



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:16 AM GMT

PDB ID : 3OJV  
Title : Crystal Structure of FGF1 complexed with the ectodomain of FGFR1c exhibiting an ordered ligand specificity-determining betaC'-betaE loop  
Authors : Beenken, A.; Mohammadi, M.  
Deposited on : 2010-08-23  
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](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 (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

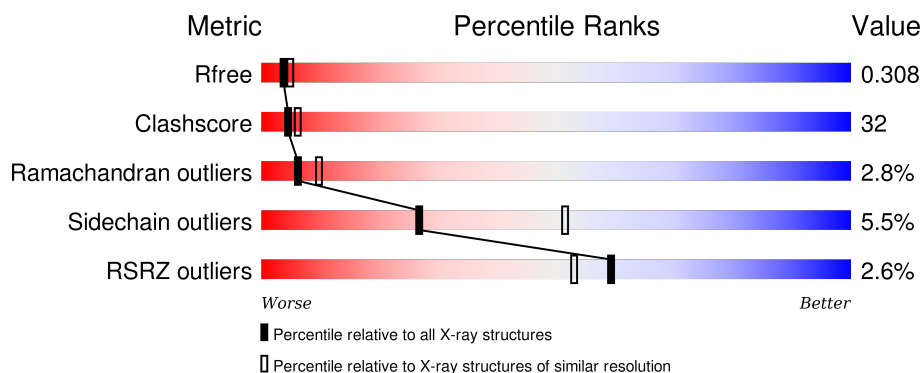
# 1 Overall quality at a glance

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  $\geq 3$ , 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	136	<div> <div>50%</div> <div>44%</div> <div>• •</div> </div>
1	B	136	<div> <div>%</div> <div>44%</div> <div>51%</div> <div>• •</div> </div>
2	C	226	<div> <div>4%</div> <div>49%</div> <div>42%</div> <div>• 6%</div> </div>
2	D	226	<div> <div>4%</div> <div>50%</div> <div>39%</div> <div>5% 6%</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
3	UAP	A	301	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5465 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 Heparin-binding growth factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1052	665	184	199	4			
1	B	133	Total	C	N	O	S	0	0	0
			1052	665	184	199	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	INITIATING METHIONINE	UNP P05230
B	20	MET	-	INITIATING METHIONINE	UNP P05230

- Molecule 2 is a protein called Basic fibroblast growth factor receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	213	Total	C	N	O	S	0	0	0
			1608	1026	278	295	9			
2	D	213	Total	C	N	O	S	0	0	0
			1617	1028	283	297	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	140	MET	-	INITIATING METHIONINE	UNP P11362
C	141	ALA	-	EXPRESSION TAG	UNP P11362
C	185	GLN	ASN	ENGINEERED MUTATION	UNP P11362
D	140	MET	-	INITIATING METHIONINE	UNP P11362
D	141	ALA	-	EXPRESSION TAG	UNP P11362
D	185	GLN	ASN	ENGINEERED MUTATION	UNP P11362

- Molecule 3 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	6	Total	C	N	O	S	0	0
			104	36	3	56	9		

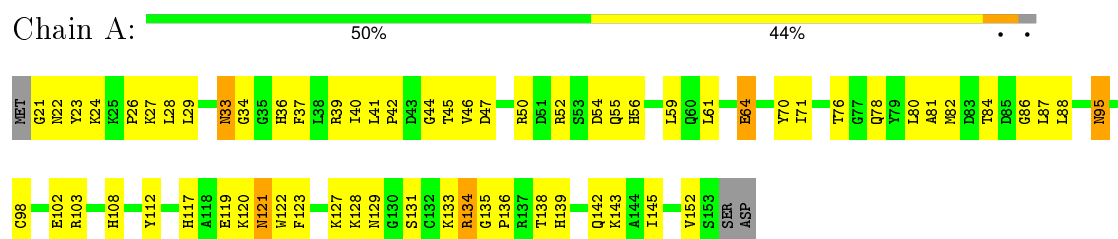
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	2	Total	O	0	0
			2	2		
4	C	13	Total	O	0	0
			13	13		
4	D	11	Total	O	0	0
			11	11		

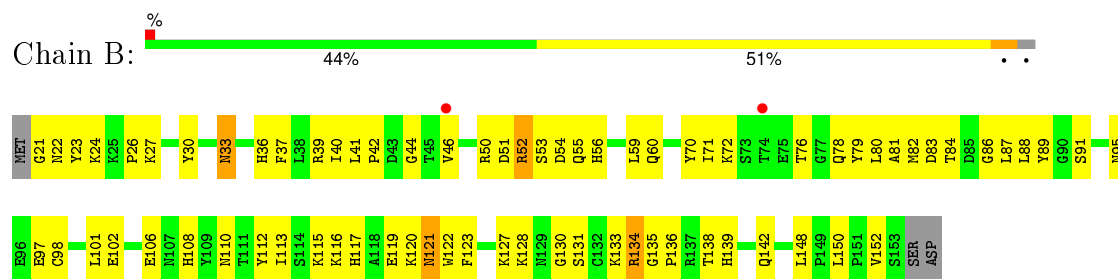
### 3 Residue-property plots

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.

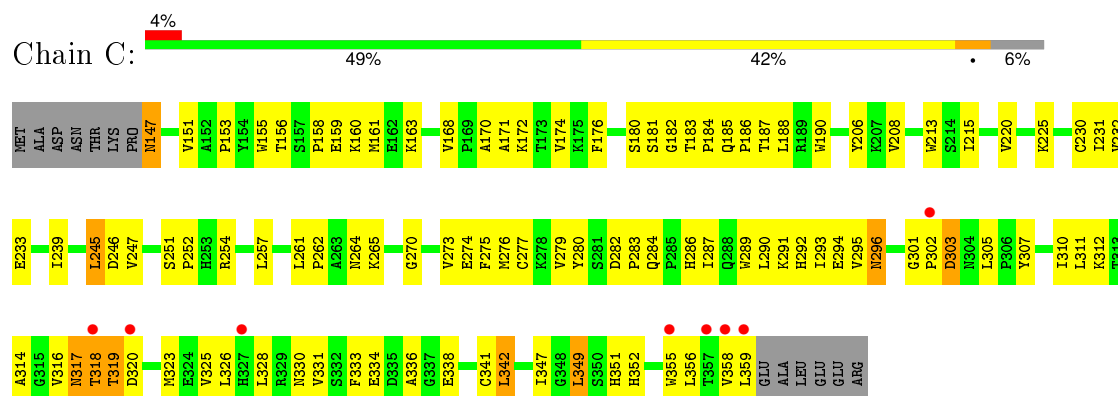
#### • Molecule 1: Heparin-binding growth factor 1



#### • Molecule 1: Heparin-binding growth factor 1

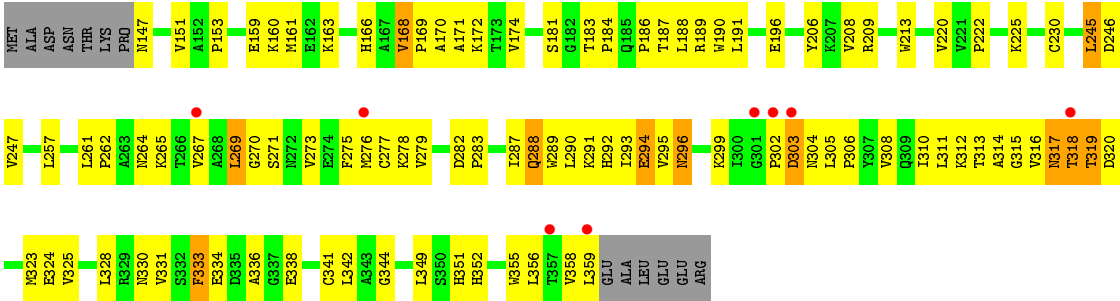


#### • Molecule 2: Basic fibroblast growth factor receptor 1



#### • Molecule 2: Basic fibroblast growth factor receptor 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.32Å 53.42Å 80.46Å 106.44° 106.40° 94.44°	Depositor
Resolution (Å)	25.00 – 2.60 36.58 – 2.59	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.60) 85.9 (36.58-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 2.58Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.251 , 0.309 0.253 , 0.308	Depositor DCC
$R_{free}$ test set	2349 reflections (9.91%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.8	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 29.6	EDS
Estimated twinning fraction	0.018 for k,h,-h-k-l 0.478 for -k,-h,-l 0.017 for -h,-k,h+k+l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 24626 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5465	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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, 0.375 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: UAP, IDS, SGN

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	0.40	0/1076	0.68	0/1453
1	B	0.41	0/1076	0.69	0/1453
2	C	0.41	0/1655	0.70	0/2268
2	D	0.41	0/1664	0.70	0/2279
All	All	0.41	0/5471	0.69	0/7453

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
2	C	0	1
3	A	1	0
All	All	1	1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	301	UAP	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	280	TYR	Sidechain

## 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	1052	0	1023	79	0
1	B	1052	0	1023	72	0
2	C	1608	0	1531	94	0
2	D	1617	0	1537	97	0
3	A	104	0	46	10	0
4	A	6	0	0	2	0
4	B	2	0	0	0	0
4	C	13	0	0	0	0
4	D	11	0	0	0	0
All	All	5465	0	5160	339	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 32.

All (339) 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)
3:A:305:IDS:H5	3:A:306:SGN:H4	1.30	1.09
3:A:305:IDS:H4	1:B:128:LYS:HD2	1.32	1.06
1:A:123:PHE:HB2	1:A:138:THR:HG21	1.37	1.05
1:B:123:PHE:HB2	1:B:138:THR:HG21	1.37	1.02
2:D:318:THR:HG23	2:D:319:THR:H	1.33	0.93
2:C:318:THR:HG21	2:C:323:MET:HG2	1.56	0.86
2:C:265:LYS:O	2:C:356:LEU:HA	1.76	0.86
1:A:133:LYS:NZ	1:A:142:GLN:HE22	1.74	0.85
2:D:333:PHE:HA	2:D:358:VAL:HG11	1.58	0.85
3:A:305:IDS:C5	3:A:306:SGN:H4	2.06	0.85
2:C:333:PHE:HA	2:C:358:VAL:HG11	1.59	0.85
1:A:143:LYS:HD3	3:A:302:SGN:O3	1.76	0.84
2:D:265:LYS:O	2:D:356:LEU:HA	1.78	0.84
2:C:257:LEU:HD23	2:C:279:VAL:HG22	1.61	0.82
2:D:257:LEU:CD2	2:D:279:VAL:HG22	2.08	0.82
1:A:59:LEU:HD22	1:A:71:ILE:HG22	1.61	0.82
1:B:42:PRO:HD3	1:B:56:HIS:CD2	2.15	0.81
2:C:314:ALA:HB2	2:C:323:MET:HG3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:291:LYS:HB2	2:C:311:LEU:HD11	1.66	0.78
2:C:257:LEU:CD2	2:C:279:VAL:HG22	2.14	0.77
2:D:277:CYS:HG	2:D:341:CYS:HG	0.91	0.77
2:D:222:PRO:O	2:D:225:LYS:HG2	1.85	0.77
2:D:209:ARG:HH11	2:D:209:ARG:HG2	1.49	0.75
2:D:277:CYS:O	2:D:324:GLU:HG3	1.86	0.75
2:D:314:ALA:HB2	2:D:323:MET:HG3	1.69	0.74
2:D:183:THR:HA	2:D:184:PRO:C	2.08	0.72
2:D:257:LEU:HD23	2:D:279:VAL:HG22	1.72	0.72
2:D:336:ALA:HB2	2:D:358:VAL:HG23	1.73	0.71
2:C:292:HIS:HD2	2:C:338:GLU:HB3	1.56	0.70
2:D:318:THR:HG23	2:D:319:THR:N	2.07	0.70
3:A:305:IDS:H5	3:A:306:SGN:C4	2.14	0.69
1:B:59:LEU:HD22	1:B:71:ILE:HG22	1.74	0.69
1:A:133:LYS:HZ3	1:A:142:GLN:NE2	1.91	0.69
2:C:183:THR:HA	2:C:184:PRO:C	2.13	0.69
2:C:262:PRO:HD2	2:C:352:HIS:HB3	1.74	0.68
1:B:139:HIS:HB3	1:B:142:GLN:HG3	1.73	0.68
2:D:187:THR:HG22	2:D:188:LEU:N	2.08	0.68
1:A:134:ARG:C	1:A:136:PRO:HD2	2.14	0.68
2:D:291:LYS:HB2	2:D:311:LEU:HD11	1.76	0.67
2:C:273:VAL:HG13	2:C:328:LEU:HD12	1.77	0.67
2:C:336:ALA:HB2	2:C:358:VAL:HG23	1.76	0.67
1:B:133:LYS:NZ	1:B:142:GLN:HE22	1.93	0.67
2:D:292:HIS:HD2	2:D:308:VAL:HG12	1.59	0.67
1:A:26:PRO:O	1:A:27:LYS:HD2	1.95	0.67
1:A:76:THR:OG1	1:A:78:GLN:HG3	1.96	0.66
1:B:76:THR:OG1	1:B:78:GLN:HG3	1.96	0.65
2:C:187:THR:HG22	2:C:188:LEU:N	2.10	0.65
2:C:188:LEU:HD11	2:C:190:TRP:NE1	2.11	0.65
2:D:261:LEU:CD1	2:D:278:LYS:HG3	2.27	0.65
1:B:119:GLU:C	1:B:121:ASN:H	1.99	0.65
2:D:269:LEU:H	2:D:269:LEU:HD23	1.61	0.65
2:D:294:GLU:HG2	2:D:299:LYS:HG2	1.76	0.65
1:A:133:LYS:NZ	1:A:142:GLN:NE2	2.44	0.65
2:C:282:ASP:HB3	2:C:283:PRO:CD	2.25	0.65
1:A:71:ILE:HD12	1:A:80:LEU:HD23	1.79	0.65
1:A:22:ASN:O	1:A:27:LYS:NZ	2.30	0.65
1:A:133:LYS:HZ1	1:A:142:GLN:HE22	1.43	0.64
2:C:292:HIS:CD2	2:C:338:GLU:HB3	2.32	0.64
1:B:133:LYS:NZ	1:B:142:GLN:NE2	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ASN:ND2	1:A:128:LYS:HG2	2.13	0.63
2:D:316:VAL:O	2:D:317:ASN:CB	2.45	0.63
1:B:127:LYS:HD2	1:B:131:SER:OG	1.97	0.63
1:B:54:ASP:OD1	1:B:56:HIS:N	2.27	0.63
1:A:119:GLU:C	1:A:121:ASN:H	2.02	0.63
1:A:29:LEU:HD12	1:A:59:LEU:HD13	1.79	0.63
1:A:42:PRO:HD3	1:A:56:HIS:CD2	2.33	0.63
2:D:317:ASN:O	2:D:319:THR:N	2.32	0.62
1:B:71:ILE:HD12	1:B:80:LEU:HD23	1.81	0.62
2:D:269:LEU:N	2:D:269:LEU:HD23	2.15	0.62
2:D:188:LEU:HD23	2:D:189:ARG:N	2.13	0.62
1:B:26:PRO:O	1:B:27:LYS:HD2	1.99	0.62
1:A:34:GLY:HA3	1:A:36:HIS:CE1	2.34	0.62
2:D:287:ILE:HD12	2:D:287:ILE:N	2.14	0.62
2:D:290:LEU:HD22	2:D:310:ILE:HD13	1.81	0.62
2:C:316:VAL:O	2:C:317:ASN:CB	2.48	0.61
2:C:317:ASN:O	2:C:319:THR:N	2.32	0.61
2:D:257:LEU:HD21	2:D:279:VAL:HG22	1.81	0.61
2:C:282:ASP:HB3	2:C:283:PRO:HD2	1.81	0.61
2:C:187:THR:HG22	2:C:188:LEU:H	1.66	0.61
1:A:102:GLU:HG3	1:A:112:TYR:CE1	2.35	0.61
1:A:50:ARG:HE	2:C:163:LYS:HA	1.65	0.61
2:C:147:ASN:HD22	2:C:147:ASN:N	1.97	0.60
1:B:133:LYS:CE	1:B:142:GLN:HE22	2.14	0.60
2:C:312:LYS:HE2	2:C:323:MET:HE2	1.83	0.60
2:D:209:ARG:NH1	2:D:209:ARG:HG2	2.12	0.60
1:B:22:ASN:O	1:B:27:LYS:NZ	2.34	0.60
2:D:262:PRO:HD2	2:D:352:HIS:HB3	1.82	0.60
2:D:261:LEU:HD12	2:D:278:LYS:HG3	1.83	0.60
2:D:295:VAL:HG22	2:D:296:ASN:ND2	2.17	0.60
2:D:318:THR:CG2	2:D:319:THR:H	2.11	0.60
1:A:54:ASP:OD1	1:A:55:GLN:N	2.33	0.60
1:B:123:PHE:CB	1:B:138:THR:HG21	2.24	0.60
2:D:261:LEU:HB3	2:D:276:MET:O	2.02	0.59
2:D:282:ASP:HB3	2:D:283:PRO:CD	2.32	0.59
2:D:163:LYS:HD2	2:D:166:HIS:CE1	2.36	0.59
1:A:127:LYS:HD2	1:A:131:SER:OG	2.02	0.59
1:B:82:MET:HA	1:B:87:LEU:O	2.03	0.59
1:A:135:GLY:N	1:A:136:PRO:HD2	2.18	0.59
1:A:40:ILE:O	1:A:56:HIS:HB3	2.02	0.58
2:C:225:LYS:HE2	2:C:246:ASP:OD1	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:318:THR:O	2:C:319:THR:HG23	2.03	0.58
1:A:33:ASN:HD21	1:A:128:LYS:HG2	1.69	0.58
2:D:318:THR:O	2:D:319:THR:HG23	2.04	0.58
1:A:70:TYR:CE2	2:C:316:VAL:HB	2.39	0.58
1:A:82:MET:HA	1:A:87:LEU:O	2.04	0.58
2:D:344:GLY:HA3	2:D:349:LEU:HD23	1.86	0.58
1:A:123:PHE:HD1	1:A:138:THR:HG22	1.68	0.57
1:A:39:ARG:NE	1:A:41:LEU:HD21	2.18	0.57
1:B:134:ARG:C	1:B:136:PRO:HD2	2.24	0.57
2:C:287:ILE:N	2:C:287:ILE:HD12	2.19	0.57
1:A:95:ASN:N	1:A:95:ASN:ND2	2.53	0.57
1:A:120:LYS:HB3	1:A:122:TRP:NE1	2.20	0.57
1:B:40:ILE:O	1:B:56:HIS:HB3	2.04	0.57
1:A:133:LYS:HZ3	1:A:142:GLN:CD	2.09	0.56
1:B:122:TRP:HB3	1:B:135:GLY:HA3	1.86	0.56
2:C:159:GLU:C	2:C:161:MET:H	2.09	0.56
2:C:261:LEU:HB3	2:C:276:MET:O	2.05	0.56
2:D:190:TRP:CZ3	2:D:230:CYS:HB3	2.40	0.56
2:D:316:VAL:O	2:D:317:ASN:HB2	2.06	0.56
2:D:264:ASN:O	2:D:265:LYS:HG3	2.05	0.56
2:D:292:HIS:ND1	2:D:338:GLU:HB3	2.20	0.56
2:D:277:CYS:HB2	2:D:289:TRP:CH2	2.41	0.56
2:D:317:ASN:OD1	2:D:318:THR:N	2.38	0.55
2:D:187:THR:CG2	2:D:188:LEU:N	2.68	0.55
2:D:159:GLU:C	2:D:161:MET:H	2.10	0.55
1:A:84:THR:HA	1:A:117:HIS:NE2	2.21	0.55
1:A:95:ASN:HD22	1:A:95:ASN:N	2.03	0.55
1:B:119:GLU:C	1:B:121:ASN:N	2.59	0.55
1:B:39:ARG:O	1:B:46:VAL:HG13	2.07	0.55
2:C:312:LYS:HG2	2:C:323:MET:HE1	1.88	0.55
2:C:174:VAL:HG23	2:C:220:VAL:HG11	1.88	0.55
2:C:301:GLY:HA2	2:C:307:TYR:CE1	2.42	0.54
1:A:119:GLU:C	1:A:121:ASN:N	2.61	0.54
1:B:133:LYS:HZ3	1:B:142:GLN:NE2	2.05	0.54
1:A:128:LYS:HG3	3:A:303:IDS:O1S	2.07	0.54
2:D:264:ASN:H	2:D:264:ASN:HD22	1.56	0.53
2:D:277:CYS:HG	2:D:341:CYS:CB	2.22	0.53
2:D:333:PHE:HA	2:D:358:VAL:CG1	2.35	0.53
2:C:295:VAL:O	2:C:296:ASN:HB2	2.08	0.53
1:A:133:LYS:O	1:A:134:ARG:O	2.25	0.53
1:B:135:GLY:N	1:B:136:PRO:HD2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LYS:HB3	1:B:122:TRP:NE1	2.23	0.53
1:B:133:LYS:O	1:B:134:ARG:O	2.27	0.53
2:D:314:ALA:CB	2:D:323:MET:HG3	2.39	0.53
2:C:265:LYS:NZ	2:C:274:GLU:O	2.40	0.53
1:B:133:LYS:HG2	1:B:133:LYS:O	2.08	0.53
2:C:264:ASN:O	2:C:265:LYS:HG3	2.10	0.52
2:C:317:ASN:OD1	2:C:318:THR:N	2.37	0.52
1:A:59:LEU:HD22	1:A:71:ILE:CG2	2.38	0.52
2:C:277:CYS:HG	2:C:341:CYS:CB	2.21	0.52
2:C:333:PHE:HA	2:C:358:VAL:CG1	2.36	0.52
2:D:159:GLU:O	2:D:161:MET:N	2.42	0.52
2:D:147:ASN:N	2:D:147:ASN:HD22	2.06	0.52
2:C:159:GLU:O	2:C:161:MET:N	2.42	0.52
1:B:133:LYS:HE2	1:B:142:GLN:HE22	1.75	0.52
2:C:314:ALA:CB	2:C:323:MET:HG3	2.38	0.52
2:D:293:ILE:CG2	2:D:294:GLU:N	2.71	0.52
2:D:294:GLU:HG2	2:D:299:LYS:CG	2.40	0.52
2:C:273:VAL:CG1	2:C:328:LEU:HD12	2.40	0.52
1:B:97:GLU:HG2	1:B:116:LYS:CD	2.41	0.51
2:D:273:VAL:CG1	2:D:328:LEU:HD12	2.40	0.51
2:C:172:LYS:O	2:C:220:VAL:HG13	2.10	0.51
2:D:245:LEU:HD22	2:D:246:ASP:N	2.26	0.51
2:C:358:VAL:O	2:C:359:LEU:HG	2.10	0.51
2:D:187:THR:HG22	2:D:188:LEU:H	1.75	0.51
2:D:273:VAL:HG13	2:D:328:LEU:HD12	1.92	0.51
2:C:273:VAL:HG12	2:C:331:VAL:HG21	1.91	0.51
2:C:257:LEU:HD21	2:C:279:VAL:HG22	1.93	0.51
1:B:89:TYR:CE1	1:B:91:SER:HB2	2.46	0.51
2:C:170:ALA:O	2:C:171:ALA:HB3	2.10	0.51
1:A:135:GLY:O	1:A:138:THR:HB	2.11	0.51
2:C:186:PRO:HG2	2:C:213:TRP:HH2	1.75	0.51
2:C:158:PRO:O	2:C:161:MET:HB2	2.11	0.51
2:C:186:PRO:HG2	2:C:213:TRP:CH2	2.46	0.50
1:A:128:LYS:HZ1	3:A:302:SGN:H3	1.76	0.50
1:A:122:TRP:HB3	1:A:135:GLY:HA3	1.92	0.50
2:C:290:LEU:HD22	2:C:310:ILE:CD1	2.40	0.50
2:D:267:VAL:HG22	2:D:356:LEU:HD11	1.93	0.50
1:B:70:TYR:CE2	2:D:316:VAL:HB	2.46	0.50
1:B:89:TYR:HE1	1:B:91:SER:HB2	1.76	0.50
2:C:303:ASP:OD2	2:C:305:LEU:HD12	2.12	0.50
1:B:148:LEU:O	1:B:150:LEU:HD23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LYS:O	1:A:134:ARG:C	2.50	0.50
1:B:135:GLY:O	1:B:138:THR:HB	2.11	0.49
2:D:312:LYS:HG2	2:D:323:MET:HE1	1.92	0.49
1:A:123:PHE:CB	1:A:138:THR:HG21	2.26	0.49
2:D:187:THR:CG2	2:D:188:LEU:H	2.24	0.49
2:C:252:PRO:C	2:C:347:ILE:HD13	2.33	0.49
2:C:302:PRO:O	2:C:303:ASP:HB3	2.12	0.49
2:C:277:CYS:HB2	2:C:289:TRP:CH2	2.48	0.49
1:B:36:HIS:NE2	1:B:130:GLY:HA3	2.28	0.49
2:C:187:THR:CG2	2:C:188:LEU:N	2.77	0.48
2:C:292:HIS:HD2	2:C:338:GLU:CB	2.26	0.48
1:B:24:LYS:HG2	2:D:320:ASP:HB3	1.95	0.48
2:C:290:LEU:HD22	2:C:310:ILE:HD13	1.95	0.48
2:C:342:LEU:HD21	2:C:349:LEU:HB2	1.96	0.48
1:B:133:LYS:O	1:B:134:ARG:C	2.51	0.48
1:B:40:ILE:HA	1:B:46:VAL:HG22	1.95	0.48
2:C:293:ILE:CG2	2:C:294:GLU:N	2.75	0.48
1:B:52:ARG:O	1:B:52:ARG:HG2	2.14	0.48
1:B:30:TYR:HB3	1:B:150:LEU:HD23	1.96	0.48
1:B:54:ASP:OD1	1:B:55:GLN:N	2.47	0.48
2:D:282:ASP:HB3	2:D:283:PRO:HD2	1.96	0.48
1:A:39:ARG:O	1:A:46:VAL:HG13	2.13	0.48
1:A:21:GLY:N	1:A:27:LYS:HE3	2.29	0.47
2:C:270:GLY:HA2	2:C:330:ASN:ND2	2.29	0.47
2:D:344:GLY:HA3	2:D:349:LEU:CD2	2.44	0.47
1:A:127:LYS:HB2	1:A:129:ASN:OD1	2.14	0.47
2:C:220:VAL:HG23	2:C:247:VAL:HG13	1.95	0.47
2:D:170:ALA:O	2:D:171:ALA:HB3	2.14	0.47
1:B:84:THR:HA	1:B:117:HIS:NE2	2.29	0.47
1:A:36:HIS:HE1	1:A:128:LYS:O	1.97	0.47
1:A:95:ASN:O	1:A:98:CYS:HB2	2.14	0.47
1:A:123:PHE:HB2	1:A:138:THR:CG2	2.27	0.47
1:A:33:ASN:HD22	1:A:128:LYS:HA	1.78	0.47
1:A:139:HIS:HB3	1:A:142:GLN:HG3	1.97	0.47
2:C:190:TRP:CZ3	2:C:230:CYS:HB3	2.49	0.47
2:C:151:VAL:HB	2:C:183:THR:H	1.79	0.47
1:A:52:ARG:HG2	1:A:52:ARG:O	2.14	0.47
2:C:275:PHE:O	2:C:325:VAL:HA	2.15	0.47
2:D:275:PHE:O	2:D:325:VAL:HA	2.15	0.47
1:B:127:LYS:HD2	1:B:131:SER:HG	1.79	0.47
2:D:265:LYS:O	2:D:356:LEU:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ARG:HE	2:D:163:LYS:HA	1.80	0.47
1:B:50:ARG:NE	2:D:163:LYS:HA	2.30	0.47
1:A:103:ARG:HG3	4:A:4015:HOH:O	2.15	0.46
2:D:264:ASN:ND2	2:D:264:ASN:H	2.14	0.46
2:D:151:VAL:HB	2:D:183:THR:H	1.80	0.46
1:A:139:HIS:H	1:A:142:GLN:HG3	1.80	0.46
2:D:271:SER:O	2:D:331:VAL:HG23	2.16	0.46
2:C:153:PRO:HA	2:C:181:SER:O	2.15	0.46
1:A:22:ASN:O	1:A:24:LYS:N	2.49	0.46
2:D:312:LYS:HE2	2:D:323:MET:HE2	1.98	0.46
2:C:155:TRP:HB3	2:C:161:MET:HE3	1.98	0.46
1:B:102:GLU:HG3	1:B:112:TYR:CE1	2.50	0.46
1:A:139:HIS:O	1:A:142:GLN:HB2	2.16	0.45
1:B:84:THR:O	1:B:84:THR:HG22	2.16	0.45
1:A:128:LYS:NZ	3:A:303:IDS:O61	2.48	0.45
2:C:187:THR:CG2	2:C:188:LEU:H	2.29	0.45
1:B:76:THR:CB	1:B:78:GLN:HG3	2.47	0.45
1:B:113:ILE:HG23	1:B:122:TRP:O	2.16	0.45
2:D:153:PRO:HA	2:D:181:SER:O	2.16	0.45
1:B:97:GLU:HG2	1:B:116:LYS:HD2	1.98	0.45
1:A:28:LEU:HD11	1:A:152:VAL:HA	1.99	0.45
1:B:119:GLU:OE1	1:B:119:GLU:HA	2.16	0.45
1:B:120:LYS:O	1:B:122:TRP:HD1	2.00	0.45
2:D:290:LEU:CD2	2:D:310:ILE:HD13	2.46	0.45
2:D:168:VAL:HG22	2:D:169:PRO:HD2	1.98	0.45
2:C:245:LEU:HD22	2:C:246:ASP:N	2.32	0.45
2:C:295:VAL:O	2:C:295:VAL:HG13	2.16	0.45
2:D:206:TYR:HE1	2:D:208:VAL:CG2	2.29	0.45
2:C:155:TRP:CE2	2:C:239:ILE:HD12	2.52	0.45
1:B:101:LEU:HD21	1:B:115:LYS:HG2	1.98	0.45
1:A:64:GLU:O	1:A:64:GLU:OE1	2.35	0.45
2:D:315:GLY:O	2:D:318:THR:HG22	2.16	0.45
2:D:220:VAL:HG23	2:D:247:VAL:HG13	1.98	0.45
2:C:176:PHE:HB2	2:C:215:ILE:HG22	1.99	0.45
3:A:303:IDS:C1	3:A:304:SGN:H62	2.47	0.45
2:C:312:LYS:HE2	2:C:323:MET:CE	2.47	0.44
1:B:21:GLY:N	1:B:27:LYS:HE3	2.32	0.44
1:B:83:ASP:C	1:B:83:ASP:OD2	2.55	0.44
2:C:251:SER:HB2	2:C:282:ASP:HB2	1.98	0.44
1:A:81:ALA:O	1:A:88:LEU:HA	2.17	0.44
2:D:344:GLY:CA	2:D:349:LEU:HD23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ALA:O	1:B:88:LEU:HA	2.18	0.44
1:A:138:THR:HG23	1:A:145:ILE:CG2	2.48	0.44
2:D:318:THR:O	2:D:319:THR:OG1	2.33	0.44
1:A:39:ARG:O	1:A:46:VAL:HA	2.18	0.44
1:B:39:ARG:O	1:B:46:VAL:HA	2.17	0.44
1:A:39:ARG:NH2	1:A:47:ASP:OD2	2.50	0.44
1:B:37:PHE:CE2	1:B:52:ARG:HB2	2.53	0.44
1:A:133:LYS:HG2	1:A:133:LYS:O	2.18	0.44
2:C:188:LEU:HD23	2:C:232:VAL:HG22	2.00	0.44
1:A:76:THR:CB	1:A:78:GLN:HG3	2.47	0.44
2:D:302:PRO:O	2:D:303:ASP:HB3	2.18	0.44
2:D:295:VAL:HG13	2:D:295:VAL:O	2.17	0.44
2:D:174:VAL:HG23	2:D:220:VAL:HG11	2.00	0.44
2:C:318:THR:HG21	2:C:323:MET:CE	2.48	0.44
1:A:84:THR:O	1:A:122:TRP:HH2	2.00	0.43
1:A:120:LYS:O	1:A:122:TRP:HD1	2.01	0.43
1:B:42:PRO:HD3	1:B:56:HIS:HD2	1.76	0.43
2:C:188:LEU:HD11	2:C:190:TRP:HE1	1.80	0.43
2:D:295:VAL:O	2:D:296:ASN:HB2	2.18	0.43
1:B:86:GLY:O	1:B:134:ARG:HA	2.18	0.43
2:D:190:TRP:CH2	2:D:230:CYS:HB3	2.53	0.43
1:B:39:ARG:NE	1:B:41:LEU:HD21	2.33	0.43
1:B:22:ASN:O	1:B:24:LYS:N	2.51	0.43
2:D:288:GLN:HB3	2:D:288:GLN:HE21	1.48	0.43
2:C:289:TRP:CD2	2:C:326:LEU:HB2	2.53	0.43
2:D:270:GLY:HA2	2:D:330:ASN:ND2	2.32	0.43
1:A:61:LEU:N	1:A:61:LEU:HD12	2.34	0.43
1:A:24:LYS:HE2	4:A:4002:HOH:O	2.18	0.43
1:A:86:GLY:O	1:A:134:ARG:HA	2.19	0.43
1:A:61:LEU:HB3	2:C:284:GLN:HG3	2.01	0.43
2:D:186:PRO:HG2	2:D:213:TRP:CH2	2.54	0.43
1:B:119:GLU:O	1:B:121:ASN:N	2.52	0.42
1:A:37:PHE:CE2	1:A:52:ARG:HB2	2.54	0.42
2:D:172:LYS:O	2:D:220:VAL:HG13	2.19	0.42
1:B:110:ASN:HB3	1:B:112:TYR:CE2	2.54	0.42
1:B:113:ILE:HD13	1:B:121:ASN:ND2	2.33	0.42
2:D:318:THR:CG2	2:D:319:THR:N	2.76	0.42
2:C:286:HIS:C	2:C:287:ILE:HD12	2.40	0.42
2:D:358:VAL:O	2:D:359:LEU:HD23	2.20	0.42
2:C:252:PRO:HA	2:C:347:ILE:CD1	2.50	0.42
1:B:51:ASP:C	1:B:53:SER:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:PHE:HD1	1:B:138:THR:HG22	1.85	0.42
1:B:95:ASN:H	1:B:98:CYS:HB2	1.85	0.42
2:C:186:PRO:HB2	2:C:232:VAL:HG13	2.02	0.42
1:B:41:LEU:O	1:B:44:GLY:N	2.49	0.42
1:A:95:ASN:H	1:A:98:CYS:HB2	1.84	0.42
2:C:231:ILE:HG22	2:C:233:GLU:HG2	2.00	0.42
2:C:316:VAL:O	2:C:317:ASN:HB2	2.19	0.42
2:C:282:ASP:CB	2:C:283:PRO:CD	2.96	0.42
1:B:24:LYS:O	1:B:60:GLN:NE2	2.52	0.42
2:C:286:HIS:CD2	2:C:314:ALA:HB3	2.55	0.41
2:D:333:PHE:CA	2:D:358:VAL:HG11	2.41	0.41
2:C:182:GLY:O	2:C:185:GLN:HA	2.19	0.41
2:C:316:VAL:O	2:C:317:ASN:HB3	2.18	0.41
1:A:26:PRO:C	1:A:27:LYS:HD2	2.39	0.41
2:C:183:THR:CA	2:C:184:PRO:C	2.88	0.41
1:A:119:GLU:O	1:A:121:ASN:N	2.53	0.41
2:C:159:GLU:C	2:C:161:MET:N	2.74	0.41
2:C:206:TYR:HE1	2:C:208:VAL:CG2	2.34	0.41
2:D:305:LEU:HA	2:D:306:PRO:HD2	1.89	0.41
2:D:159:GLU:C	2:D:161:MET:N	2.74	0.41
2:D:191:LEU:HD23	2:D:196:GLU:HA	2.01	0.41
2:C:147:ASN:ND2	2:C:147:ASN:N	2.68	0.41
1:A:54:ASP:OD1	1:A:56:HIS:N	2.42	0.41
2:C:188:LEU:HD21	2:C:230:CYS:HB2	2.03	0.41
1:A:41:LEU:O	1:A:44:GLY:N	2.49	0.41
2:D:318:THR:O	2:D:319:THR:CB	2.69	0.41
1:A:123:PHE:CD1	1:A:138:THR:HG22	2.50	0.40
1:B:84:THR:O	1:B:122:TRP:HH2	2.04	0.40
1:B:72:LYS:HD2	1:B:79:TYR:CZ	2.56	0.40
2:D:282:ASP:CB	2:D:283:PRO:CD	2.99	0.40
2:C:254:ARG:HG2	2:C:254:ARG:H	1.60	0.40
2:C:334:GLU:C	2:C:336:ALA:H	2.25	0.40
1:A:143:LYS:HD3	3:A:302:SGN:HO3	1.82	0.40
1:A:41:LEU:HD12	1:A:45:THR:HB	2.04	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	131/136 (96%)	113 (86%)	15 (12%)	3 (2%)	8	14
1	B	131/136 (96%)	113 (86%)	14 (11%)	4 (3%)	5	8
2	C	211/226 (93%)	184 (87%)	21 (10%)	6 (3%)	6	10
2	D	211/226 (93%)	185 (88%)	20 (10%)	6 (3%)	6	10
All	All	684/724 (94%)	595 (87%)	70 (10%)	19 (3%)	6	10

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	134	ARG
1	B	33	ASN
1	B	134	ARG
2	C	160	LYS
2	C	303	ASP
2	C	317	ASN
2	C	318	THR
2	C	319	THR
2	D	160	LYS
2	D	303	ASP
2	D	317	ASN
2	D	318	THR
2	D	319	THR
1	A	23	TYR
1	B	23	TYR
2	C	296	ASN
2	D	296	ASN
1	B	52	ARG

### 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	113/119 (95%)	109 (96%)	4 (4%)	43	71
1	B	113/119 (95%)	108 (96%)	5 (4%)	35	63
2	C	170/198 (86%)	160 (94%)	10 (6%)	24	47
2	D	171/198 (86%)	159 (93%)	12 (7%)	19	37
All	All	567/634 (89%)	536 (94%)	31 (6%)	27	51

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	GLU
1	A	95	ASN
1	A	108	HIS
1	A	121	ASN
1	B	33	ASN
1	B	106	GLU
1	B	108	HIS
1	B	121	ASN
1	B	152	VAL
2	C	147	ASN
2	C	156	THR
2	C	168	VAL
2	C	180	SER
2	C	245	LEU
2	C	320	ASP
2	C	342	LEU
2	C	349	LEU
2	C	351	HIS
2	C	355	TRP
2	D	168	VAL
2	D	245	LEU
2	D	269	LEU
2	D	288	GLN
2	D	294	GLU

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Mol	Chain	Res	Type
2	D	304	ASN
2	D	313	THR
2	D	333	PHE
2	D	334	GLU
2	D	342	LEU
2	D	351	HIS
2	D	355	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	60	GLN
1	A	78	GLN
1	A	92	GLN
1	A	95	ASN
1	A	121	ASN
1	A	142	GLN
1	B	60	GLN
1	B	78	GLN
1	B	92	GLN
1	B	121	ASN
1	B	142	GLN
2	C	185	GLN
2	C	284	GLN
2	C	288	GLN
2	C	296	ASN
2	C	330	ASN
2	D	166	HIS
2	D	185	GLN
2	D	201	HIS
2	D	264	ASN
2	D	284	GLN
2	D	288	GLN
2	D	296	ASN
2	D	330	ASN
2	D	351	HIS

### 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 ⓘ

6 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	UAP	A	301	3	12,15,16	2.77	6 (50%)	11,22,24	1.34	1 (9%)
3	SGN	A	302	3	17,19,20	1.51	4 (23%)	19,29,31	1.76	5 (26%)
3	IDS	A	303	3	13,16,17	2.41	4 (30%)	17,24,26	1.49	4 (23%)
3	SGN	A	304	3	17,19,20	1.98	3 (17%)	19,29,31	2.35	5 (26%)
3	IDS	A	305	3	13,16,17	2.23	5 (38%)	17,24,26	0.95	0
3	SGN	A	306	3	17,19,20	2.47	4 (23%)	19,29,31	2.03	6 (31%)

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	UAP	A	301	3	1/1/5/7	0/5/22/25	0/1/1/1
3	SGN	A	302	3	-	0/11/28/31	0/1/1/1
3	IDS	A	303	3	-	0/5/26/29	0/1/1/1
3	SGN	A	304	3	-	0/11/28/31	0/1/1/1
3	IDS	A	305	3	-	0/5/26/29	0/1/1/1
3	SGN	A	306	3	-	0/11/28/31	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	306	SGN	C2-N	-3.35	1.41	1.47
3	A	304	SGN	C2-N	-2.86	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	IDS	C4-C3	2.01	1.57	1.52
3	A	302	SGN	C4-C3	2.07	1.57	1.52
3	A	302	SGN	O2S-S1	2.07	1.44	1.42
3	A	304	SGN	O5-C1	2.22	1.47	1.43
3	A	302	SGN	O5-C5	2.35	1.48	1.43
3	A	305	IDS	O5-C1	2.67	1.48	1.43
3	A	305	IDS	C3-C2	2.88	1.59	1.53
3	A	301	UAP	O2-C2	2.89	1.52	1.47
3	A	301	UAP	C4-C5	2.89	1.36	1.32
3	A	306	SGN	O4-C4	3.05	1.50	1.43
3	A	301	UAP	O3S-S	3.10	1.56	1.45
3	A	305	IDS	C4-C3	3.31	1.61	1.52
3	A	302	SGN	O5-C1	3.36	1.49	1.43
3	A	305	IDS	C1-C2	3.40	1.57	1.51
3	A	303	IDS	O5-C1	3.53	1.49	1.43
3	A	301	UAP	C2-C3	4.06	1.59	1.52
3	A	301	UAP	C3-C4	4.27	1.55	1.50
3	A	305	IDS	O5-C5	4.29	1.47	1.43
3	A	303	IDS	C3-C2	4.83	1.63	1.53
3	A	303	IDS	O5-C5	5.00	1.48	1.43
3	A	301	UAP	C1-C2	5.00	1.60	1.51
3	A	306	SGN	O1S-S1	5.34	1.47	1.42
3	A	304	SGN	O2S-S1	6.35	1.48	1.42
3	A	306	SGN	O2S-S1	6.77	1.49	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	304	SGN	C2-N-S1	-6.51	108.17	121.35
3	A	304	SGN	C4-C3-C2	-5.37	102.88	111.23
3	A	306	SGN	C2-N-S1	-4.55	112.14	121.35
3	A	306	SGN	O2S-S1-N	-4.24	102.84	108.50
3	A	302	SGN	O1S-S1-N	-3.64	103.63	108.50
3	A	302	SGN	C4-C3-C2	-3.12	106.38	111.23
3	A	306	SGN	O6-C6-C5	-2.90	102.31	107.90
3	A	306	SGN	C4-C3-C2	-2.74	106.98	111.23
3	A	303	IDS	O3-C3-C4	-2.46	104.80	110.34
3	A	304	SGN	O2S-S1-N	-2.39	105.30	108.50
3	A	306	SGN	O1S-S1-N	-2.28	105.45	108.50
3	A	303	IDS	C6-C5-C4	-2.00	107.34	113.00
3	A	303	IDS	O4-C4-C3	2.08	115.03	110.34
3	A	304	SGN	O5S-S2-O4S	2.08	121.54	112.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	IDS	O2S-S-O1S	2.23	122.16	112.46
3	A	306	SGN	O5S-S2-O4S	2.29	122.41	112.46
3	A	302	SGN	O5S-S2-O4S	2.33	122.59	112.46
3	A	302	SGN	C1-O5-C5	2.70	115.67	112.25
3	A	301	UAP	O1S-S-O2S	3.04	120.00	108.56
3	A	302	SGN	O6-C6-C5	3.20	114.06	107.90
3	A	304	SGN	O6-C6-C5	3.37	114.38	107.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	301	UAP	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	SGN	3	0
3	A	303	IDS	3	0
3	A	304	SGN	1	0
3	A	305	IDS	4	0
3	A	306	SGN	3	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 ⓘ

### 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<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	133/136 (97%)	-0.07	0 100 100	21, 44, 60, 63	0
1	B	133/136 (97%)	0.05	2 (1%) 76 71	23, 44, 59, 65	0
2	C	213/226 (94%)	0.06	8 (3%) 44 36	19, 38, 74, 79	0
2	D	213/226 (94%)	0.01	8 (3%) 44 36	20, 37, 74, 79	0
All	All	692/724 (95%)	0.02	18 (2%) 59 53	19, 40, 69, 79	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	358	VAL	4.3
2	C	318	THR	3.4
2	D	267	VAL	3.2
2	D	302	PRO	3.0
2	C	302	PRO	2.9
2	C	355	TRP	2.8
1	B	46	VAL	2.7
2	D	301	GLY	2.5
2	C	359	LEU	2.5
2	C	320	ASP	2.3
2	C	327	HIS	2.3
2	D	357	THR	2.3
2	D	318	THR	2.2
2	D	359	LEU	2.2
1	B	74	THR	2.2
2	D	303	ASP	2.2
2	D	276	MET	2.2
2	C	357	THR	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	IDS	A	303	16/17	0.89	0.18	0.09	74,79,79,80	0
3	IDS	A	305	16/17	0.82	0.21	-0.28	82,83,84,85	0
3	SGN	A	304	19/20	0.89	0.18	-0.38	78,79,81,81	0
3	SGN	A	302	19/20	0.89	0.17	-0.48	78,81,85,85	0
3	SGN	A	306	19/20	0.76	0.22	-	87,90,94,94	0
3	UAP	A	301	15/16	0.69	0.20	-	84,86,87,87	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.