



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:27 PM GMT

PDB ID : 1FQ9  
Title : CRYSTAL STRUCTURE OF A TERNARY FGF2-FGFR1-HEPARIN COMPLEX  
Authors : Schlessinger, J.; Plotnikov, A.N.; Ibrahimi, O.A.; Eliseenkova, A.V.; Yeh, B.K.; Yayon, A.; Linhardt, R.J.; Mohammadi, M.  
Deposited on : 2000-09-04  
Resolution : 3.00 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

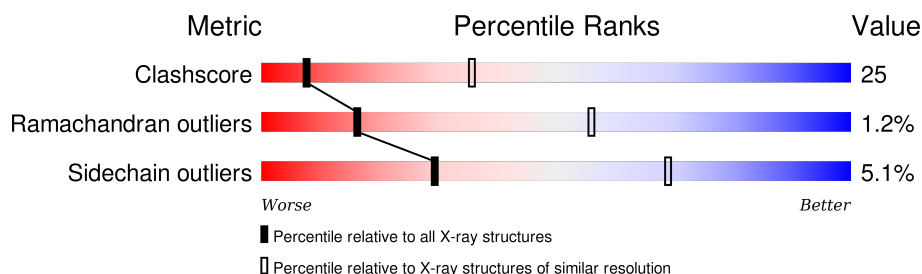
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	132	
1	B	132	
2	C	225	
2	D	225	

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	SGN	A	306	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5496 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 FIBROBLAST GROWTH FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1040	660	190	186	4			
1	B	129	Total	C	N	O	S	0	0	0
			1040	660	190	186	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	SER	CYS	ENGINEERED	UNP P09038
A	87	SER	CYS	ENGINEERED	UNP P09038
B	69	SER	CYS	ENGINEERED	UNP P09038
B	87	SER	CYS	ENGINEERED	UNP P09038

- Molecule 2 is a protein called FIBROBLAST GROWTH FACTOR RECEPTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	211	Total	C	N	O	S	0	0	0
			1638	1047	280	302	9			
2	D	196	Total	C	N	O	S	0	0	0
			1533	980	263	281	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	185	GLN	ASN	ENGINEERED	UNP P11362
D	185	GLN	ASN	ENGINEERED	UNP P11362

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	8	Total	C	N	O	S	0	0
			140	48	4	76	12		

- Molecule 4 is a polymer of unknown type called SUGAR (HEPARIN).

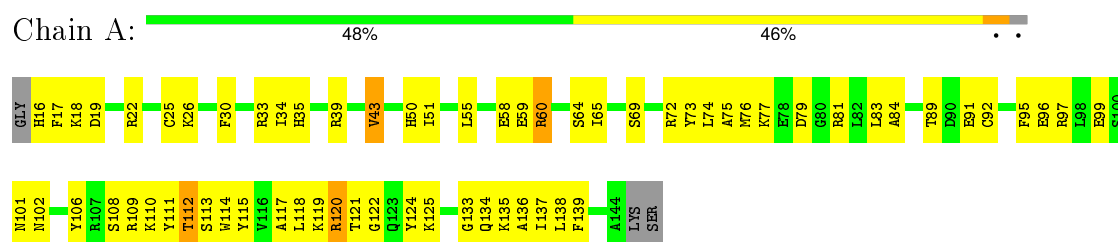
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	6	Total	C	N	O	S	0	0
			105	36	3	57	9		

### 3 Residue-property plots

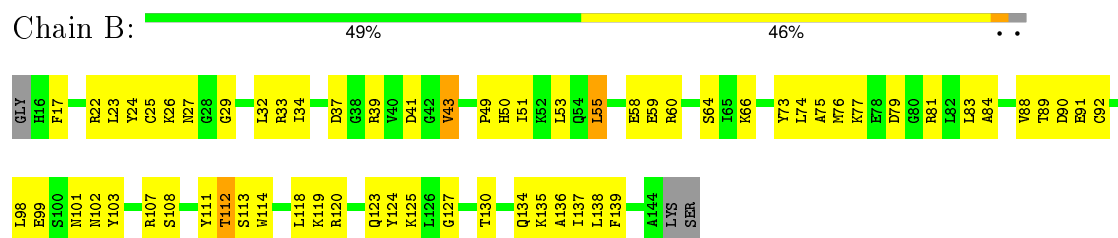
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

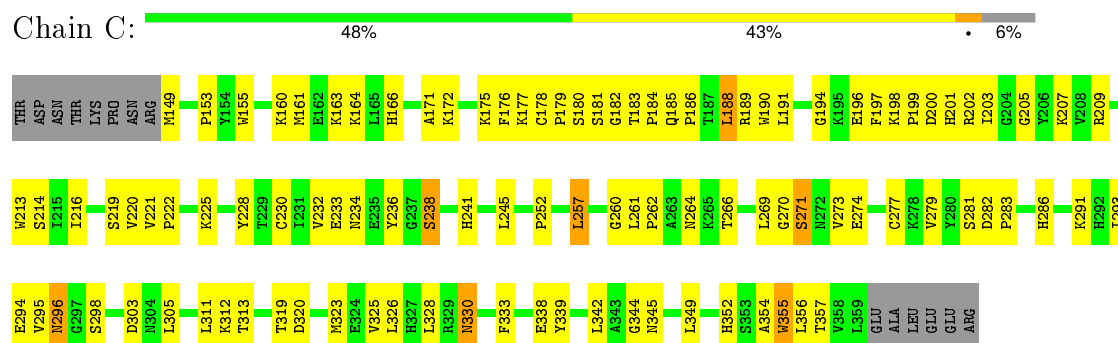
#### • Molecule 1: FIBROBLAST GROWTH FACTOR 2



#### • Molecule 1: FIBROBLAST GROWTH FACTOR 2



#### • Molecule 2: FIBROBLAST GROWTH FACTOR RECEPTOR 1



#### • Molecule 2: FIBROBLAST GROWTH FACTOR RECEPTOR 1



THR	S223	GLY
ASP	D224	PRO
ASN	K225	ASN
THR		LEU
LYS	Y228	PRO
PRO	T229	TYR
ASN	C230	Y308
ARG	I231	
M149	V232	L311
	E233	
P153	N234	A314
Y154	P235	G315
H155	Y236	Y316
T156	G237	N317
S157	S238	T318
P158		T319
E159	L245	T320
	D246	K321
H166		E322
	S251	K323
A170	P252	E324
A171	H253	Y325
K172		L326
T173	L257	
V174		H330
K175	P262	Y331
F176	A263	
K177	N264	D335
G178	K265	
P179		Y339
S180	L269	
S181	G270	L342
	S271	A343
P186	E274	G344
T187		L349
L188	C277	
R189	R278	H352
H190	V279	S353
L191	Y280	A354
	S281	K355
E196	D282	L356
F197	P283	
		L359
D200	H286	GLU
H201	I287	ALA
R202	Q288	LEU
I203		
	W289	GLU
Y206	L290	GLU
K207	K291	ARG
Y208	H292	
R209		
Y210	ILE	
A211	GLU	
	VAL	
S214	ASN	
T215	GLY	
I216	SER	
	LYS	
S219	ILE	

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.89Å 98.89Å 196.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-3.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.229 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5496	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP



## 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: UAP, IDU, 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	0.44	0/1063	0.70	1/1425 (0.1%)
1	B	0.45	0/1063	0.68	1/1425 (0.1%)
2	C	0.44	0/1685	0.68	0/2299
2	D	0.42	0/1576	0.69	0/2146
All	All	0.44	0/5387	0.69	2/7295 (0.0%)

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
3	A	1	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	SER	N-CA-C	-5.30	96.68	111.00
1	B	64	SER	N-CA-C	-5.16	97.08	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	306	SGN	C1

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	1040	0	1040	59	0
1	B	1040	0	1040	61	0
2	C	1638	0	1603	92	0
2	D	1533	0	1506	82	0
3	A	140	0	53	4	0
4	B	105	0	40	1	0
All	All	5496	0	5282	273	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 25.

All (273) 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:D:175:LYS:HG3	2:D:216:ILE:HG12	1.42	0.99
2:D:282:ASP:HB3	2:D:283:PRO:HD3	1.44	0.98
2:C:282:ASP:HB3	2:C:283:PRO:HD3	1.45	0.96
2:D:286:HIS:HD2	2:D:314:ALA:HB3	1.37	0.90
2:C:207:LYS:HE2	2:C:209:ARG:HE	1.35	0.89
2:C:207:LYS:CE	2:C:209:ARG:HE	1.85	0.88
1:B:88:VAL:HG21	2:D:316:VAL:HG11	1.55	0.88
2:D:286:HIS:CD2	2:D:314:ALA:HB3	2.08	0.88
1:B:76:MET:HE3	1:B:114:TRP:HE3	1.38	0.85
1:A:77:LYS:HD2	1:A:83:LEU:HD21	1.60	0.83
2:C:273:VAL:HG13	2:C:328:LEU:HB2	1.60	0.83
1:B:27:ASN:HA	1:B:135:LYS:HE2	1.60	0.82
1:A:59:GLU:HA	2:C:286:HIS:CD2	2.15	0.81
2:D:344:GLY:HA3	2:D:349:LEU:HD12	1.61	0.81
2:C:344:GLY:HA3	2:C:349:LEU:HD13	1.65	0.78
1:B:76:MET:HE3	1:B:114:TRP:CE3	2.18	0.78
1:A:133:GLY:HA3	2:D:200:ASP:HA	1.66	0.77
2:C:149:MET:O	2:C:149:MET:HG3	1.83	0.77
2:C:164:LYS:HE3	2:C:241:HIS:CE1	2.20	0.77
2:D:171:ALA:O	2:D:219:SER:HA	1.86	0.76
2:D:262:PRO:HG2	2:D:354:ALA:HB2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LYS:HD3	1:A:138:LEU:HD12	1.67	0.74
1:B:79:ASP:CG	1:B:81:ARG:HH11	1.91	0.73
2:D:269:LEU:HD23	2:D:270:GLY:N	2.04	0.72
1:B:59:GLU:HA	2:D:286:HIS:ND1	2.04	0.72
1:A:120:ARG:HD3	3:A:305:IDS:O3S	1.92	0.70
2:C:262:PRO:HG2	2:C:354:ALA:HB2	1.73	0.69
2:C:171:ALA:O	2:C:219:SER:HA	1.93	0.69
1:A:25:CYS:HB2	1:A:139:PHE:CE2	2.28	0.69
1:B:119:LYS:HA	4:B:305:IDS:O3S	1.92	0.69
1:B:76:MET:HE1	1:B:114:TRP:HB2	1.75	0.69
2:C:291:LYS:HB2	2:C:311:LEU:HD11	1.74	0.69
2:D:188:LEU:HD11	2:D:190:TRP:HE1	1.58	0.69
2:C:185:GLN:HE21	2:C:185:GLN:HA	1.59	0.68
2:C:342:LEU:HD11	2:C:349:LEU:HD12	1.75	0.68
1:A:118:LEU:HD23	1:A:124:TYR:HA	1.75	0.67
1:A:97:ARG:HD3	1:A:99:GLU:OE1	1.94	0.67
2:D:209:ARG:CD	2:D:211:ALA:HB3	2.26	0.66
2:D:209:ARG:HE	2:D:211:ALA:H	1.42	0.66
2:D:282:ASP:HB3	2:D:283:PRO:CD	2.23	0.66
1:B:33:ARG:NH1	1:B:43:VAL:HG11	2.11	0.66
2:C:260:GLY:O	2:C:261:LEU:HD23	1.95	0.65
1:A:76:MET:HE3	1:A:114:TRP:HE3	1.61	0.65
2:C:282:ASP:HB3	2:C:283:PRO:CD	2.25	0.65
1:B:55:LEU:N	1:B:55:LEU:HD23	2.11	0.64
2:D:257:LEU:HB2	2:D:352:HIS:CE1	2.32	0.64
1:A:16:HIS:HB3	1:A:19:ASP:OD2	1.96	0.64
1:B:76:MET:CE	1:B:114:TRP:HB2	2.27	0.64
1:B:75:ALA:HB2	1:B:92:CYS:SG	2.38	0.64
1:B:58:GLU:OE1	2:D:316:VAL:HG23	1.98	0.63
2:D:342:LEU:HD11	2:D:349:LEU:HG	1.79	0.63
1:A:135:LYS:HZ1	2:D:207:LYS:HD3	1.63	0.63
3:A:301:UAP:H4	2:D:216:ILE:HD13	1.81	0.63
1:B:119:LYS:HE2	1:B:123:GLN:HB2	1.79	0.63
1:B:79:ASP:OD1	1:B:81:ARG:HD3	1.98	0.63
2:C:296:ASN:C	2:C:298:SER:H	2.01	0.62
1:B:119:LYS:CE	1:B:123:GLN:HB2	2.29	0.62
1:A:135:LYS:NZ	2:D:207:LYS:HD3	2.15	0.62
1:A:16:HIS:CE1	1:A:18:LYS:H	2.17	0.62
2:C:185:GLN:NE2	2:C:185:GLN:HA	2.15	0.61
2:C:222:PRO:O	2:C:225:LYS:HG3	2.00	0.61
2:D:209:ARG:HD3	2:D:211:ALA:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PHE:CE1	1:A:109:ARG:HA	2.35	0.61
1:A:60:ARG:NH1	2:C:345:ASN:O	2.33	0.61
2:D:190:TRP:CZ3	2:D:230:CYS:HB3	2.36	0.61
1:A:73:TYR:O	1:A:84:ALA:HA	2.01	0.61
2:C:166:HIS:CD2	2:C:176:PHE:HE1	2.19	0.60
2:D:292:HIS:HD2	2:D:308:VAL:HG12	1.67	0.60
1:B:79:ASP:OD2	1:B:81:ARG:HG2	2.02	0.60
1:B:73:TYR:O	1:B:84:ALA:HA	2.02	0.59
1:B:107:ARG:HD2	1:B:112:THR:O	2.03	0.59
1:A:55:LEU:HD23	1:A:55:LEU:N	2.16	0.59
1:B:66:LYS:HD2	1:B:73:TYR:CZ	2.38	0.59
1:A:91:GLU:HG2	1:A:110:LYS:HD3	1.85	0.59
2:D:291:LYS:HG2	2:D:339:TYR:CE2	2.38	0.59
1:A:96:GLU:HG3	1:A:106:TYR:CE1	2.38	0.58
2:C:160:LYS:HD2	2:C:179:PRO:HG2	1.85	0.58
3:A:301:UAP:H4	2:D:216:ILE:CD1	2.34	0.58
2:C:185:GLN:HE21	2:C:185:GLN:CA	2.16	0.58
1:B:22:ARG:HD3	1:B:51:ILE:HD12	1.86	0.58
2:D:251:SER:HB3	2:D:253:HIS:NE2	2.17	0.58
1:B:24:TYR:CZ	1:B:29:GLY:HA2	2.39	0.57
2:D:157:SER:HB2	2:D:179:PRO:HG3	1.86	0.57
2:C:266:THR:HG23	2:C:357:THR:HG22	1.86	0.57
2:C:163:LYS:HE2	2:C:166:HIS:CE1	2.39	0.57
1:A:101:ASN:O	1:A:102:ASN:HB2	2.03	0.57
2:C:188:LEU:HD12	2:C:213:TRP:HA	1.86	0.57
1:B:119:LYS:HG2	1:B:125:LYS:HZ3	1.70	0.57
2:C:207:LYS:HE2	2:C:209:ARG:HG2	1.87	0.56
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.68	0.56
2:D:159:GLU:OE1	2:D:159:GLU:HA	2.03	0.56
1:A:72:ARG:HD3	1:A:84:ALA:O	2.06	0.56
1:B:101:ASN:O	1:B:102:ASN:HB2	2.06	0.56
2:C:221:VAL:HB	2:C:222:PRO:HD2	1.86	0.56
2:C:338:GLU:HB2	2:C:355:TRP:CE2	2.41	0.56
2:C:293:ILE:HG22	2:C:294:GLU:N	2.22	0.54
2:D:172:LYS:HD3	2:D:173:THR:O	2.07	0.54
2:D:233:GLU:HB3	2:D:238:SER:HB2	1.89	0.54
2:D:155:TRP:CE3	2:D:180:SER:HB3	2.43	0.54
1:A:59:GLU:CA	2:C:286:HIS:CD2	2.90	0.53
2:C:191:LEU:HD13	2:C:194:GLY:O	2.07	0.53
1:B:60:ARG:HD2	2:D:349:LEU:HD13	1.89	0.53
2:D:186:PRO:HB2	2:D:232:VAL:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:HD3	1:A:99:GLU:CD	2.29	0.53
2:C:257:LEU:HD22	2:C:279:VAL:HG22	1.92	0.52
2:C:257:LEU:HB2	2:C:352:HIS:CE1	2.45	0.52
2:D:318:THR:CG2	2:D:323:MET:SD	2.98	0.52
2:C:303:ASP:CG	2:C:305:LEU:HD23	2.30	0.52
2:C:207:LYS:HE2	2:C:209:ARG:NE	2.16	0.52
2:D:180:SER:OG	2:D:232:VAL:HG11	2.10	0.52
1:A:97:ARG:HG3	1:A:97:ARG:NH1	2.25	0.52
2:D:190:TRP:CH2	2:D:230:CYS:HB3	2.45	0.52
1:B:49:PRO:HG2	1:B:50:HIS:CD2	2.45	0.52
2:C:155:TRP:CE3	2:C:180:SER:HB3	2.44	0.52
2:C:177:LYS:HB3	2:C:214:SER:OG	2.09	0.52
2:D:291:LYS:HB2	2:D:311:LEU:HD11	1.92	0.51
1:A:58:GLU:O	1:A:59:GLU:HB3	2.10	0.51
2:C:257:LEU:HD13	2:C:277:CYS:SG	2.49	0.51
1:A:79:ASP:CG	1:A:81:ARG:HH11	2.13	0.51
2:C:295:VAL:O	2:C:295:VAL:HG12	2.10	0.51
1:A:125:LYS:NZ	1:A:134:GLN:NE2	2.58	0.51
1:B:79:ASP:OD2	1:B:81:ARG:NH1	2.41	0.51
2:C:153:PRO:HG3	2:C:233:GLU:HA	1.91	0.51
1:A:111:TYR:O	1:A:113:SER:N	2.43	0.51
1:A:16:HIS:CE1	1:A:18:LYS:CB	2.93	0.51
2:C:153:PRO:HA	2:C:181:SER:O	2.10	0.51
2:D:157:SER:HB2	2:D:179:PRO:CG	2.40	0.51
2:C:236:TYR:CD1	2:C:236:TYR:N	2.79	0.51
2:C:260:GLY:C	2:C:261:LEU:HD23	2.31	0.51
2:C:264:ASN:OD1	2:C:355:TRP:N	2.30	0.51
1:A:115:TYR:HB2	1:A:137:ILE:HG22	1.93	0.51
2:C:296:ASN:C	2:C:298:SER:N	2.64	0.51
1:A:95:PHE:CZ	1:A:109:ARG:HG3	2.46	0.51
2:D:236:TYR:N	2:D:236:TYR:CD1	2.78	0.51
2:D:170:ALA:O	2:D:171:ALA:HB3	2.10	0.51
2:D:153:PRO:HA	2:D:181:SER:O	2.11	0.51
3:A:302:SGN:H3	2:D:207:LYS:NZ	2.26	0.50
1:B:59:GLU:HA	2:D:286:HIS:CG	2.46	0.50
1:B:17:PHE:HE1	2:D:320:ASP:HB3	1.77	0.50
2:C:172:LYS:O	2:C:220:VAL:HG22	2.11	0.49
1:A:125:LYS:HZ2	1:A:134:GLN:NE2	2.10	0.49
2:C:262:PRO:HD2	2:C:352:HIS:HB3	1.94	0.49
1:B:26:LYS:O	1:B:135:LYS:HE2	2.11	0.49
2:D:262:PRO:HD2	2:D:352:HIS:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HD23	1:B:124:TYR:HA	1.94	0.49
2:C:295:VAL:O	2:C:296:ASN:CG	2.51	0.49
1:A:30:PHE:CD2	1:A:122:GLY:HA2	2.48	0.49
2:C:175:LYS:HG3	2:C:216:ILE:HD13	1.93	0.49
2:D:188:LEU:HD23	2:D:232:VAL:HG22	1.95	0.49
1:A:120:ARG:H	1:A:120:ARG:HD3	1.77	0.48
1:B:33:ARG:NH2	1:B:43:VAL:HG13	2.28	0.48
1:B:83:LEU:C	1:B:83:LEU:HD12	2.34	0.48
2:C:269:LEU:HD12	2:C:333:PHE:CD2	2.49	0.48
1:A:60:ARG:HD2	2:C:349:LEU:HD11	1.94	0.48
1:B:111:TYR:O	1:B:113:SER:N	2.47	0.48
1:B:33:ARG:NH1	1:B:43:VAL:CG1	2.76	0.48
1:A:76:MET:HE1	1:A:114:TRP:HB2	1.96	0.48
2:C:266:THR:HG23	2:C:357:THR:CG2	2.44	0.48
1:B:134:GLN:O	1:B:137:ILE:HG12	2.14	0.47
1:A:33:ARG:NH1	1:A:43:VAL:HG11	2.29	0.47
1:A:22:ARG:HD3	1:A:51:ILE:HD12	1.95	0.47
2:D:245:LEU:HD12	2:D:246:ASP:N	2.29	0.47
1:B:25:CYS:HB2	1:B:139:PHE:CE2	2.50	0.47
2:C:291:LYS:HD3	2:C:339:TYR:CZ	2.50	0.47
2:D:188:LEU:HD11	2:D:190:TRP:NE1	2.26	0.47
1:B:37:ASP:OD1	1:B:39:ARG:HG3	2.15	0.47
1:A:83:LEU:C	1:A:83:LEU:HD12	2.36	0.46
2:D:271:SER:O	2:D:330:ASN:HA	2.14	0.46
1:B:33:ARG:HG3	1:B:50:HIS:O	2.15	0.46
1:A:33:ARG:CZ	1:A:43:VAL:HG13	2.45	0.46
1:B:26:LYS:HB2	1:B:103:TYR:CE1	2.50	0.46
2:C:191:LEU:O	2:C:228:TYR:HA	2.16	0.46
2:D:191:LEU:HD23	2:D:196:GLU:HA	1.97	0.46
2:C:153:PRO:HD3	2:C:234:ASN:CG	2.35	0.46
2:C:271:SER:O	2:C:330:ASN:HA	2.16	0.46
2:D:153:PRO:HG3	2:D:233:GLU:HA	1.98	0.46
1:A:76:MET:O	1:A:111:TYR:HE2	1.99	0.46
2:C:186:PRO:HG2	2:C:213:TRP:CH2	2.51	0.46
1:A:115:TYR:HB2	1:A:137:ILE:CG2	2.46	0.46
1:B:27:ASN:ND2	1:B:120:ARG:N	2.63	0.46
1:A:16:HIS:ND1	1:A:17:PHE:N	2.64	0.45
2:C:221:VAL:HB	2:C:222:PRO:CD	2.45	0.45
1:B:77:LYS:HA	1:B:91:GLU:OE2	2.15	0.45
2:D:318:THR:HG21	2:D:323:MET:SD	2.57	0.45
2:D:245:LEU:HD12	2:D:246:ASP:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ILE:HD12	1:A:74:LEU:HD23	1.97	0.45
1:B:23:LEU:HG	1:B:53:LEU:HD12	1.97	0.45
2:C:274:GLU:HA	2:C:326:LEU:O	2.17	0.45
1:A:60:ARG:CZ	2:C:349:LEU:HD21	2.47	0.45
2:D:189:ARG:HD3	2:D:233:GLU:OE1	2.17	0.45
2:D:189:ARG:HG3	2:D:231:ILE:HB	1.99	0.45
2:D:277:CYS:O	2:D:324:GLU:HG2	2.17	0.45
2:C:198:LYS:N	2:C:201:HIS:CD2	2.85	0.45
1:B:98:LEU:HD21	2:D:252:PRO:HB3	1.99	0.45
2:C:188:LEU:HD23	2:C:189:ARG:N	2.31	0.45
2:D:318:THR:O	2:D:318:THR:HG22	2.15	0.45
1:B:32:LEU:HD21	1:B:74:LEU:HD22	1.98	0.45
2:C:319:THR:HG22	2:C:320:ASP:N	2.31	0.45
2:C:213:TRP:CZ3	2:C:232:VAL:HG13	2.52	0.45
1:A:117:ALA:HB1	1:A:136:ALA:HB1	1.99	0.44
2:C:257:LEU:HD23	2:C:257:LEU:N	2.32	0.44
1:A:60:ARG:NE	2:C:349:LEU:HD21	2.33	0.44
1:B:34:ILE:O	1:B:50:HIS:HB3	2.18	0.44
1:B:127:GLY:HA2	1:B:130:THR:HG23	1.98	0.44
2:C:196:GLU:OE1	2:C:198:LYS:HE3	2.17	0.44
2:D:263:ALA:O	2:D:265:LYS:HG3	2.18	0.44
2:D:191:LEU:O	2:D:228:TYR:HA	2.16	0.44
2:C:270:GLY:O	2:C:330:ASN:HA	2.18	0.44
2:D:319:THR:HG21	2:D:321:LYS:NZ	2.33	0.44
2:C:293:ILE:HG22	2:C:294:GLU:H	1.82	0.44
1:B:33:ARG:HH21	1:B:41:ASP:CG	2.20	0.44
1:B:33:ARG:CZ	1:B:43:VAL:HG13	2.47	0.44
2:C:180:SER:OG	2:C:232:VAL:HG11	2.17	0.44
2:D:331:VAL:HA	2:D:335:ASP:OD2	2.18	0.44
2:D:270:GLY:O	2:D:330:ASN:HA	2.18	0.43
2:C:186:PRO:HB2	2:C:232:VAL:HG12	2.00	0.43
1:B:88:VAL:HG21	2:D:316:VAL:CG1	2.36	0.43
2:C:261:LEU:HA	2:C:262:PRO:C	2.39	0.43
2:D:156:THR:HG23	2:D:180:SER:HA	2.00	0.43
2:D:291:LYS:HE3	2:D:339:TYR:CE1	2.53	0.43
2:C:338:GLU:HB2	2:C:355:TRP:CZ2	2.53	0.43
2:C:233:GLU:HB3	2:C:238:SER:HB2	2.01	0.43
1:B:99:GLU:HB2	1:B:101:ASN:OD1	2.18	0.43
2:C:202:ARG:HG2	2:C:205:GLY:HA2	2.01	0.43
2:C:190:TRP:CZ3	2:C:230:CYS:HB3	2.53	0.43
1:B:99:GLU:HB3	2:C:203:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:161:MET:CE	2:C:178:CYS:HA	2.49	0.43
2:C:171:ALA:HA	2:C:219:SER:HA	2.01	0.43
1:A:26:LYS:CD	1:A:138:LEU:HD12	2.43	0.42
2:C:188:LEU:CD1	2:C:213:TRP:HA	2.49	0.42
2:D:166:HIS:CG	2:D:176:PHE:HE1	2.37	0.42
1:A:76:MET:CE	1:A:114:TRP:HB2	2.49	0.42
1:B:125:LYS:HE2	1:B:136:ALA:CB	2.49	0.42
2:D:234:ASN:OD1	2:D:234:ASN:C	2.58	0.42
1:A:77:LYS:HE2	1:A:77:LYS:HA	2.01	0.42
1:B:26:LYS:HD3	1:B:138:LEU:HD12	2.00	0.42
2:D:155:TRP:HE3	2:D:180:SER:HB3	1.82	0.42
1:A:119:LYS:C	1:A:121:THR:H	2.23	0.42
2:C:325:VAL:O	2:C:325:VAL:HG13	2.20	0.42
1:A:75:ALA:HB2	1:A:92:CYS:SG	2.59	0.42
1:B:27:ASN:HB2	1:B:136:ALA:HA	2.02	0.42
1:A:60:ARG:HD2	2:C:349:LEU:CD1	2.49	0.42
1:A:35:HIS:CD2	1:A:39:ARG:HB2	2.54	0.41
2:D:257:LEU:CD2	2:D:279:VAL:HG22	2.50	0.41
2:D:279:VAL:HG12	2:D:280:TYR:N	2.35	0.41
2:C:303:ASP:O	2:C:305:LEU:HD22	2.20	0.41
2:D:288:GLN:HG2	2:D:290:LEU:CD1	2.50	0.41
1:B:125:LYS:HZ3	1:B:125:LYS:HB2	1.86	0.41
1:B:60:ARG:HH11	2:D:349:LEU:HD13	1.85	0.41
1:B:81:ARG:HB2	1:B:124:TYR:OH	2.21	0.41
1:B:33:ARG:NH2	1:B:41:ASP:OD1	2.53	0.41
2:C:166:HIS:O	2:C:245:LEU:HD12	2.21	0.41
2:C:186:PRO:HG2	2:C:213:TRP:HH2	1.86	0.41
2:C:203:ILE:C	2:C:205:GLY:H	2.24	0.41
1:A:22:ARG:HD3	1:A:51:ILE:CD1	2.51	0.41
2:D:225:LYS:HE2	2:D:246:ASP:OD2	2.21	0.41
2:C:198:LYS:H	2:C:201:HIS:CD2	2.39	0.41
2:C:190:TRP:CH2	2:C:230:CYS:HB3	2.55	0.41
1:B:88:VAL:CG2	2:D:316:VAL:HG11	2.39	0.41
2:D:269:LEU:C	2:D:269:LEU:HD23	2.39	0.41
2:C:312:LYS:HG2	2:C:323:MET:SD	2.61	0.41
1:A:34:ILE:O	1:A:50:HIS:HB3	2.20	0.41
2:C:182:GLY:O	2:C:186:PRO:HD3	2.21	0.40
2:D:177:LYS:HB3	2:D:214:SER:HB3	2.03	0.40
2:D:153:PRO:HB3	2:D:186:PRO:HB3	2.03	0.40
1:B:108:SER:O	1:B:112:THR:HA	2.20	0.40
1:A:81:ARG:HB2	1:A:124:TYR:OH	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:287:ILE:HG22	2:D:288:GLN:N	2.36	0.40
2:D:274:GLU:HA	2:D:326:LEU:O	2.22	0.40
2:D:197:PHE:HD1	2:D:206:TYR:CZ	2.39	0.40
1:A:108:SER:O	1:A:112:THR:HA	2.21	0.40
2:C:161:MET:HE3	2:C:178:CYS:HA	2.04	0.40
2:C:183:THR:HA	2:C:184:PRO:C	2.41	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	127/132 (96%)	116 (91%)	10 (8%)	1 (1%)	24	66
1	B	127/132 (96%)	116 (91%)	10 (8%)	1 (1%)	24	66
2	C	209/225 (93%)	194 (93%)	11 (5%)	4 (2%)	10	43
2	D	192/225 (85%)	176 (92%)	14 (7%)	2 (1%)	19	61
All	All	655/714 (92%)	602 (92%)	45 (7%)	8 (1%)	16	56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	THR
1	B	112	THR
2	C	271	SER
2	C	296	ASN
2	C	281	SER
2	D	219	SER
2	D	330	ASN
2	C	330	ASN

### 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	110/113 (97%)	105 (96%)	5 (4%)	34	74
1	B	110/113 (97%)	106 (96%)	4 (4%)	42	79
2	C	180/198 (91%)	170 (94%)	10 (6%)	26	65
2	D	169/198 (85%)	159 (94%)	10 (6%)	24	63
All	All	569/622 (92%)	540 (95%)	29 (5%)	29	69

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	60	ARG
1	A	69	SER
1	A	89	THR
1	A	120	ARG
1	B	43	VAL
1	B	55	LEU
1	B	89	THR
1	B	90	ASP
2	C	188	LEU
2	C	197	PHE
2	C	199	PRO
2	C	200	ASP
2	C	238	SER
2	C	252	PRO
2	C	257	LEU
2	C	313	THR
2	C	355	TRP
2	C	356	LEU
2	D	172	LYS
2	D	197	PHE
2	D	201	HIS
2	D	203	ILE
2	D	206	TYR

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Mol	Chain	Res	Type
2	D	223	SER
2	D	238	SER
2	D	317	ASN
2	D	355	TRP
2	D	356	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	134	GLN
1	B	27	ASN
2	C	166	HIS
2	C	185	GLN
2	C	201	HIS
2	C	286	HIS
2	C	317	ASN
2	C	330	ASN
2	D	292	HIS
2	D	317	ASN

### 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](#)

14 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	5.04	6 (50%)	11,22,24	2.69	3 (27%)
3	SGN	A	302	3	18,20,20	1.73	3 (16%)	20,31,31	1.46	2 (10%)
3	IDS	A	303	3	12,15,17	2.61	2 (16%)	12,22,26	2.42	3 (25%)
3	SGN	A	304	3	18,20,20	1.63	2 (11%)	20,31,31	0.94	1 (5%)
3	IDS	A	305	3	12,15,17	2.43	3 (25%)	12,22,26	2.45	2 (16%)
3	SGN	A	306	3	18,20,20	1.91	3 (16%)	20,31,31	1.34	3 (15%)
3	IDU	A	307	3	12,15,17	2.39	3 (25%)	12,22,26	2.52	2 (16%)
3	SGN	A	308	3	18,20,20	2.02	2 (11%)	20,31,31	1.15	1 (5%)
4	UAP	B	301	4	12,15,16	5.22	5 (41%)	11,22,24	2.87	3 (27%)
4	SGN	B	302	4	18,20,20	1.73	2 (11%)	20,31,31	1.13	3 (15%)
4	IDS	B	303	4	12,15,17	2.51	3 (25%)	12,22,26	2.37	3 (25%)
4	SGN	B	304	4	18,20,20	1.62	1 (5%)	20,31,31	1.03	1 (5%)
4	IDS	B	305	4	12,15,17	2.47	4 (33%)	12,22,26	3.39	4 (33%)
4	SGN	B	306	4	18,20,20	1.75	3 (16%)	20,31,31	1.05	1 (5%)

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	-	0/5/22/25	0/1/1/1
3	SGN	A	302	3	-	0/11/31/31	0/1/1/1
3	IDS	A	303	3	-	0/5/22/29	0/1/1/1
3	SGN	A	304	3	-	0/11/31/31	0/1/1/1
3	IDS	A	305	3	-	0/5/22/29	0/1/1/1
3	SGN	A	306	3	1/1/7/8	0/11/31/31	0/1/1/1
3	IDU	A	307	3	-	0/5/22/29	0/1/1/1
3	SGN	A	308	3	-	0/11/31/31	0/1/1/1
4	UAP	B	301	4	-	0/5/22/25	0/1/1/1
4	SGN	B	302	4	-	0/11/31/31	0/1/1/1
4	IDS	B	303	4	-	0/5/22/29	0/1/1/1
4	SGN	B	304	4	-	0/11/31/31	0/1/1/1
4	IDS	B	305	4	-	0/5/22/29	0/1/1/1
4	SGN	B	306	4	-	0/11/31/31	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	IDS	O2-C2	-5.66	1.38	1.47
4	B	301	UAP	O2-C2	-5.36	1.39	1.47
4	B	303	IDS	O2-C2	-5.10	1.39	1.47
3	A	301	UAP	O2-C2	-4.93	1.39	1.47
3	A	305	IDS	O2-C2	-4.79	1.40	1.47
3	A	307	IDU	O2-C2	-3.92	1.41	1.47
4	B	305	IDS	O2-C2	-3.14	1.42	1.47
3	A	305	IDS	O3-C3	-2.77	1.37	1.43
4	B	305	IDS	O3-C3	-2.54	1.37	1.43
3	A	301	UAP	O3-C3	-2.37	1.38	1.43
3	A	302	SGN	C2-N	-2.34	1.43	1.47
3	A	304	SGN	C2-N	-2.30	1.43	1.47
4	B	303	IDS	O3-C3	-2.20	1.38	1.43
4	B	306	SGN	C2-N	-2.18	1.44	1.47
3	A	306	SGN	C2-N	-2.06	1.44	1.47
3	A	307	IDU	C1-C2	2.28	1.55	1.51
4	B	306	SGN	O1S-S1	2.32	1.44	1.42
4	B	302	SGN	O1S-S1	2.37	1.44	1.42
3	A	302	SGN	O1S-S1	2.40	1.44	1.42
4	B	305	IDS	C1-C2	2.40	1.55	1.51
3	A	308	SGN	O1S-S1	2.66	1.44	1.42
3	A	301	UAP	O5-C5	2.69	1.41	1.37
3	A	306	SGN	O1S-S1	3.02	1.45	1.42
4	B	301	UAP	O5-C5	3.07	1.42	1.37
3	A	301	UAP	C3-C4	3.79	1.55	1.50
4	B	301	UAP	C3-C4	4.24	1.55	1.50
3	A	305	IDS	O2-S	5.25	1.73	1.57
4	B	301	UAP	O2-S	5.45	1.74	1.57
4	B	304	SGN	O6-S2	5.72	1.75	1.57
3	A	301	UAP	O2-S	5.77	1.75	1.57
3	A	303	IDS	O2-S	5.79	1.75	1.57
4	B	303	IDS	O2-S	5.82	1.75	1.57
3	A	302	SGN	O6-S2	5.95	1.76	1.57
4	B	306	SGN	O6-S2	5.97	1.76	1.57
4	B	302	SGN	O6-S2	5.99	1.76	1.57
3	A	304	SGN	O6-S2	6.03	1.76	1.57
3	A	307	IDU	O2-S	6.17	1.76	1.57
4	B	305	IDS	O2-S	6.39	1.77	1.57
3	A	306	SGN	O6-S2	6.88	1.78	1.57
3	A	308	SGN	O6-S2	7.08	1.79	1.57
3	A	301	UAP	C4-C5	14.65	1.52	1.32
4	B	301	UAP	C4-C5	15.21	1.53	1.32

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	UAP	C3-C4-C5	-4.72	113.61	121.60
3	A	302	SGN	C3-C2-N	-4.67	101.35	110.64
3	A	301	UAP	C3-C4-C5	-4.51	113.98	121.60
3	A	308	SGN	C4-C3-C2	-3.53	105.53	110.43
3	A	306	SGN	C3-C2-N	-3.20	104.29	110.64
4	B	304	SGN	C3-C2-N	-2.77	105.14	110.64
4	B	306	SGN	C3-C2-N	-2.64	105.40	110.64
4	B	302	SGN	C4-C3-C2	-2.55	106.89	110.43
3	A	302	SGN	C3-C4-C5	-2.46	105.90	110.20
3	A	306	SGN	C1-O5-C5	-2.34	109.15	113.47
4	B	302	SGN	C3-C2-N	-2.30	106.08	110.64
3	A	304	SGN	C3-C2-N	-2.05	106.56	110.64
3	A	301	UAP	C1-O5-C5	2.01	119.75	115.30
4	B	301	UAP	C1-O5-C5	2.04	119.82	115.30
4	B	302	SGN	O5-C5-C6	2.16	111.01	106.61
3	A	306	SGN	O1-C1-O5	2.42	116.86	110.25
3	A	303	IDS	C1-O5-C5	2.89	118.17	113.47
4	B	305	IDS	O2-C2-C1	2.96	116.22	107.50
4	B	303	IDS	C1-O5-C5	3.37	118.94	113.47
3	A	305	IDS	C1-C2-C3	3.64	114.87	109.89
3	A	307	IDU	C1-O5-C5	3.88	119.77	113.47
4	B	305	IDS	C1-O5-C5	3.89	119.78	113.47
4	B	303	IDS	C1-C2-C3	4.08	115.46	109.89
3	A	303	IDS	C1-C2-C3	5.29	117.12	109.89
3	A	303	IDS	O5-C5-C4	5.47	119.08	110.56
4	B	305	IDS	O5-C5-C4	5.81	119.60	110.56
4	B	303	IDS	O5-C5-C4	6.03	119.94	110.56
3	A	305	IDS	O5-C5-C4	7.17	121.72	110.56
3	A	307	IDU	O5-C5-C4	7.32	121.96	110.56
3	A	301	UAP	C1-C2-C3	7.34	118.04	109.32
4	B	301	UAP	C1-C2-C3	7.82	118.60	109.32
4	B	305	IDS	C1-C2-C3	8.65	121.70	109.89

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	306	SGN	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	UAP	2	0
3	A	302	SGN	1	0
3	A	305	IDS	1	0
4	B	305	IDS	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](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.