



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2017 – 05:32 PM EST

PDB ID : 4GLP  
Title : The crystal structure of soluble human CD14 reveals a bent solenoid with a hydrophobic amino-terminal pocket.  
Authors : Kelley, S.L.; Lukk, T.; Nair, S.K.; Tapping, R.I.  
Deposited on : unknown  
Resolution : 4.00 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
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-20030345

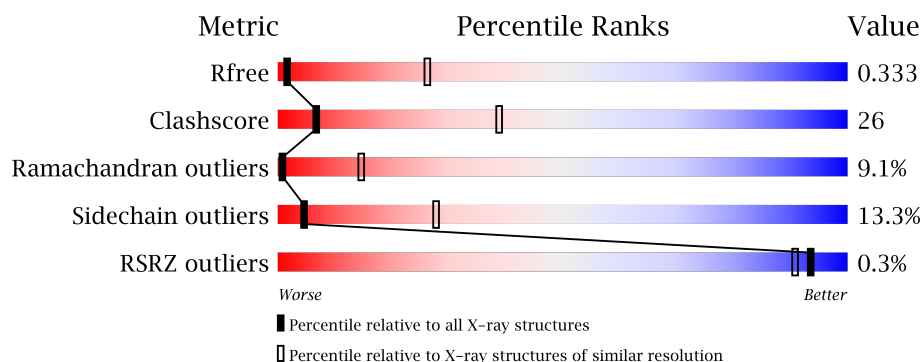
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

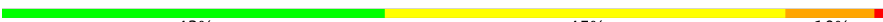
The reported resolution of this entry is 4.00 Å.

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	1088 (4.40-3.60)
Clashscore	112137	1187 (4.40-3.60)
Ramachandran outliers	110173	1139 (4.40-3.60)
Sidechain outliers	110143	1126 (4.40-3.60)
RSRZ outliers	101464	1099 (4.40-3.60)

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  $\geq 3$ , 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	310	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2346 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 Monocyte differentiation antigen CD14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2346	1479	415	441	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	SER	CYS	ENGINEERED MUTATION	UNP P08571

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:  43% 45% 10%

Node ID	Status
P330	Good
R262	Good
A263	Good
T264	Good
V265	Good
N266	Good
P267	Good
C272	Good
M273	Good
W274	Good
S275	Good
S276	Good
A277	Good
N278	Good
L279	Good
S280	Good
L281	Good
N282	Good
L283	Good
E289	Good
Q290	Good
V291	Good
P292	Good
K293	Good
G294	Good
L295	Good
P296	Good
A297	Good
K298	Good
L299	Good
R300	Good
V301	Good
L302	Good
D303	Good
L304	Good
S305	Good
S306	Good
N307	Good
R308	Good
L309	Good
N310	Good
R311	Good
A312	Good
P313	Good
Q314	Good
E317	Good
L318	Good
P319	Good
E320	Good
V321	Good
D322	Good
R323	Good
L324	Good
T325	Good
L326	Good
D327	Good
G328	Good
W329	Good
F185	Warning
S186	Warning
C187	Warning
E188	Warning
Q189	Warning
V190	Warning
R191	Warning
A192	Warning
F193	Warning
L196	Warning
T197	Warning
S198	Warning
L199	Warning
D200	Warning
L201	Warning
S202	Warning
D203	Warning
N204	Warning
P205	Warning
G206	Warning
R210	Warning
M213	Warning
L216	Warning
C217	Warning
P218	Warning
H219	Warning
K220	Warning
F221	Warning
L224	Warning
L227	Warning
R230	Warning
E235	Warning
V240	Warning
C241	Warning
A242	Warning
A243	Warning
L244	Warning
A247	Warning
G248	Warning
H252	Warning
S253	Warning
L254	Warning
D255	Warning
L256	Warning
S257	Warning
H258	Warning
N259	Warning
S260	Warning
L261	Warning
F185	Error
S186	Error
C187	Error
E188	Error
Q189	Error
V190	Error
R191	Error
A192	Error
F193	Error
L196	Error
T197	Error
S198	Error
L199	Error
D200	Error
L201	Error
S202	Error
D203	Error
N204	Error
P205	Error
G206	Error
R210	Error
M213	Error
L216	Error
C217	Error
P218	Error
H219	Error
K220	Error
F221	Error
L224	Error
L227	Error
R230	Error
E235	Error
V240	Error
C241	Error
A242	Error
A243	Error
L244	Error
A247	Error
G248	Error
H252	Error
S253	Error
L254	Error
D255	Error
L256	Error
S257	Error
H258	Error
N259	Error
S260	Error
L261	Error
F185	Critical
S186	Critical
C187	Critical
E188	Critical
Q189	Critical
V190	Critical
R191	Critical
A192	Critical
F193	Critical
L196	Critical
T197	Critical
S198	Critical
L199	Critical
D200	Critical
L201	Critical
S202	Critical
D203	Critical
N204	Critical
P205	Critical
G206	Critical
R210	Critical
M213	Critical
L216	Critical
C217	Critical
P218	Critical
H219	Critical
K220	Critical
F221	Critical
L224	Critical
L227	Critical
R230	Critical
E235	Critical
V240	Critical
C241	Critical
A242	Critical
A243	Critical

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.52Å 147.52Å 44.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.88 – 4.00 29.31 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (27.88-4.00) 100.0 (29.31-4.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	421.48 (at 3.98Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.283 , 0.321 0.294 , 0.333	Depositor DCC
$R_{free}$ test set	216 reflections (4.74%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 80.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.059 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.76	EDS
Total number of atoms	2346	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.48	1/2396 (0.0%)	0.81	5/3271 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	ALA	CA-CB	-5.25	1.41	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	ARG	NE-CZ-NH1	-11.55	114.53	120.30
1	A	175	LEU	CB-CG-CD2	5.72	120.73	111.00
1	A	210	ARG	NE-CZ-NH2	5.69	123.15	120.30
1	A	289	GLU	CB-CA-C	5.25	120.90	110.40
1	A	295	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	75	ALA	Peptide

## 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	2346	0	2353	122	0
All	All	2346	0	2353	122	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 26.

All (122) 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:221:PHE:HB3	1:A:224:ILE:HD11	1.60	0.81
1:A:79:PRO:HG2	1:A:82:TYR:H	1.44	0.80
1:A:295:LEU:HD23	1:A:319:PRO:HD3	1.64	0.79
1:A:235:GLU:O	1:A:261:LEU:HD12	1.84	0.77
1:A:143:ALA:HB2	1:A:169:LYS:HE2	1.67	0.76
1:A:189:GLN:OE1	1:A:189:GLN:N	2.18	0.76
1:A:76:ASP:OD2	1:A:76:ASP:N	2.18	0.76
1:A:73:VAL:HG23	1:A:76:ASP:HB3	1.70	0.73
1:A:304:LEU:O	1:A:307:ASN:ND2	2.24	0.70
1:A:274:TRP:NE1	1:A:294:GLY:O	2.24	0.70
1:A:122:THR:HG22	1:A:148:ARG:HB2	1.73	0.70
1:A:301:VAL:HA	1:A:323:ASN:HD21	1.57	0.69
1:A:38:PHE:O	1:A:39:SER:OG	2.09	0.69
1:A:89:LEU:O	1:A:91:VAL:N	2.27	0.68
1:A:138:GLU:HG2	1:A:139:ALA:H	1.58	0.67
1:A:137:LEU:HD12	1:A:137:LEU:N	2.11	0.65
1:A:93:ARG:HG3	1:A:93:ARG:HH11	1.63	0.64
1:A:190:VAL:HG12	1:A:220:LYS:CE	2.27	0.64
1:A:240:VAL:O	1:A:244:LEU:HD13	1.98	0.64
1:A:264:THR:OG1	1:A:265:VAL:N	2.29	0.64
1:A:158:ARG:O	1:A:185:PHE:HA	1.98	0.63
1:A:58:GLU:OE1	1:A:59:ILE:N	2.33	0.61
1:A:186:SER:OG	1:A:189:GLN:OE1	2.18	0.61
1:A:191:ARG:O	1:A:220:LYS:NZ	2.34	0.61
1:A:318:LEU:HD12	1:A:319:PRO:HD2	1.82	0.60
1:A:193:PHE:N	1:A:220:LYS:HZ3	1.98	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:SER:O	1:A:258:HIS:ND1	2.34	0.60
1:A:301:VAL:HG12	1:A:323:ASN:OD1	2.02	0.60
1:A:278:LEU:HD21	1:A:281:LEU:HD11	1.85	0.58
1:A:67:GLU:OE2	1:A:100:GLN:NE2	2.36	0.58
1:A:321:VAL:HG22	1:A:322:ASP:H	1.68	0.58
1:A:151:ASN:H	1:A:179:GLN:HB2	1.69	0.58
1:A:279:ASN:O	1:A:299:LEU:HD12	2.03	0.57
1:A:28:ASP:N	1:A:28:ASP:OD2	2.37	0.57
1:A:204:ASN:O	1:A:206:GLY:N	2.38	0.56
1:A:111:ARG:HH11	1:A:167:TRP:HZ3	1.55	0.55
1:A:218:PRO:C	1:A:220:LYS:H	2.10	0.54
1:A:314:GLN:HB2	1:A:317:GLU:HG2	1.89	0.54
1:A:200:ASP:OD1	1:A:202:SER:OG	2.16	0.54
1:A:67:GLU:OE1	1:A:67:GLU:N	2.41	0.54
1:A:188:GLU:HG3	1:A:189:GLN:OE1	2.08	0.54
1:A:73:VAL:HG13	1:A:105:LEU:HD12	1.89	0.54
1:A:176:SER:HA	1:A:200:ASP:HB3	1.90	0.54
1:A:35:VAL:HG12	1:A:37:ASN:H	1.74	0.53
1:A:309:LEU:O	1:A:330:PRO:HG2	2.09	0.53
1:A:323:ASN:N	1:A:323:ASN:HD22	2.06	0.53
1:A:301:VAL:HA	1:A:323:ASN:ND2	2.23	0.53
1:A:35:VAL:HG12	1:A:37:ASN:N	2.24	0.53
1:A:43:PRO:HB2	1:A:45:TRP:CE2	2.45	0.52
1:A:108:GLY:O	1:A:112:VAL:HG12	2.09	0.52
1:A:185:PHE:CD2	1:A:185:PHE:N	2.79	0.51
1:A:220:LYS:HG3	1:A:221:PHE:HD1	1.75	0.51
1:A:333:VAL:N	1:A:334:PRO:HD2	2.26	0.50
1:A:79:PRO:HD2	1:A:83:ALA:HB2	1.92	0.50
1:A:302:LEU:O	1:A:324:LEU:HD12	2.10	0.50
1:A:333:VAL:H	1:A:334:PRO:HD2	1.76	0.50
1:A:175:LEU:O	1:A:200:ASP:N	2.28	0.49
1:A:305:SER:O	1:A:307:ASN:ND2	2.45	0.49
1:A:135:LEU:H	1:A:135:LEU:HD23	1.77	0.49
1:A:255:ASP:C	1:A:256:LEU:HD12	2.33	0.49
1:A:159:SER:OG	1:A:159:SER:O	2.29	0.49
1:A:272:CYS:O	1:A:274:TRP:N	2.44	0.49
1:A:52:VAL:HG22	1:A:89:LEU:HD11	1.95	0.49
1:A:77:ALA:HB2	1:A:111:ARG:HH21	1.77	0.49
1:A:58:GLU:C	1:A:58:GLU:OE1	2.51	0.48
1:A:68:PRO:O	1:A:70:LEU:HD22	2.13	0.48
1:A:280:SER:HA	1:A:301:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ASP:OD1	1:A:304:LEU:N	2.46	0.48
1:A:53:SER:OG	1:A:53:SER:O	2.30	0.48
1:A:297:ALA:HA	1:A:319:PRO:HB2	1.95	0.48
1:A:241:CYS:HB2	1:A:274:TRP:CE2	2.49	0.48
1:A:142:LEU:HD12	1:A:144:LEU:HD13	1.96	0.48
1:A:168:LEU:HD23	1:A:172:LEU:HD22	1.95	0.48
1:A:220:LYS:HG3	1:A:221:PHE:CD1	2.49	0.47
1:A:291:VAL:CG1	1:A:295:LEU:HD21	2.45	0.47
1:A:193:PHE:CD1	1:A:221:PHE:CE1	3.03	0.46
1:A:321:VAL:HG21	1:A:324:LEU:HB2	1.96	0.46
1:A:47:GLU:N	1:A:47:GLU:OE1	2.49	0.46
1:A:282:ASN:O	1:A:283:LEU:HD23	2.16	0.46
1:A:121:LEU:HB2	1:A:144:LEU:HD11	1.98	0.45
1:A:142:LEU:C	1:A:169:LYS:HG3	2.37	0.45
1:A:241:CYS:HB2	1:A:274:TRP:CZ2	2.52	0.45
1:A:46:SER:O	1:A:49:PHE:HD2	1.99	0.45
1:A:64:LEU:HD23	1:A:65:ASN:C	2.36	0.45
1:A:190:VAL:HG12	1:A:220:LYS:HE2	1.98	0.45
1:A:275:SER:O	1:A:277:ALA:N	2.51	0.44
1:A:291:VAL:HA	1:A:292:PRO:HD3	1.83	0.44
1:A:298:LYS:O	1:A:299:LEU:HD13	2.17	0.44
1:A:186:SER:O	1:A:186:SER:OG	2.22	0.44
1:A:175:LEU:HB3	1:A:199:LEU:HD12	1.99	0.44
1:A:71:LYS:HE3	1:A:71:LYS:HB3	1.76	0.44
1:A:133:PRO:HA	1:A:134:PRO:HD3	1.80	0.44
1:A:227:LEU:HD23	1:A:254:LEU:CD1	2.48	0.44
1:A:126:LEU:HB3	1:A:127:LYS:H	1.72	0.44
1:A:119:LYS:O	1:A:145:SER:N	2.40	0.44
1:A:165:GLN:HE22	1:A:220:LYS:HZ1	1.65	0.44
1:A:218:PRO:C	1:A:220:LYS:N	2.71	0.43
1:A:295:LEU:HB3	1:A:319:PRO:HG3	1.99	0.43
1:A:66:LEU:HD23	1:A:66:LEU:O	2.18	0.43
1:A:144:LEU:HD12	1:A:144:LEU:HA	1.65	0.43
1:A:137:LEU:HD11	1:A:140:THR:CG2	2.49	0.43
1:A:218:PRO:O	1:A:220:LYS:N	2.50	0.43
1:A:58:GLU:OE2	1:A:60:HIS:ND1	2.51	0.43
1:A:200:ASP:CG	1:A:202:SER:HG	2.15	0.43
1:A:137:LEU:CD1	1:A:140:THR:CG2	2.97	0.42
1:A:299:LEU:HB3	1:A:300:ARG:H	1.65	0.42
1:A:326:LEU:HD12	1:A:326:LEU:HA	1.90	0.42
1:A:190:VAL:HG12	1:A:220:LYS:HE3	1.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ASN:HB2	1:A:261:LEU:HD11	2.02	0.41
1:A:306:SER:H	1:A:328:GLY:HA3	1.85	0.41
1:A:94:LEU:HD23	1:A:121:LEU:CD1	2.49	0.41
1:A:114:ALA:HA	1:A:142:LEU:HB3	2.02	0.41
1:A:256:LEU:O	1:A:258:HIS:N	2.47	0.41
1:A:197:THR:OG1	1:A:198:SER:N	2.53	0.41
1:A:281:LEU:O	1:A:302:LEU:HD12	2.21	0.41
1:A:192:ALA:C	1:A:220:LYS:HZ3	2.24	0.41
1:A:71:LYS:HB3	1:A:72:ARG:HA	2.02	0.41
1:A:160:TRP:HH2	1:A:177:ILE:HD13	1.85	0.41
1:A:151:ASN:N	1:A:179:GLN:HB2	2.34	0.40
1:A:213:MET:HG2	1:A:243:ALA:HB1	2.02	0.40
1:A:311:ARG:HB2	1:A:312:ALA:H	1.63	0.40
1:A:101:VAL:O	1:A:128:ILE:HA	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	308/310 (99%)	210 (68%)	70 (23%)	28 (9%)	<b>1</b> <b>14</b>

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	73	VAL
1	A	77	ALA
1	A	90	ARG
1	A	136	PRO
1	A	137	LEU
1	A	139	ALA

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Mol	Chain	Res	Type
1	A	230	ARG
1	A	257	SER
1	A	273	MET
1	A	276	SER
1	A	35	VAL
1	A	45	TRP
1	A	98	ALA
1	A	187	CYS
1	A	219	HIS
1	A	248	GLY
1	A	75	ALA
1	A	179	GLN
1	A	196	LEU
1	A	206	GLY
1	A	247	ALA
1	A	313	PRO
1	A	205	PRO
1	A	321	VAL
1	A	323	ASN
1	A	79	PRO
1	A	62	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	255/256 (100%)	221 (87%)	34 (13%)	4 28

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

Mol	Chain	Res	Type
1	A	28	ASP
1	A	34	CYS
1	A	36	CYS
1	A	47	GLU
1	A	57	VAL

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Mol	Chain	Res	Type
1	A	58	GLU
1	A	66	LEU
1	A	70	LEU
1	A	74	ASP
1	A	76	ASP
1	A	82	TYR
1	A	105	LEU
1	A	112	VAL
1	A	123	LEU
1	A	131	THR
1	A	132	MET
1	A	137	LEU
1	A	142	LEU
1	A	158	ARG
1	A	172	LEU
1	A	175	LEU
1	A	181	HIS
1	A	185	PHE
1	A	186	SER
1	A	216	LEU
1	A	252	HIS
1	A	261	LEU
1	A	262	ARG
1	A	273	MET
1	A	295	LEU
1	A	304	LEU
1	A	310	ASN
1	A	322	ASP
1	A	323	ASN

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	307	ASN
1	A	323	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	310/310 (100%)	-0.37	1 (0%) 93 91	9, 51, 100, 126	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	PRO	3.9

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.