



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:59 am GMT

PDB ID : 2D9Q  
Title : Crystal Structure of the Human GCSF-Receptor Signaling Complex  
Authors : Tamada, T.; Kuroki, R.  
Deposited on : 2005-12-12  
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](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  
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

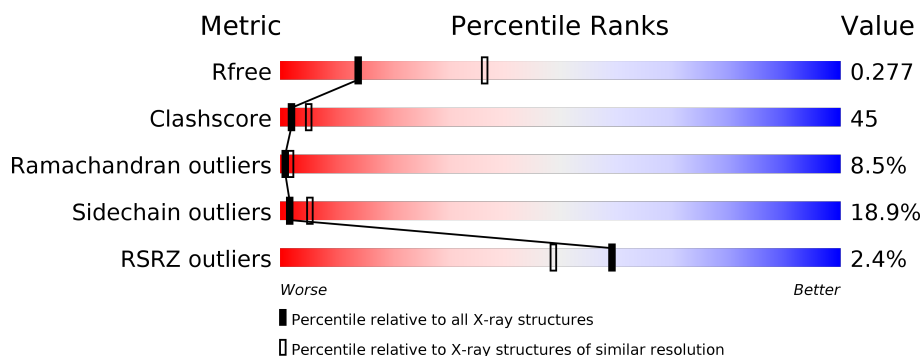
# 1 Overall quality at a glance

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  $\geq 3$ , 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	174	 29% 47% 17% . .
2	B	313	 33% 41% 19% . .

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3647 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 CSF3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1274	815	216	235	8			

- Molecule 2 is a protein called Granulocyte colony-stimulating factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	299	Total	C	N	O	S	0	0	0
			2331	1472	410	429	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	79	SER	CYS	ENGINEERED	UNP Q99062
B	164	SER	CYS	ENGINEERED	UNP Q99062
B	229	SER	CYS	ENGINEERED	UNP Q99062
B	310	ALA	-	CLONING ARTIFACT	UNP Q99062
B	311	ALA	-	CLONING ARTIFACT	UNP Q99062
B	312	ALA	-	CLONING ARTIFACT	UNP Q99062
B	313	PRO	-	CLONING ARTIFACT	UNP Q99062
B	314	ARG	-	CLONING ARTIFACT	UNP Q99062

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		

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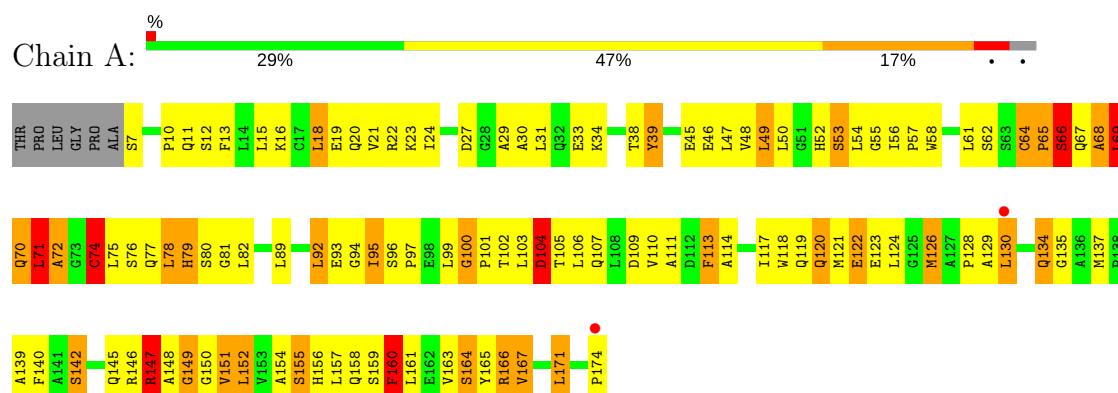
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	9	Total	O	0	0
			9	9		

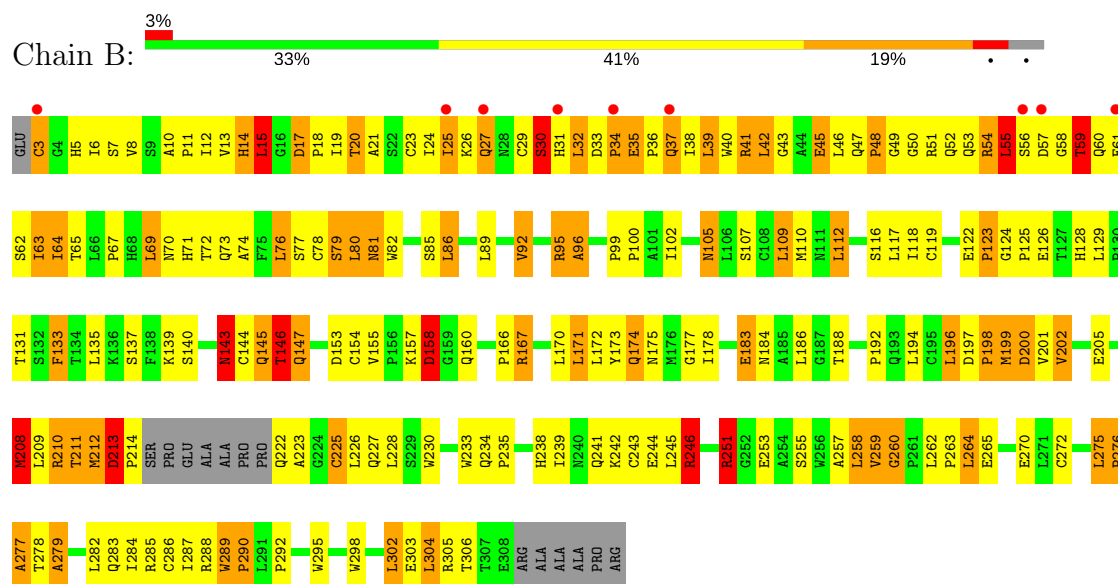
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: CSF3



#### • Molecule 2: Granulocyte colony-stimulating factor receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.78Å 134.78Å 105.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 40.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (20.00-2.80) 91.2 (40.70-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.251 , 0.284 0.242 , 0.277	Depositor DCC
$R_{free}$ test set	1266 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.9	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 36.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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

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	1.61	10/1302 (0.8%)	1.37	8/1769 (0.5%)
2	B	1.59	13/2396 (0.5%)	1.52	34/3273 (1.0%)
All	All	1.59	23/3698 (0.6%)	1.47	42/5042 (0.8%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	208	MET	CG-SD	14.39	2.18	1.81
1	A	147	ARG	CG-CD	7.34	1.70	1.51
2	B	208	MET	CB-CG	7.08	1.74	1.51
1	A	166	ARG	CB-CG	6.60	1.70	1.52
1	A	39	TYR	CE1-CZ	-6.34	1.30	1.38
2	B	146	THR	CA-CB	6.15	1.69	1.53
1	A	113	PHE	CD2-CE2	-6.14	1.26	1.39
2	B	230	TRP	CE3-CZ3	-6.01	1.28	1.38
2	B	290	PRO	CA-C	5.97	1.64	1.52
1	A	137	MET	CG-SD	5.92	1.96	1.81
1	A	160	PHE	CB-CG	-5.85	1.41	1.51
2	B	143	ASN	CB-CG	5.84	1.64	1.51
2	B	96	ALA	CA-CB	-5.71	1.40	1.52
2	B	183	GLU	CD-OE2	5.71	1.31	1.25
2	B	92	VAL	CA-CB	-5.70	1.42	1.54
1	A	74	CYS	CB-SG	-5.56	1.72	1.81
1	A	69	LEU	CA-C	5.46	1.67	1.52
1	A	147	ARG	NE-CZ	5.43	1.40	1.33
2	B	133	PHE	CB-CG	-5.23	1.42	1.51
1	A	33	GLU	CD-OE1	5.23	1.31	1.25
2	B	202	VAL	CA-CB	-5.21	1.43	1.54
2	B	122	GLU	CD-OE2	5.15	1.31	1.25
2	B	201	VAL	CB-CG1	-5.06	1.42	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	200	ASP	CB-CG-OD1	10.71	127.94	118.30
2	B	290	PRO	N-CD-CG	-8.83	89.95	103.20
2	B	305	ARG	NE-CZ-NH1	8.58	124.59	120.30
2	B	118	ILE	CG1-CB-CG2	-8.15	93.47	111.40
2	B	123	PRO	N-CD-CG	-8.06	91.11	103.20
2	B	264	LEU	CB-CG-CD1	-7.90	97.57	111.00
2	B	258	LEU	CA-CB-CG	7.52	132.60	115.30
2	B	153	ASP	CB-CG-OD2	6.91	124.52	118.30
2	B	17	ASP	CB-CG-OD2	6.83	124.45	118.30
2	B	208	MET	CB-CG-SD	6.53	131.99	112.40
2	B	3	CYS	CA-CB-SG	-6.40	102.48	114.00
1	A	69	LEU	CB-CA-C	6.24	122.06	110.20
2	B	251	ARG	NE-CZ-NH1	6.23	123.42	120.30
2	B	183	GLU	OE1-CD-OE2	6.17	130.70	123.30
1	A	151	VAL	CB-CA-C	-6.08	99.84	111.40
1	A	15	LEU	CB-CG-CD1	-6.05	100.71	111.00
2	B	192	PRO	N-CD-CG	-5.98	94.24	103.20
2	B	55	LEU	CA-CB-CG	5.94	128.96	115.30
2	B	246	ARG	NE-CZ-NH2	-5.85	117.37	120.30
2	B	109	LEU	CB-CA-C	-5.80	99.19	110.20
2	B	155	VAL	CB-CA-C	-5.63	100.70	111.40
2	B	15	LEU	CA-CB-CG	5.54	128.04	115.30
2	B	57	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	104	ASP	CB-CG-OD2	5.53	123.27	118.30
2	B	259	VAL	CB-CA-C	-5.51	100.93	111.40
1	A	122	GLU	OE1-CD-OE2	-5.50	116.70	123.30
2	B	253	GLU	N-CA-C	-5.48	96.21	111.00
2	B	272	CYS	CA-CB-SG	-5.48	104.14	114.00
2	B	76	LEU	CA-CB-CG	5.44	127.80	115.30
2	B	213	ASP	CB-CG-OD2	5.40	123.16	118.30
2	B	95	ARG	NE-CZ-NH2	-5.39	117.60	120.30
2	B	225	CYS	CA-CB-SG	-5.39	104.31	114.00
2	B	199	MET	CG-SD-CE	-5.34	91.66	100.20
1	A	152	LEU	CB-CG-CD1	5.30	120.01	111.00
2	B	17	ASP	CB-CA-C	-5.26	99.87	110.40
2	B	112	LEU	CB-CG-CD1	5.20	119.84	111.00
2	B	158	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	31	LEU	CB-CG-CD2	-5.13	102.27	111.00
1	A	49	LEU	CB-CG-CD2	-5.12	102.30	111.00
2	B	246	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	B	14	HIS	CA-C-N	-5.11	105.96	117.20
2	B	41	ARG	NE-CZ-NH1	-5.03	117.79	120.30



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	1274	0	1283	129	0
2	B	2331	0	2287	196	0
3	B	28	0	25	1	0
4	A	5	0	0	1	0
4	B	9	0	0	1	0
All	All	3647	0	3595	322	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 45.

All (322) 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)
2:B:212:MET:SD	2:B:212:MET:CE	2.05	1.45
2:B:208:MET:CG	2:B:208:MET:SD	2.18	1.31
2:B:276:PRO:O	2:B:278:THR:HG23	1.03	1.16
1:A:7:SER:HB2	1:A:174:PRO:HG2	1.25	1.12
2:B:276:PRO:O	2:B:278:THR:CG2	1.99	1.09
2:B:143:ASN:H	2:B:143:ASN:HD22	1.12	0.95
2:B:63:ILE:HD12	2:B:63:ILE:C	1.88	0.94
1:A:71:LEU:O	1:A:72:ALA:O	1.86	0.93
1:A:45:GLU:O	1:A:48:VAL:HG23	1.71	0.90
2:B:259:VAL:O	2:B:260:GLY:O	1.88	0.88
1:A:7:SER:CB	1:A:174:PRO:HG2	2.03	0.87
2:B:205:GLU:HB2	2:B:233:TRP:CE2	2.10	0.86
2:B:25:ILE:HG21	2:B:38:ILE:HG21	1.57	0.86
2:B:246:ARG:HG2	2:B:298:TRP:CZ3	2.12	0.84
1:A:38:THR:O	1:A:38:THR:HG22	1.76	0.84
1:A:71:LEU:O	1:A:74:CYS:HB3	1.76	0.83
2:B:183:GLU:HB3	2:B:188:THR:HG23	1.61	0.83
2:B:33:ASP:O	2:B:35:GLU:N	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLU:HB2	1:A:146:ARG:NH1	1.95	0.81
2:B:86:LEU:N	2:B:86:LEU:HD12	1.96	0.81
2:B:86:LEU:HD12	2:B:86:LEU:H	1.47	0.80
1:A:120:GLN:OE1	1:A:120:GLN:HA	1.83	0.79
2:B:23:CYS:HB2	2:B:40:TRP:CH2	2.18	0.79
2:B:19:ILE:CD1	2:B:69:LEU:HD12	2.14	0.78
1:A:72:ALA:HB2	1:A:126:MET:SD	2.23	0.78
2:B:143:ASN:H	2:B:143:ASN:ND2	1.83	0.76
1:A:7:SER:HB2	1:A:174:PRO:CG	2.12	0.76
2:B:27:GLN:HG2	2:B:34:PRO:HG2	1.67	0.76
2:B:19:ILE:HD11	2:B:69:LEU:HD12	1.67	0.76
2:B:264:LEU:C	2:B:264:LEU:HD12	2.07	0.75
1:A:159:SER:O	1:A:161:LEU:N	2.19	0.75
2:B:23:CYS:HB2	2:B:40:TRP:CZ2	2.22	0.74
2:B:39:LEU:N	2:B:39:LEU:HD23	2.02	0.74
1:A:20:GLN:NE2	4:A:176:HOH:O	2.19	0.74
2:B:39:LEU:HB2	2:B:46:LEU:HD21	1.70	0.73
2:B:302:LEU:HD22	2:B:304:LEU:HD22	1.69	0.73
2:B:19:ILE:HA	4:B:405:HOH:O	1.87	0.73
2:B:278:THR:O	2:B:279:ALA:HB2	1.89	0.72
2:B:37:GLN:HA	2:B:52:GLN:HE21	1.54	0.72
1:A:38:THR:O	1:A:38:THR:CG2	2.37	0.72
2:B:80:LEU:HD13	2:B:89:LEU:HD11	1.71	0.71
2:B:226:LEU:HD21	2:B:304:LEU:HG	1.73	0.70
2:B:275:LEU:C	2:B:277:ALA:H	1.92	0.70
2:B:137:SER:HA	2:B:177:GLY:O	1.91	0.69
1:A:82:LEU:HD22	1:A:82:LEU:H	1.57	0.69
2:B:37:GLN:HG3	2:B:52:GLN:HG3	1.74	0.69
1:A:71:LEU:C	1:A:72:ALA:O	2.30	0.68
2:B:285:ARG:HD3	2:B:298:TRP:CE2	2.29	0.68
1:A:79:HIS:ND1	1:A:79:HIS:C	2.47	0.67
2:B:26:LYS:HA	2:B:59:THR:HG22	1.76	0.67
2:B:37:GLN:HA	2:B:52:GLN:NE2	2.09	0.67
2:B:222:GLN:HG2	2:B:223:ALA:H	1.58	0.67
1:A:171:LEU:O	1:A:171:LEU:HD23	1.95	0.66
1:A:81:GLY:O	1:A:82:LEU:C	2.32	0.66
2:B:55:LEU:HD13	2:B:58:GLY:HA3	1.77	0.66
1:A:12:SER:OG	1:A:13:PHE:N	2.28	0.66
2:B:212:MET:HG2	2:B:227:GLN:HE21	1.60	0.65
2:B:289:TRP:HB3	2:B:290:PRO:HD3	1.78	0.65
1:A:130:LEU:HD22	1:A:130:LEU:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:SER:O	1:A:160:PHE:C	2.33	0.65
1:A:38:THR:HG22	1:A:39:TYR:CE2	2.31	0.65
1:A:47:LEU:HD22	1:A:148:ALA:HB1	1.79	0.65
2:B:251:ARG:NH1	2:B:279:ALA:HB3	2.12	0.64
2:B:128:HIS:O	2:B:129:LEU:HG	1.97	0.64
1:A:34:LYS:O	1:A:99:LEU:HD21	1.98	0.64
1:A:78:LEU:O	1:A:79:HIS:C	2.36	0.63
2:B:63:ILE:CD1	2:B:63:ILE:C	2.62	0.63
2:B:184:ASN:C	2:B:184:ASN:OD1	2.37	0.62
2:B:239:ILE:HG23	2:B:288:ARG:HG3	1.81	0.62
2:B:143:ASN:N	2:B:143:ASN:HD22	1.90	0.61
2:B:211:THR:HG22	2:B:212:MET:H	1.64	0.61
2:B:14:HIS:HB3	2:B:15:LEU:HG	1.84	0.60
2:B:8:VAL:HG12	2:B:21:ALA:HB2	1.82	0.60
2:B:64:ILE:HD12	2:B:65:THR:H	1.67	0.60
1:A:95:ILE:HG21	1:A:99:LEU:HD12	1.83	0.60
1:A:159:SER:C	1:A:161:LEU:N	2.55	0.60
1:A:20:GLN:O	1:A:24:ILE:HG13	2.00	0.60
2:B:145:GLN:O	2:B:147:GLN:N	2.34	0.60
2:B:212:MET:HE3	2:B:212:MET:HA	1.83	0.60
2:B:212:MET:HA	2:B:212:MET:CE	2.32	0.60
2:B:41:ARG:HG2	2:B:45:GLU:C	2.22	0.60
2:B:287:ILE:HG23	2:B:287:ILE:O	2.02	0.59
1:A:82:LEU:HD22	1:A:82:LEU:N	2.16	0.59
1:A:167:VAL:O	1:A:167:VAL:HG12	2.03	0.59
2:B:63:ILE:HD12	2:B:63:ILE:O	2.02	0.59
2:B:277:ALA:O	2:B:278:THR:C	2.41	0.59
1:A:61:LEU:HD23	1:A:163:VAL:CG1	2.33	0.59
2:B:6:ILE:HD11	2:B:78:CYS:CB	2.34	0.58
2:B:80:LEU:HD23	2:B:81:ASN:N	2.18	0.58
2:B:278:THR:HA	2:B:306:THR:H	1.67	0.58
1:A:99:LEU:C	1:A:101:PRO:HD2	2.23	0.58
2:B:275:LEU:C	2:B:277:ALA:N	2.56	0.58
2:B:259:VAL:C	2:B:260:GLY:O	2.42	0.58
1:A:99:LEU:O	1:A:101:PRO:HD2	2.03	0.58
1:A:16:LYS:O	1:A:20:GLN:HG3	2.04	0.58
1:A:69:LEU:O	1:A:70:GLN:OE1	2.21	0.58
1:A:71:LEU:O	1:A:72:ALA:C	2.42	0.58
1:A:92:LEU:HD11	1:A:150:GLY:HA2	1.85	0.58
2:B:233:TRP:CD2	2:B:235:PRO:HG2	2.39	0.58
2:B:233:TRP:CE2	2:B:235:PRO:HG2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:ILE:HD11	2:B:78:CYS:HB2	1.85	0.57
1:A:34:LYS:HG2	1:A:99:LEU:HD23	1.86	0.57
2:B:26:LYS:HD3	2:B:59:THR:HG23	1.86	0.57
1:A:39:TYR:CE1	1:A:147:ARG:HD2	2.39	0.57
2:B:80:LEU:C	2:B:80:LEU:HD23	2.25	0.57
2:B:41:ARG:HG2	2:B:45:GLU:O	2.04	0.57
1:A:34:LYS:O	1:A:34:LYS:HG3	2.05	0.56
1:A:99:LEU:O	1:A:101:PRO:CD	2.53	0.56
1:A:52:HIS:O	1:A:54:LEU:N	2.38	0.56
2:B:17:ASP:HB3	2:B:18:PRO:HD2	1.86	0.56
2:B:304:LEU:N	2:B:304:LEU:HD23	2.21	0.56
1:A:77:GLN:O	1:A:78:LEU:O	2.24	0.56
1:A:64:CYS:O	1:A:66:SER:N	2.39	0.56
2:B:80:LEU:HD13	2:B:89:LEU:CD1	2.36	0.55
2:B:26:LYS:CD	2:B:59:THR:HG23	2.36	0.55
2:B:116:SER:HB2	2:B:166:PRO:HA	1.87	0.55
2:B:278:THR:O	2:B:279:ALA:CB	2.55	0.55
1:A:151:VAL:HG12	1:A:151:VAL:O	2.07	0.55
2:B:173:TYR:O	2:B:174:GLN:OE1	2.25	0.55
2:B:173:TYR:CE1	2:B:199:MET:HG2	2.42	0.54
1:A:10:PRO:O	1:A:11:GLN:C	2.41	0.54
1:A:23:LYS:HB2	2:B:238:HIS:ND1	2.22	0.54
2:B:197:ASP:O	2:B:199:MET:N	2.41	0.54
2:B:24:ILE:HG22	2:B:24:ILE:O	2.08	0.54
2:B:20:THR:OG1	2:B:65:THR:OG1	2.26	0.54
2:B:6:ILE:HD13	2:B:76:LEU:CD1	2.37	0.54
1:A:99:LEU:O	1:A:101:PRO:N	2.41	0.54
2:B:157:LYS:HB2	2:B:160:GLN:NE2	2.23	0.54
2:B:284:ILE:HG12	2:B:285:ARG:N	2.22	0.54
1:A:13:PHE:C	1:A:13:PHE:CD2	2.81	0.54
1:A:56:ILE:HD12	1:A:152:LEU:HD23	1.90	0.54
2:B:262:LEU:HB3	2:B:263:PRO:HD2	1.90	0.53
2:B:41:ARG:HH21	2:B:79:SER:CB	2.22	0.53
1:A:56:ILE:HG21	1:A:58:TRP:CH2	2.43	0.53
2:B:275:LEU:HD23	2:B:275:LEU:H	1.74	0.53
1:A:13:PHE:CE1	1:A:120:GLN:HB2	2.44	0.53
2:B:72:THR:HA	2:B:96:ALA:O	2.09	0.53
1:A:19:GLU:HA	1:A:22:ARG:NH2	2.24	0.53
2:B:239:ILE:CG2	2:B:288:ARG:HG3	2.38	0.53
2:B:54:ARG:NE	2:B:60:GLN:NE2	2.57	0.53
1:A:134:GLN:HG3	1:A:135:GLY:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ILE:HG22	1:A:96:SER:N	2.22	0.52
1:A:119:GLN:O	1:A:120:GLN:C	2.46	0.52
1:A:61:LEU:HD23	1:A:163:VAL:HG12	1.91	0.52
1:A:93:GLU:C	1:A:95:ILE:H	2.12	0.52
2:B:19:ILE:HD12	2:B:69:LEU:HD12	1.89	0.52
1:A:159:SER:C	1:A:161:LEU:H	2.13	0.52
1:A:45:GLU:O	1:A:47:LEU:N	2.43	0.52
2:B:123:PRO:HB3	2:B:133:PHE:CE2	2.43	0.52
2:B:275:LEU:O	2:B:277:ALA:N	2.43	0.52
1:A:50:LEU:HD13	1:A:54:LEU:HD12	1.92	0.52
1:A:38:THR:O	1:A:39:TYR:CG	2.63	0.52
2:B:172:LEU:HD22	2:B:199:MET:SD	2.50	0.52
1:A:130:LEU:HD22	1:A:130:LEU:H	1.72	0.51
2:B:38:ILE:HD11	2:B:62:SER:CB	2.40	0.51
2:B:107:SER:O	2:B:119:CYS:HA	2.10	0.51
2:B:109:LEU:O	2:B:117:LEU:HD12	2.10	0.51
2:B:110:MET:HB3	2:B:202:VAL:HA	1.93	0.51
2:B:285:ARG:HD3	2:B:298:TRP:CZ2	2.46	0.51
1:A:24:ILE:CD1	1:A:110:VAL:HA	2.41	0.51
1:A:20:GLN:NE2	1:A:113:PHE:HA	2.26	0.50
2:B:139:LYS:HD2	2:B:171:LEU:HB2	1.91	0.50
2:B:63:ILE:HD12	2:B:64:ILE:N	2.26	0.50
2:B:234:GLN:N	2:B:235:PRO:HD2	2.27	0.50
1:A:167:VAL:O	1:A:171:LEU:HB2	2.11	0.50
1:A:93:GLU:O	1:A:95:ILE:N	2.45	0.50
2:B:60:GLN:HG2	2:B:60:GLN:O	2.12	0.50
1:A:82:LEU:CD2	1:A:82:LEU:H	2.24	0.50
2:B:245:LEU:HD12	2:B:246:ARG:H	1.76	0.50
2:B:33:ASP:O	2:B:35:GLU:HG3	2.12	0.50
1:A:154:ALA:O	1:A:158:GLN:HB2	2.10	0.50
2:B:38:ILE:HD11	2:B:62:SER:HB3	1.92	0.50
2:B:12:ILE:C	2:B:13:VAL:HG13	2.32	0.49
2:B:196:LEU:HD12	2:B:196:LEU:C	2.33	0.49
2:B:80:LEU:HD22	2:B:89:LEU:HD11	1.94	0.49
1:A:148:ALA:C	1:A:150:GLY:N	2.66	0.49
1:A:164:SER:O	1:A:165:TYR:C	2.49	0.49
2:B:29:CYS:O	2:B:30:SER:CB	2.58	0.49
2:B:226:LEU:CD2	2:B:304:LEU:HG	2.41	0.49
2:B:239:ILE:O	2:B:239:ILE:HG22	2.11	0.49
2:B:200:ASP:HB3	2:B:292:PRO:HB2	1.94	0.49
2:B:197:ASP:C	2:B:199:MET:N	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:LEU:HD23	2:B:303:GLU:N	2.28	0.48
1:A:93:GLU:C	1:A:95:ILE:N	2.65	0.48
2:B:288:ARG:HD3	2:B:292:PRO:O	2.13	0.48
2:B:226:LEU:O	2:B:270:GLU:HA	2.13	0.48
1:A:100:GLY:O	1:A:104:ASP:HB2	2.13	0.48
1:A:38:THR:CG2	1:A:39:TYR:CE2	2.96	0.48
2:B:234:GLN:HB2	2:B:235:PRO:CD	2.43	0.48
2:B:86:LEU:N	2:B:86:LEU:CD1	2.69	0.48
2:B:209:LEU:C	2:B:210:ARG:HG3	2.34	0.48
2:B:27:GLN:NE2	2:B:33:ASP:HB3	2.29	0.48
1:A:55:GLY:O	1:A:57:PRO:HD3	2.14	0.48
2:B:39:LEU:H	2:B:39:LEU:HD23	1.77	0.48
1:A:27:ASP:OD1	1:A:109:ASP:OD2	2.31	0.47
1:A:38:THR:HG22	1:A:39:TYR:CZ	2.49	0.47
1:A:50:LEU:HD13	1:A:54:LEU:CD1	2.44	0.47
1:A:24:ILE:HD13	1:A:110:VAL:CG2	2.44	0.47
2:B:304:LEU:N	2:B:304:LEU:CD2	2.77	0.47
1:A:13:PHE:CE1	1:A:120:GLN:CB	2.98	0.47
1:A:148:ALA:O	1:A:149:GLY:C	2.53	0.47
2:B:175:ASN:HA	2:B:196:LEU:O	2.15	0.47
2:B:42:LEU:HD13	2:B:74:ALA:HB1	1.97	0.47
2:B:246:ARG:NH1	2:B:283:GLN:OE1	2.44	0.47
1:A:123:GLU:O	1:A:124:LEU:HD22	2.15	0.47
1:A:163:VAL:HG12	1:A:164:SER:N	2.28	0.47
2:B:245:LEU:HD12	2:B:246:ARG:N	2.29	0.47
2:B:242:LYS:HE3	2:B:289:TRP:NE1	2.30	0.47
2:B:6:ILE:HG22	2:B:7:SER:N	2.30	0.47
2:B:209:LEU:O	2:B:210:ARG:HG3	2.14	0.47
1:A:119:GLN:O	1:A:122:GLU:N	2.48	0.47
2:B:205:GLU:HB2	2:B:233:TRP:CD2	2.51	0.46
2:B:55:LEU:O	2:B:55:LEU:HD23	2.15	0.46
2:B:6:ILE:HD13	2:B:76:LEU:HD13	1.96	0.46
1:A:24:ILE:HD13	1:A:110:VAL:HA	1.96	0.46
2:B:264:LEU:HD12	2:B:265:GLU:N	2.31	0.46
1:A:13:PHE:CE1	1:A:120:GLN:HG2	2.51	0.46
1:A:72:ALA:C	1:A:74:CYS:H	2.19	0.46
2:B:157:LYS:O	2:B:158:ASP:C	2.55	0.45
1:A:130:LEU:CD2	1:A:130:LEU:N	2.77	0.45
2:B:126:GLU:HG3	2:B:128:HIS:H	1.81	0.45
1:A:145:GLN:O	1:A:149:GLY:N	2.44	0.45
2:B:131:THR:HB	2:B:184:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:ILE:CG2	2:B:287:ILE:O	2.64	0.45
2:B:55:LEU:CD1	2:B:58:GLY:HA3	2.46	0.45
1:A:64:CYS:O	1:A:65:PRO:C	2.56	0.45
2:B:173:TYR:CZ	2:B:199:MET:HG2	2.52	0.45
2:B:245:LEU:HD12	2:B:283:GLN:O	2.17	0.45
1:A:18:LEU:HB3	1:A:22:ARG:HH12	1.82	0.45
1:A:45:GLU:C	1:A:47:LEU:H	2.21	0.45
2:B:41:ARG:HA	2:B:45:GLU:O	2.15	0.45
1:A:119:GLN:O	1:A:121:MET:N	2.50	0.44
1:A:61:LEU:HD23	1:A:163:VAL:HG11	1.97	0.44
2:B:133:PHE:N	2:B:133:PHE:CD1	2.82	0.44
2:B:49:GLY:O	2:B:50:GLY:C	2.54	0.44
2:B:119:CYS:HB2	2:B:135:LEU:CD2	2.48	0.44
2:B:197:ASP:O	2:B:198:PRO:C	2.54	0.44
2:B:242:LYS:HE3	2:B:289:TRP:CD1	2.53	0.44
2:B:205:GLU:OE1	3:B:401:NAG:H81	2.18	0.44
1:A:93:GLU:HB2	1:A:146:ARG:HH11	1.75	0.44
2:B:82:TRP:O	2:B:85:SER:OG	2.36	0.44
1:A:50:LEU:O	1:A:53:SER:OG	2.26	0.44
1:A:167:VAL:O	1:A:167:VAL:CG1	2.63	0.44
2:B:178:ILE:HG21	2:B:178:ILE:HD13	1.68	0.44
2:B:25:ILE:HG21	2:B:38:ILE:CG2	2.40	0.44
2:B:32:LEU:HB3	2:B:36:PRO:HG3	2.00	0.44
2:B:105:ASN:HD22	2:B:105:ASN:N	2.16	0.43
2:B:99:PRO:HB3	2:B:186:LEU:HB3	2.00	0.43
1:A:52:HIS:O	1:A:53:SER:C	2.56	0.43
1:A:94:GLY:HA2	1:A:103:LEU:HD23	2.00	0.43
2:B:123:PRO:HB3	2:B:133:PHE:CZ	2.52	0.43
2:B:213:ASP:HB2	2:B:214:PRO:HD3	1.98	0.43
2:B:276:PRO:C	2:B:278:THR:N	2.71	0.43
2:B:241:GLN:HE21	2:B:286:CYS:HB3	1.83	0.43
1:A:151:VAL:O	1:A:155:SER:HB3	2.18	0.43
1:A:19:GLU:OE1	2:B:173:TYR:OH	2.25	0.43
2:B:38:ILE:CG1	2:B:38:ILE:O	2.67	0.43
1:A:78:LEU:O	1:A:80:SER:N	2.52	0.43
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.77	0.43
2:B:275:LEU:HD23	2:B:275:LEU:N	2.34	0.43
2:B:47:GLN:O	2:B:48:PRO:O	2.37	0.43
1:A:156:HIS:O	1:A:157:LEU:C	2.58	0.43
1:A:74:CYS:C	1:A:76:SER:N	2.67	0.43
2:B:167:ARG:NH1	2:B:172:LEU:CD1	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ASP:HB3	2:B:18:PRO:CD	2.45	0.43
2:B:19:ILE:HD11	2:B:69:LEU:CD1	2.42	0.43
2:B:86:LEU:H	2:B:86:LEU:CD1	2.26	0.43
1:A:52:HIS:C	1:A:54:LEU:N	2.71	0.42
1:A:67:GLN:O	1:A:68:ALA:HB2	2.19	0.42
2:B:25:ILE:HG13	2:B:34:PRO:HG3	2.00	0.42
2:B:275:LEU:HB2	2:B:277:ALA:HB2	2.01	0.42
1:A:106:LEU:O	1:A:107:GLN:C	2.56	0.42
2:B:244:GLU:HG2	2:B:295:TRP:CH2	2.53	0.42
1:A:34:LYS:HG2	1:A:99:LEU:CD2	2.50	0.42
1:A:62:SER:HA	1:A:65:PRO:HD2	2.01	0.42
2:B:117:LEU:HB2	2:B:170:LEU:HD11	2.02	0.42
2:B:167:ARG:NH1	2:B:172:LEU:HD12	2.35	0.42
2:B:53:GLN:HG3	2:B:54:ARG:H	1.85	0.42
2:B:171:LEU:O	2:B:172:LEU:C	2.56	0.42
1:A:148:ALA:O	1:A:150:GLY:N	2.52	0.42
2:B:146:THR:O	2:B:147:GLN:C	2.57	0.42
1:A:67:GLN:HG2	1:A:67:GLN:O	2.19	0.42
2:B:69:LEU:CD2	2:B:71:HIS:H	2.32	0.42
2:B:241:GLN:HG2	2:B:264:LEU:HD23	2.02	0.42
2:B:225:CYS:N	2:B:306:THR:HG22	2.34	0.42
1:A:142:SER:OG	1:A:145:GLN:HG3	2.20	0.41
1:A:68:ALA:C	1:A:69:LEU:HG	2.40	0.41
2:B:32:LEU:HD22	2:B:36:PRO:HD3	2.00	0.41
1:A:129:ALA:HB3	1:A:130:LEU:HD22	2.01	0.41
1:A:77:GLN:O	1:A:78:LEU:C	2.59	0.41
1:A:21:VAL:O	1:A:22:ARG:C	2.58	0.41
2:B:12:ILE:C	2:B:13:VAL:CG1	2.87	0.41
2:B:186:LEU:HA	2:B:186:LEU:HD23	1.71	0.41
2:B:243:CYS:HB3	2:B:285:ARG:O	2.19	0.41
1:A:103:LEU:O	1:A:107:GLN:HG3	2.20	0.41
2:B:20:THR:HG1	2:B:65:THR:HG1	1.63	0.41
2:B:212:MET:HG2	2:B:227:GLN:NE2	2.32	0.41
1:A:111:ALA:O	1:A:114:ALA:HB3	2.21	0.41
1:A:74:CYS:SG	1:A:75:LEU:N	2.89	0.41
2:B:183:GLU:HG3	2:B:183:GLU:O	2.20	0.41
2:B:246:ARG:HA	2:B:257:ALA:O	2.21	0.41
2:B:245:LEU:HD11	2:B:282:LEU:HB3	2.02	0.41
1:A:140:PHE:HB3	1:A:146:ARG:HG2	2.02	0.41
2:B:26:LYS:HA	2:B:59:THR:CG2	2.48	0.41
2:B:54:ARG:NE	2:B:60:GLN:HE21	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:TYR:CG	1:A:147:ARG:HG2	2.56	0.41
2:B:197:ASP:C	2:B:199:MET:H	2.23	0.41
1:A:29:ALA:O	1:A:30:ALA:C	2.56	0.41
2:B:29:CYS:SG	2:B:29:CYS:O	2.78	0.41
2:B:46:LEU:HA	2:B:46:LEU:HD23	1.65	0.41
1:A:117:ILE:O	1:A:118:TRP:C	2.60	0.41
1:A:20:GLN:HG2	2:B:173:TYR:CE2	2.55	0.41
2:B:10:ALA:HA	2:B:11:PRO:HD2	1.83	0.41
2:B:73:GLN:HG2	2:B:74:ALA:N	2.35	0.41
2:B:259:VAL:HG12	2:B:260:GLY:N	2.35	0.41
2:B:209:LEU:HD22	2:B:228:LEU:CD1	2.51	0.40
2:B:276:PRO:C	2:B:278:THR:H	2.24	0.40
1:A:148:ALA:O	1:A:151:VAL:N	2.55	0.40
1:A:79:HIS:HB2	1:A:117:ILE:HG21	2.04	0.40
1:A:89:LEU:O	1:A:92:LEU:HB2	2.21	0.40
1:A:130:LEU:CD2	1:A:130:LEU:H	2.31	0.40
2:B:233:TRP:O	2:B:234:GLN:C	2.60	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	166/174 (95%)	125 (75%)	23 (14%)	18 (11%)	0	1
2	B	295/313 (94%)	241 (82%)	33 (11%)	21 (7%)	1	3
All	All	461/487 (95%)	366 (79%)	56 (12%)	39 (8%)	1	2

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	ALA

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Mol	Chain	Res	Type
1	A	71	LEU
1	A	72	ALA
1	A	78	LEU
1	A	79	HIS
1	A	100	GLY
2	B	15	LEU
2	B	34	PRO
2	B	48	PRO
2	B	56	SER
2	B	260	GLY
2	B	277	ALA
2	B	279	ALA
1	A	66	SER
1	A	139	ALA
1	A	149	GLY
1	A	160	PHE
2	B	30	SER
2	B	124	GLY
2	B	289	TRP
1	A	46	GLU
1	A	53	SER
1	A	120	GLN
1	A	128	PRO
2	B	31	HIS
2	B	67	PRO
2	B	69	LEU
2	B	158	ASP
2	B	213	ASP
1	A	95	ILE
2	B	59	THR
2	B	144	CYS
2	B	146	THR
2	B	276	PRO
1	A	167	VAL
1	A	64	CYS
1	A	65	PRO
2	B	35	GLU
2	B	43	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	137/141 (97%)	116 (85%)	21 (15%)	3	9
2	B	265/274 (97%)	210 (79%)	55 (21%)	1	4
All	All	402/415 (97%)	326 (81%)	76 (19%)	2	5

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	49	LEU
1	A	66	SER
1	A	69	LEU
1	A	70	GLN
1	A	71	LEU
1	A	74	CYS
1	A	92	LEU
1	A	97	PRO
1	A	102	THR
1	A	104	ASP
1	A	105	THR
1	A	126	MET
1	A	130	LEU
1	A	134	GLN
1	A	142	SER
1	A	147	ARG
1	A	155	SER
1	A	164	SER
1	A	166	ARG
1	A	171	LEU
2	B	3	CYS
2	B	5	HIS
2	B	15	LEU
2	B	20	THR
2	B	25	ILE
2	B	27	GLN

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Mol	Chain	Res	Type
2	B	30	SER
2	B	32	LEU
2	B	37	GLN
2	B	39	LEU
2	B	42	LEU
2	B	45	GLU
2	B	51	ARG
2	B	54	ARG
2	B	55	LEU
2	B	59	THR
2	B	61	GLU
2	B	63	ILE
2	B	64	ILE
2	B	70	ASN
2	B	77	SER
2	B	79	SER
2	B	80	LEU
2	B	81	ASN
2	B	86	LEU
2	B	92	VAL
2	B	95	ARG
2	B	100	PRO
2	B	102	ILE
2	B	105	ASN
2	B	112	LEU
2	B	125	PRO
2	B	140	SER
2	B	143	ASN
2	B	145	GLN
2	B	147	GLN
2	B	154	CYS
2	B	158	ASP
2	B	167	ARG
2	B	171	LEU
2	B	174	GLN
2	B	194	LEU
2	B	196	LEU
2	B	198	PRO
2	B	208	MET
2	B	210	ARG
2	B	211	THR
2	B	212	MET

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Mol	Chain	Res	Type
2	B	246	ARG
2	B	251	ARG
2	B	255	SER
2	B	258	LEU
2	B	275	LEU
2	B	302	LEU
2	B	304	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	67	GLN
2	B	27	GLN
2	B	52	GLN
2	B	81	ASN
2	B	87	GLN
2	B	105	ASN
2	B	120	GLN
2	B	143	ASN
2	B	160	GLN
2	B	227	GLN
2	B	241	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	B	401	3,2	14,14,15	1.29	2 (14%)	15,19,21	2.81	8 (53%)
3	NAG	B	402	3	14,14,15	1.86	2 (14%)	15,19,21	2.35	6 (40%)

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	B	401	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	402	3	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NAG	O5-C1	-2.45	1.39	1.43
3	B	401	NAG	O7-C7	2.99	1.30	1.23
3	B	402	NAG	C2-N2	3.71	1.52	1.46
3	B	402	NAG	C1-C2	4.12	1.58	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	NAG	C1-O5-C5	-5.55	104.52	112.17
3	B	401	NAG	O5-C1-C2	-5.18	104.27	111.47
3	B	401	NAG	O6-C6-C5	-3.88	98.28	111.34
3	B	401	NAG	C6-C5-C4	-3.41	105.02	113.00
3	B	401	NAG	C8-C7-N2	-2.70	111.24	116.11
3	B	402	NAG	O7-C7-C8	-2.26	117.95	122.06
3	B	402	NAG	O4-C4-C5	-2.06	104.10	109.28
3	B	401	NAG	O7-C7-N2	2.08	125.93	121.92
3	B	401	NAG	O3-C3-C2	2.17	114.04	109.39
3	B	402	NAG	C3-C4-C5	2.42	114.48	110.22
3	B	401	NAG	O3-C3-C4	2.78	116.41	110.36
3	B	402	NAG	C4-C3-C2	3.64	116.35	111.02
3	B	402	NAG	C2-N2-C7	4.26	129.16	122.94
3	B	402	NAG	C1-C2-N2	5.46	119.82	110.49

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	B	401	NAG	1	0

## 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	168/174 (96%)	-0.19	2 (1%) 79 72	31, 68, 120, 128	0
2	B	299/313 (95%)	-0.20	9 (3%) 51 39	33, 64, 125, 140	0
All	All	467/487 (95%)	-0.20	11 (2%) 59 49	31, 66, 121, 140	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	56	SER	5.4
2	B	57	ASP	5.3
2	B	31	HIS	5.1
2	B	61	GLU	4.1
2	B	34	PRO	4.1
2	B	37	GLN	3.5
2	B	25	ILE	3.2
2	B	3	CYS	2.9
1	A	174	PRO	2.8
1	A	130	LEU	2.2
2	B	27	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	402	14/15	0.91	0.15	-	94,96,97,98	0
3	NAG	B	401	14/15	0.96	0.10	-	73,82,86,89	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.