1175	ARG
1	A	1180	LYS
1	A	1187	GLN
1	A	1188	LEU
1	A	1223	ASP
1	A	1237	LEU
1	A	1238	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	727	ASN
1	A	738	HIS
1	A	824	ASN
1	A	919	HIS
1	A	940	GLN
1	A	1182	GLN
1	A	1187	GLN
1	A	1209	GLN
1	A	1216	HIS
1	A	1238	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](#)

2 carbohydrates 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	$\# Z > 2$
3	NAG	A	1245	1,3	14,14,15	0.53	0	15,19,21	1.43	3 (20%)
3	NAG	A	1246	3	14,14,15	0.47	0	15,19,21	1.16	1 (6%)

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	NAG	A	1245	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1246	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1245	NAG	O5-C1-C2	-2.24	108.35	111.47
3	A	1245	NAG	C4-C3-C2	2.99	115.40	111.02
3	A	1245	NAG	C1-O5-C5	3.11	116.45	112.17
3	A	1246	NAG	C1-O5-C5	3.23	116.62	112.17

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	1245	NAG	1	0

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	NAG	A	1244	1	14,14,15	0.64	0	15,19,21	0.96	1 (6%)
2	NAG	A	1247	1	14,14,15	0.50	0	15,19,21	1.61	1 (6%)
2	NAG	A	1248	1	14,14,15	0.62	0	15,19,21	1.23	3 (20%)

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	NAG	A	1244	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	1247	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1248	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1248	NAG	O5-C1-C2	-2.92	107.41	111.47
2	A	1248	NAG	C8-C7-N2	2.04	119.78	116.11
2	A	1248	NAG	C1-O5-C5	2.10	115.06	112.17
2	A	1244	NAG	C4-C3-C2	2.41	114.56	111.02
2	A	1247	NAG	C1-O5-C5	5.13	119.23	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1244	NAG	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	606/623 (97%)	0.66	40 (6%) 19 11	74, 110, 171, 210	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1132	SER	5.8
1	A	1113	LEU	4.2
1	A	1131	LEU	4.0
1	A	1098	PHE	3.5
1	A	1144	ILE	3.4
1	A	1118	TRP	3.4
1	A	1139	LEU	3.2
1	A	1153	PHE	3.2
1	A	1135	ASN	3.1
1	A	1174	GLY	3.0
1	A	1102	SER	2.9
1	A	1222	GLY	2.9
1	A	1152	VAL	2.8
1	A	1126	ILE	2.7
1	A	1157	LEU	2.7
1	A	1134	ALA	2.7
1	A	1137	ILE	2.6
1	A	1196	GLU	2.6
1	A	1175	ARG	2.6
1	A	1191	ILE	2.6
1	A	841	TYR	2.6
1	A	986	GLN	2.6
1	A	1117	PHE	2.5
1	A	1154	GLU	2.5
1	A	1167	ILE	2.4
1	A	1128	SER	2.4
1	A	1172	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1199	LEU	2.4
1	A	1147	PRO	2.3
1	A	1083	ILE	2.3
1	A	1097	PHE	2.3
1	A	936	LEU	2.2
1	A	911	GLY	2.2
1	A	892	GLU	2.2
1	A	1156	TRP	2.1
1	A	1074	THR	2.1
1	A	1109	LEU	2.1
1	A	1105	ILE	2.0
1	A	1115	LYS	2.0
1	A	864	GLN	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](#)

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	NAG	A	1245	14/15	0.91	0.27	0.88	147,148,149,149	0
3	NAG	A	1246	14/15	0.84	0.27	-	163,165,166,166	0

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(\AA^2)	Q<0.9
2	NAG	A	1248	14/15	0.84	0.30	3.29	172,173,173,174	0
2	NAG	A	1244	14/15	0.77	0.16	-	170,172,175,176	0
2	NAG	A	1247	14/15	0.63	0.21	-	178,180,181,181	0

6.5 Other polymers [i](#)

There are no such residues in this entry.