



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:36 am GMT

PDB ID : 5CMN  
Title : FLRT3 LRR domain in complex with LPHN3 Olfactomedin domain  
Authors : Lu, Y.; Salzman, G.; Arac, D.  
Deposited on : 2015-07-17  
Resolution : 3.60 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 : 1.7.2 (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

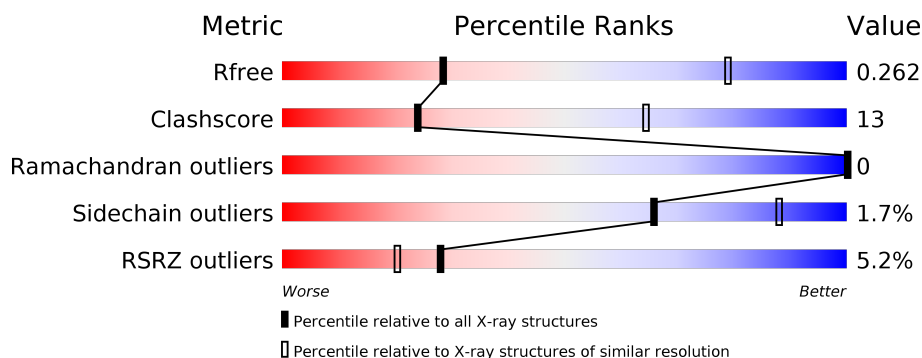
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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))
$R_{free}$	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)

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	333	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>35%</div> <div>• •</div> </div> </div>
1	B	333	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>28%</div> <div>• •</div> </div> </div>
1	C	333	<div> <div>9%</div> <div> <div></div> <div>64%</div> <div>32%</div> <div>• •</div> </div> </div>
1	D	333	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>35%</div> <div>• •</div> </div> </div>
2	E	261	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>28%</div> <div>• 5%</div> </div> </div>
2	F	261	<div> <div>7%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	261	<div><div></div><div>3%</div><div>70%</div><div>24%</div><div>5%</div></div>
2	H	261	<div><div></div><div>11%</div><div>70%</div><div>24%</div><div>• 5%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18420 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 Leucine-rich repeat transmembrane protein FLRT3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2575	1628	454	482	11			
1	B	321	Total	C	N	O	S	0	0	0
			2575	1628	454	482	11			
1	C	321	Total	C	N	O	S	0	0	0
			2575	1628	454	482	11			
1	D	321	Total	C	N	O	S	0	0	0
			2575	1628	454	482	11			

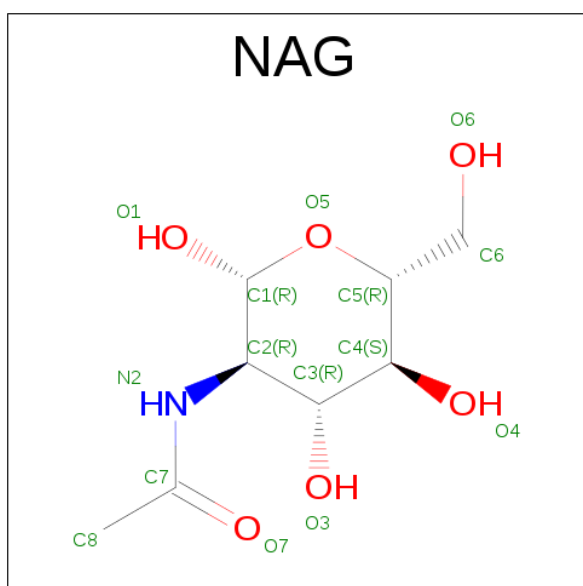
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	25	ALA	-	expression tag	UNP Q9NZU0
D	26	ASP	-	expression tag	UNP Q9NZU0
D	27	PRO	-	expression tag	UNP Q9NZU0
D	28	GLY	-	expression tag	UNP Q9NZU0
A	25	ALA	-	expression tag	UNP Q9NZU0
A	26	ASP	-	expression tag	UNP Q9NZU0
A	27	PRO	-	expression tag	UNP Q9NZU0
A	28	GLY	-	expression tag	UNP Q9NZU0
B	25	ALA	-	expression tag	UNP Q9NZU0
B	26	ASP	-	expression tag	UNP Q9NZU0
B	27	PRO	-	expression tag	UNP Q9NZU0
B	28	GLY	-	expression tag	UNP Q9NZU0
C	25	ALA	-	expression tag	UNP Q9NZU0
C	26	ASP	-	expression tag	UNP Q9NZU0
C	27	PRO	-	expression tag	UNP Q9NZU0
C	28	GLY	-	expression tag	UNP Q9NZU0

- Molecule 2 is a protein called Latrophilin-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	247	Total	C	N	O	S	0	0	0
			2015	1292	334	384	5			
2	F	247	Total	C	N	O	S	0	0	0
			2015	1292	334	384	5			
2	G	247	Total	C	N	O	S	0	0	0
			2015	1292	334	384	5			
2	H	247	Total	C	N	O	S	0	0	0
			2015	1292	334	384	5			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Ca	0	0
			1	1		
4	G	1	Total	Ca	0	0
			1	1		

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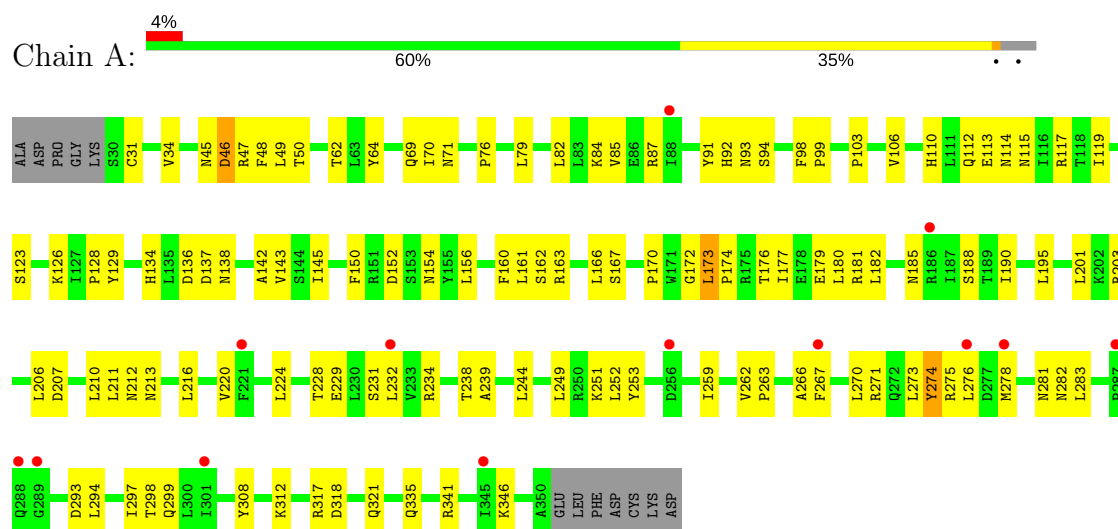
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total 1	Ca 1	0	0
4	E	1	Total 1	Ca 1	0	0

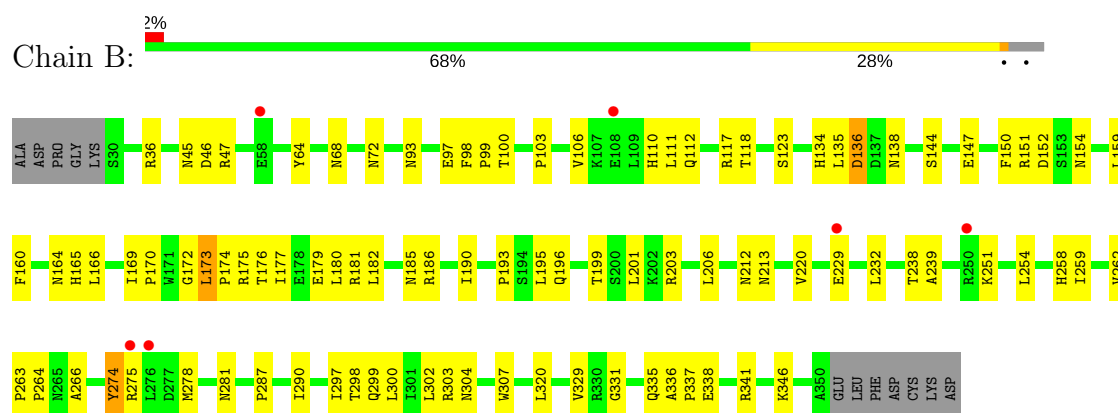
### 3 Residue-property plots [i](#)

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.

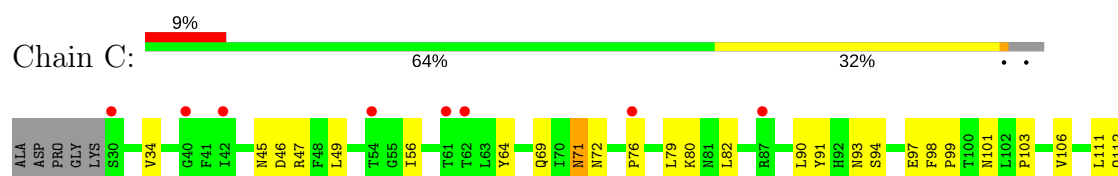
- Molecule 1: Leucine-rich repeat transmembrane protein FLRT3

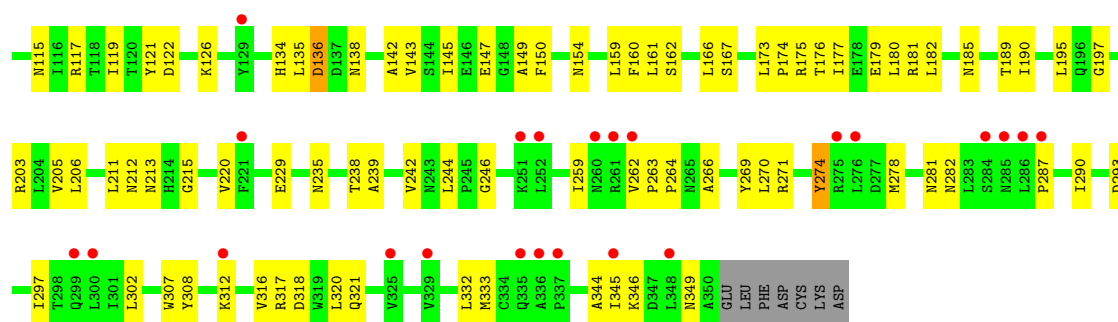


- Molecule 1: Leucine-rich repeat transmembrane protein FLRT3

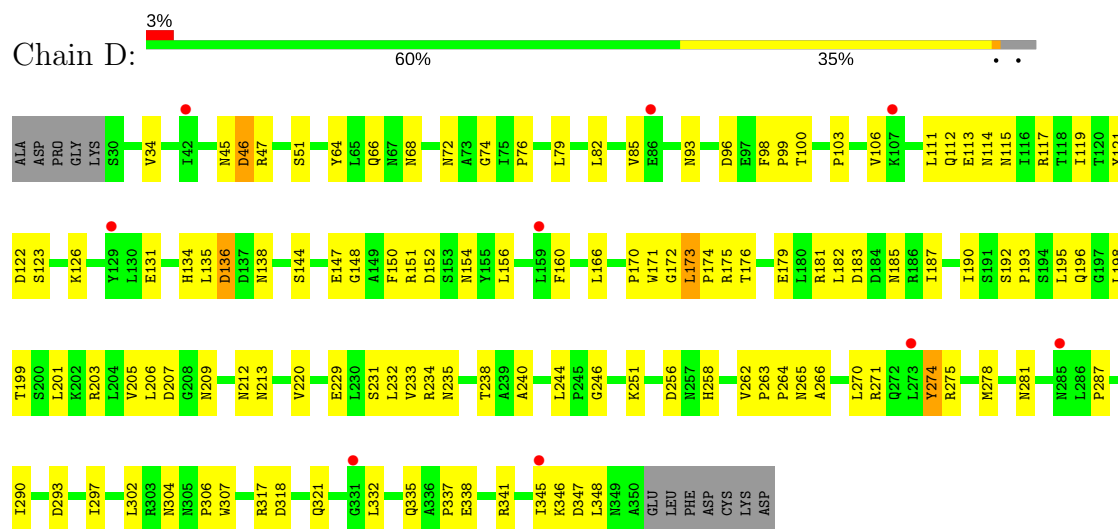


- Molecule 1: Leucine-rich repeat transmembrane protein FLRT3

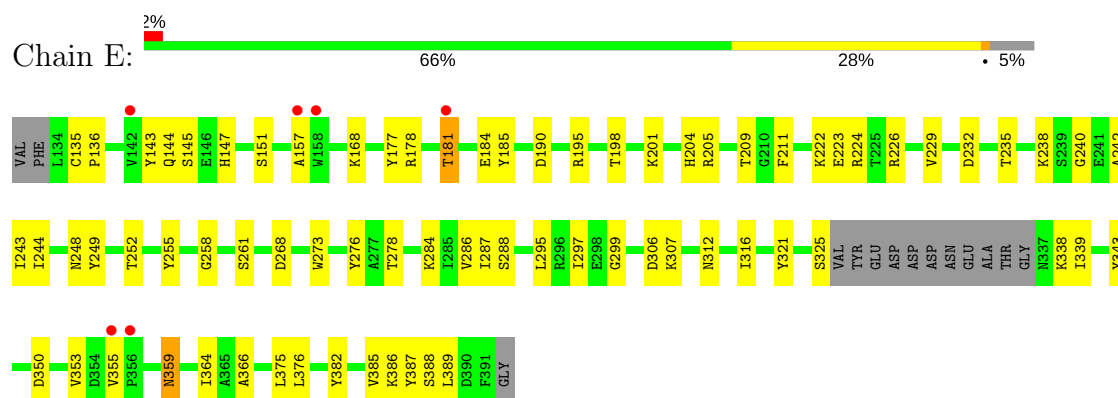




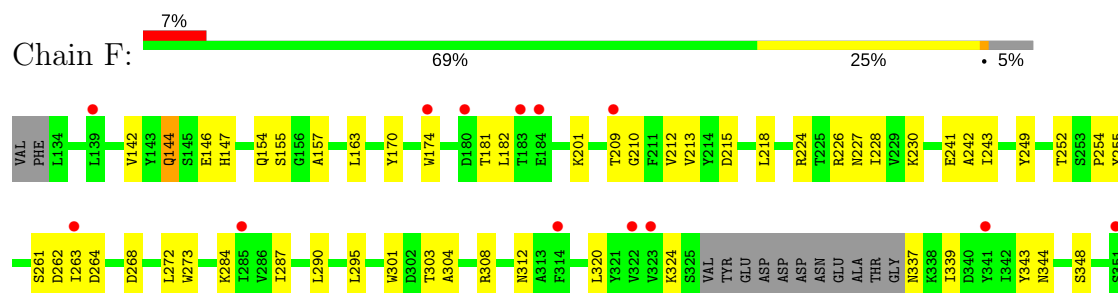
- Molecule 1: Leucine-rich repeat transmembrane protein FLRT3



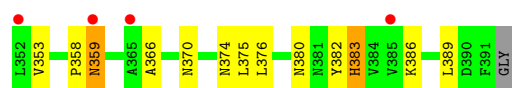
- Molecule 2: Latrophilin-3



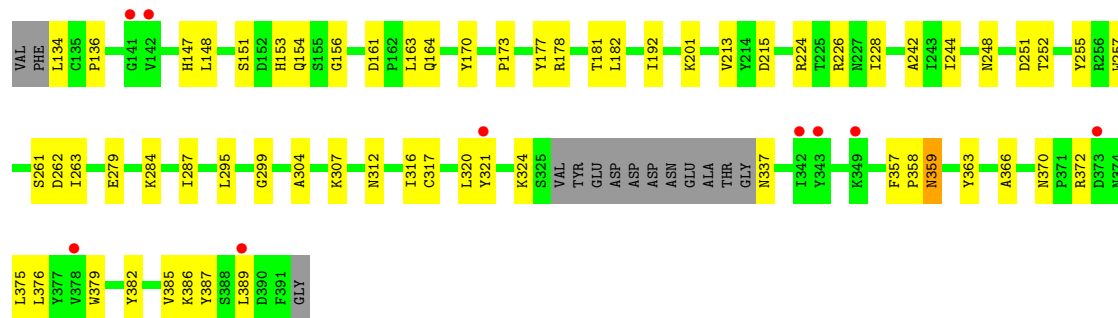
- Molecule 2: Latrophilin-3



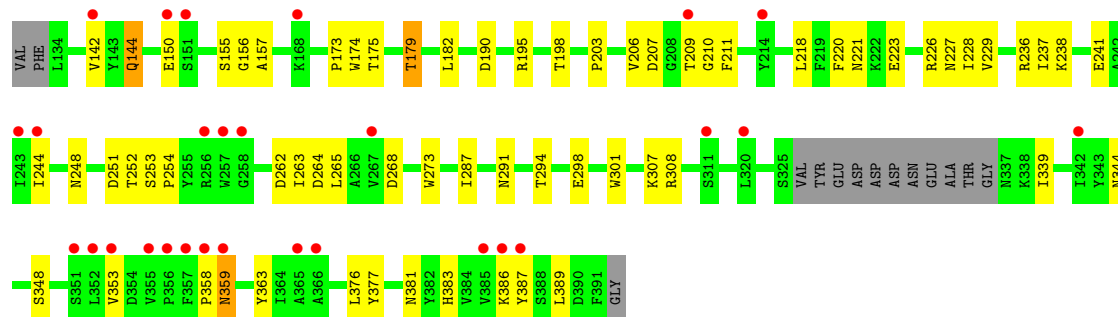




● Molecule 2: Latrophilin-3



● Molecule 2: Latrophilin-3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.27Å 102.27Å 419.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.20 – 3.60 73.20 – 3.60	Depositor EDS
% Data completeness (in resolution range)	91.7 (73.20-3.60) 91.7 (73.20-3.60)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 3.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.195 , 0.262 0.195 , 0.262	Depositor DCC
$R_{free}$ test set	1851 reflections (4.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.4	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 77.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.350 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	18420	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.28	0/2627	0.51	0/3574
1	B	0.28	0/2627	0.49	0/3574
1	C	0.28	0/2627	0.50	0/3574
1	D	0.28	0/2627	0.50	0/3574
2	E	0.30	0/2071	0.53	0/2820
2	F	0.27	0/2071	0.50	0/2820
2	G	0.28	0/2071	0.49	0/2820
2	H	0.27	0/2071	0.50	0/2820
All	All	0.28	0/18792	0.50	0/25576

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2575	0	2578	86	1
1	B	2575	0	2578	67	0
1	C	2575	0	2578	84	1
1	D	2575	0	2578	91	0
2	E	2015	0	1924	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2015	0	1924	43	0
2	G	2015	0	1924	40	0
2	H	2015	0	1924	42	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
All	All	18420	0	18060	457	1

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 13.

All (457) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:PRO:HA	1:D:290:ILE:HG22	1.64	0.80
1:A:115:ASN:OD1	1:A:117:ARG:NH1	2.16	0.78
2:H:376:LEU:HB2	2:H:387:TYR:HB2	1.68	0.76
1:D:263:PRO:HG2	1:D:266:ALA:HB2	1.68	0.74
1:A:174:PRO:HG2	1:A:177:ILE:HG12	1.70	0.73
1:D:112:GLN:HA	1:D:138:ASN:HD21	1.52	0.73
1:C:115:ASN:OD1	1:C:117:ARG:NH1	2.23	0.72
1:B:251:LYS:HG2	1:B:275:ARG:HB3	1.71	0.70
1:A:251:LYS:HG2	1:A:275:ARG:HB3	1.73	0.70
2:H:287:ILE:HG13	2:H:301:TRP:HB2	1.73	0.70
1:C:271:ARG:NH2	1:C:293:ASP:OD2	2.26	0.68
2:E:242:ALA:HB2	2:E:295:LEU:HB3	1.74	0.68
2:E:316:ILE:HB	2:E:321:TYR:HE2	1.59	0.68
1:A:166:LEU:HB2	1:A:185:ASN:HD22	1.58	0.67
1:D:98:PHE:HB2	1:D:119:ILE:HG12	1.76	0.67
2:H:210:GLY:HA3	2:H:264:ASP:HA	1.77	0.67
2:H:198:THR:HG21	2:H:236:ARG:HH22	1.61	0.66
2:G:248:ASN:HB3	2:G:252:THR:HB	1.78	0.66
2:E:190:ASP:OD1	2:E:195:ARG:NH1	2.29	0.66
1:D:251:LYS:HG2	1:D:275:ARG:HB3	1.78	0.66
1:A:282:ASN:O	1:B:335:GLN:NE2	2.29	0.65
2:E:147:HIS:HA	2:E:385:VAL:HG12	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HG21	2:F:227:ASN:HD21	1.61	0.65
1:C:263:PRO:HG2	1:C:266:ALA:HB2	1.78	0.65
2:F:375:LEU:HD13	2:F:386:LYS:HD3	1.77	0.65
1:A:134:HIS:HA	1:A:160:PHE:HB2	1.79	0.64
2:G:255:TYR:H	2:G:261:SER:HB2	1.63	0.63
1:A:136:ASP:O	1:A:138:ASN:ND2	2.32	0.63
2:F:210:GLY:HA3	2:F:264:ASP:HA	1.81	0.63
1:C:119:ILE:HD12	1:C:145:ILE:HG12	1.79	0.63
1:A:181:ARG:NH2	2:E:178:ARG:HG3	2.14	0.63
1:C:166:LEU:HB2	1:C:185:ASN:HD22	1.63	0.63
1:C:317:ARG:NH2	1:C:318:ASP:OD1	2.32	0.63
1:A:119:ILE:HD12	1:A:145:ILE:HG12	1.80	0.62
1:B:175:ARG:HD2	1:D:151:ARG:HH11	1.64	0.62
2:H:228:ILE:HD11	2:H:263:ILE:HG21	1.81	0.62
2:H:344:ASN:O	2:H:348:SER:N	2.32	0.62
1:A:166:LEU:HB2	1:A:185:ASN:ND2	2.13	0.62
1:A:45:ASN:ND2	1:A:46:ASP:OD1	2.32	0.62
2:E:284:LYS:HA	2:E:306:ASP:HA	1.81	0.62
1:D:264:PRO:HG2	2:E:299:GLY:HA3	1.80	0.62
1:B:110:HIS:HB3	1:B:112:GLN:HE22	1.65	0.62
1:C:117:ARG:NH2	1:D:113:GLU:HA	2.14	0.62
1:D:136:ASP:O	1:D:138:ASN:ND2	2.32	0.62
2:E:151:SER:N	2:E:382:TYR:O	2.31	0.62
1:B:100:THR:HG22	1:B:123:SER:HA	1.80	0.61
1:B:195:LEU:HD12	1:B:220:VAL:HG22	1.81	0.61
2:H:254:PRO:HA	2:H:262:ASP:HA	1.82	0.61
1:B:117:ARG:O	1:B:144:SER:HB3	1.99	0.61
2:G:376:LEU:HB2	2:G:387:TYR:HB2	1.82	0.61
2:E:204:HIS:HB3	2:E:222:LYS:HG3	1.82	0.61
1:C:76:PRO:HG2	1:C:79:LEU:HB2	1.81	0.61
2:G:161:ASP:HB3	2:G:164:GLN:HB2	1.82	0.61
2:G:376:LEU:HG	2:G:389:LEU:HD21	1.82	0.61
1:B:278:MET:O	1:B:281:ASN:ND2	2.34	0.60
1:C:34:VAL:HG12	1:C:47:ARG:HD3	1.83	0.60
1:D:181:ARG:NH2	1:D:203:ARG:HH12	1.99	0.60
1:B:179:GLU:HG3	1:B:203:ARG:HB3	1.83	0.60
1:C:189:THR:HG21	2:H:237:ILE:HA	1.83	0.60
1:D:117:ARG:O	1:D:144:SER:HB3	2.02	0.60
1:C:181:ARG:HH21	1:C:203:ARG:HH12	1.50	0.60
1:A:112:GLN:HA	1:A:138:ASN:HD21	1.66	0.60
1:C:112:GLN:HG3	2:G:224:ARG:HD3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:LEU:HB2	1:C:185:ASN:ND2	2.17	0.59
1:A:271:ARG:NH2	1:A:293:ASP:OD2	2.35	0.59
1:B:182:LEU:HB2	1:B:206:LEU:HD23	1.84	0.59
1:D:181:ARG:HH21	1:D:203:ARG:HH12	1.48	0.59
1:B:212:ASN:OD1	1:B:213:ASN:N	2.36	0.59
2:H:229:VAL:HG22	2:H:241:GLU:HG3	1.84	0.59
1:C:72:ASN:ND2	1:C:97:GLU:HG2	2.18	0.59
1:B:151:ARG:HH11	1:D:175:ARG:HD2	1.68	0.58
2:H:248:ASN:HB3	2:H:252:THR:HB	1.85	0.58
1:D:166:LEU:HB2	1:D:185:ASN:ND2	2.18	0.58
1:A:206:LEU:HB2	1:A:232:LEU:HD23	1.86	0.58
1:C:302:LEU:HB3	1:C:307:TRP:HZ2	1.67	0.58
2:E:343:TYR:CD2	2:E:350:ASP:HB3	2.39	0.58
1:C:143:VAL:HG21	2:H:227:ASN:HD21	1.68	0.58
2:H:175:THR:O	2:H:179:THR:OG1	2.22	0.58
1:C:274:TYR:HA	1:C:297:ILE:HA	1.85	0.57
1:A:274:TYR:HA	1:A:297:ILE:HA	1.86	0.57
1:D:45:ASN:ND2	1:D:46:ASP:OD1	2.35	0.57
1:A:112:GLN:O	1:A:114:ASN:ND2	2.36	0.57
1:A:128:PRO:HG2	1:A:129:TYR:CD2	2.40	0.57
2:G:151:SER:N	2:G:382:TYR:O	2.32	0.57
1:B:166:LEU:HB2	1:B:185:ASN:HD22	1.70	0.57
1:D:302:LEU:HB3	1:D:307:TRP:HZ2	1.70	0.57
1:A:161:LEU:HB2	1:A:182:LEU:HD23	1.87	0.56
2:E:232:ASP:OD2	2:E:235:THR:OG1	2.17	0.56
1:B:274:TYR:HA	1:B:297:ILE:HA	1.88	0.56
1:D:321:GLN:NE2	1:D:346:LYS:O	2.39	0.56
1:D:212:ASN:OD1	1:D:213:ASN:N	2.34	0.56
1:D:278:MET:O	1:D:281:ASN:ND2	2.38	0.56
1:A:308:TYR:CZ	1:B:337:PRO:HB3	2.41	0.56
2:E:157:ALA:HB2	2:E:209:THR:HB	1.88	0.56
1:A:98:PHE:HD2	1:A:123:SER:HB3	1.70	0.55
1:C:190:ILE:N	1:C:215:GLY:O	2.34	0.55
1:D:166:LEU:HB2	1:D:185:ASN:HD22	1.69	0.55
2:F:268:ASP:OD1	2:F:273:TRP:NE1	2.40	0.55
2:H:206:VAL:HG13	2:H:220:PHE:HB2	1.89	0.55
2:G:316:ILE:HB	2:G:321:TYR:HE2	1.71	0.55
1:B:174:PRO:HG2	1:B:177:ILE:HG12	1.89	0.55
2:H:359:ASN:OD1	2:H:359:ASN:N	2.39	0.55
1:A:270:LEU:HD23	1:A:273:LEU:HD22	1.89	0.55
1:B:136:ASP:OD1	1:B:136:ASP:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ASN:ND2	1:D:114:ASN:O	2.40	0.55
1:B:264:PRO:HG2	2:G:299:GLY:HA3	1.89	0.55
1:A:182:LEU:HB2	1:A:206:LEU:HD23	1.89	0.55
1:C:308:TYR:CZ	1:D:337:PRO:HB3	2.41	0.54
2:F:144:GLN:NE2	2:F:146:GLU:O	2.39	0.54
1:B:179:GLU:OE1	1:B:203:ARG:NH1	2.40	0.54
2:F:284:LYS:HD3	2:F:304:ALA:HA	1.89	0.54
1:C:278:MET:O	1:C:281:ASN:ND2	2.40	0.54
2:E:143:TYR:O	2:E:388:SER:N	2.40	0.54
1:A:150:PHE:HB3	1:A:174:PRO:HD3	1.89	0.54
1:D:111:LEU:HB2	1:D:135:LEU:HD23	1.89	0.54
1:D:346:LYS:HG3	1:D:347:ASP:OD2	2.08	0.54
2:E:268:ASP:OD1	2:E:273:TRP:NE1	2.39	0.54
1:B:181:ARG:HH21	1:B:203:ARG:HH12	1.56	0.54
2:G:359:ASN:OD1	2:G:359:ASN:N	2.41	0.54
1:B:229:GLU:HG2	1:B:251:LYS:HB2	1.90	0.54
1:D:244:LEU:HB2	1:D:270:LEU:HD11	1.90	0.54
1:D:51:SER:HA	1:D:74:GLY:HA3	1.89	0.54
1:B:36:ARG:HG2	1:B:47:ARG:HH21	1.73	0.53
1:D:190:ILE:HG22	1:D:220:VAL:HG21	1.89	0.53
2:E:255:TYR:H	2:E:261:SER:HB2	1.71	0.53
1:C:94:SER:OG	1:C:94:SER:O	2.25	0.53
1:B:103:PRO:HB2	1:B:106:VAL:HG23	1.90	0.53
1:B:68:ASN:O	1:B:93:ASN:HA	2.08	0.53
1:C:332:LEU:HG	1:C:345:ILE:HD12	1.90	0.53
1:D:179:GLU:OE1	1:D:203:ARG:NH1	2.42	0.53
2:E:276:TYR:HA	2:E:307:LYS:HE3	1.90	0.53
2:E:376:LEU:HG	2:E:389:LEU:HD21	1.89	0.53
1:C:56:ILE:HG21	1:C:82:LEU:HD11	1.90	0.53
1:D:150:PHE:HB2	1:D:172:GLY:O	2.08	0.53
1:B:110:HIS:HB3	1:B:112:GLN:NE2	2.24	0.53
1:B:303:ARG:HA	1:B:331:GLY:HA3	1.91	0.52
1:B:263:PRO:HG2	1:B:266:ALA:HB2	1.91	0.52
1:D:332:LEU:HG	1:D:345:ILE:HD12	1.90	0.52
1:D:238:THR:HA	1:D:258:HIS:O	2.09	0.52
1:D:76:PRO:HG2	1:D:79:LEU:HB2	1.91	0.52
2:E:376:LEU:HB2	2:E:387:TYR:HB2	1.91	0.52
2:G:242:ALA:HB2	2:G:295:LEU:HB3	1.90	0.52
1:C:47:ARG:NH1	2:G:279:GLU:OE2	2.43	0.52
2:E:205:ARG:HB2	2:E:223:GLU:HB2	1.91	0.52
1:A:231:SER:HA	1:A:253:TYR:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:HIS:HA	1:C:160:PHE:HB2	1.92	0.52
1:D:246:GLY:HA3	1:D:270:LEU:HA	1.91	0.52
1:C:122:ASP:O	1:C:126:LYS:HG2	2.10	0.52
1:C:181:ARG:HA	1:C:205:VAL:HB	1.92	0.52
1:D:156:LEU:HD23	1:D:174:PRO:HG3	1.92	0.52
2:E:229:VAL:HG13	2:E:238:LYS:HE2	1.92	0.52
1:B:147:GLU:HB2	1:D:196:GLN:NE2	2.25	0.52
1:B:170:PRO:HB2	1:B:173:LEU:HD13	1.92	0.52
1:C:82:LEU:O	1:C:103:PRO:HB3	2.10	0.52
2:G:228:ILE:HD11	2:G:263:ILE:HG21	1.91	0.52
1:D:317:ARG:HD2	1:D:348:LEU:O	2.09	0.52
1:C:112:GLN:HA	1:C:138:ASN:HD21	1.74	0.51
1:C:181:ARG:NH2	2:G:177:TYR:O	2.41	0.51
1:C:80:LYS:NZ	1:C:101:ASN:HA	2.26	0.51
1:C:239:ALA:HA	1:C:259:ILE:HG23	1.93	0.51
2:F:376:LEU:HG	2:F:389:LEU:HD21	1.93	0.51
1:A:113:GLU:H	1:A:137:ASP:HB2	1.75	0.51
1:A:335:GLN:HA	1:A:341:ARG:HG3	1.91	0.51
1:A:98:PHE:CD2	1:A:123:SER:HB3	2.46	0.50
1:C:181:ARG:HH22	2:G:177:TYR:C	2.13	0.50
1:B:264:PRO:HA	1:B:290:ILE:HG22	1.93	0.50
1:A:103:PRO:HB2	1:A:106:VAL:HG23	1.92	0.50
1:D:198:LEU:HB3	1:D:201:LEU:HB2	1.92	0.50
1:A:62:THR:HG21	1:A:87:ARG:HH21	1.77	0.50
2:E:359:ASN:OD1	2:E:359:ASN:N	2.42	0.50
1:A:163:ARG:HG2	1:B:186:ARG:NH2	2.27	0.50
2:H:157:ALA:HB2	2:H:209:THR:HB	1.94	0.50
1:C:181:ARG:NH2	1:C:203:ARG:HH12	2.10	0.50
1:C:203:ARG:HG3	1:C:229:GLU:HB2	1.93	0.50
1:C:321:GLN:NE2	1:C:346:LYS:O	2.45	0.50
1:D:317:ARG:NH2	1:D:318:ASP:OD1	2.44	0.50
2:G:147:HIS:HA	2:G:385:VAL:HG12	1.93	0.50
1:B:335:GLN:HA	1:B:341:ARG:HG3	1.93	0.50
1:D:72:ASN:HD21	1:D:96:ASP:H	1.60	0.50
2:E:278:THR:HG23	2:E:286:VAL:HG21	1.94	0.50
1:B:181:ARG:NH2	1:B:203:ARG:HH12	2.09	0.49
2:E:312:ASN:ND2	2:E:366:ALA:HA	2.26	0.49
1:C:179:GLU:HG3	1:C:203:ARG:HB3	1.93	0.49
1:C:212:ASN:OD1	1:C:213:ASN:N	2.45	0.49
1:D:103:PRO:O	1:D:106:VAL:HG23	2.13	0.49
1:D:34:VAL:HG12	1:D:47:ARG:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ASN:OD1	1:A:213:ASN:N	2.44	0.49
1:C:161:LEU:HD13	1:C:166:LEU:HD11	1.95	0.49
2:E:226:ARG:HD3	2:E:244:ILE:O	2.12	0.49
1:C:211:LEU:HB2	1:C:235:ASN:OD1	2.12	0.49
2:F:272:LEU:HB3	2:F:290:LEU:O	2.12	0.49
1:D:100:THR:HG22	1:D:123:SER:HA	1.94	0.49
1:B:175:ARG:HD2	1:D:151:ARG:NH1	2.28	0.49
1:C:312:LYS:HG2	1:D:338:GLU:HG3	1.95	0.49
1:C:159:LEU:HB3	1:C:180:LEU:HD12	1.93	0.49
1:C:215:GLY:HA2	2:H:237:ILE:HG22	1.95	0.49
2:E:375:LEU:HD13	2:E:386:LYS:HD3	1.95	0.49
2:H:155:SER:HB2	2:H:174:TRP:HE3	1.77	0.49
1:A:91:TYR:HB3	1:A:112:GLN:HG2	1.95	0.49
1:A:244:LEU:HB2	1:A:270:LEU:HD11	1.95	0.48
2:F:255:TYR:H	2:F:261:SER:HB2	1.77	0.48
2:F:370:ASN:O	2:F:374:ASN:HA	2.13	0.48
1:C:244:LEU:HB2	1:C:270:LEU:HD11	1.94	0.48
2:H:190:ASP:OD1	2:H:195:ARG:NH1	2.46	0.48
1:C:182:LEU:HB2	1:C:206:LEU:HD23	1.96	0.48
1:A:161:LEU:HD13	1:A:166:LEU:HD11	1.96	0.48
1:C:64:TYR:CE1	2:G:252:THR:HA	2.49	0.48
2:H:291:ASN:OD1	2:H:294:THR:N	2.40	0.48
1:B:302:LEU:HB3	1:B:307:TRP:HZ2	1.79	0.47
1:D:240:ALA:HB3	1:D:263:PRO:HD2	1.95	0.47
2:F:324:LYS:O	2:F:337:ASN:HB2	2.14	0.47
1:A:203:ARG:HG3	1:A:229:GLU:HB2	1.97	0.47
2:F:287:ILE:HD13	2:F:320:LEU:HD22	1.96	0.47
1:D:182:LEU:HB2	1:D:206:LEU:HD23	1.96	0.47
1:A:207:ASP:HB3	1:A:234:ARG:NH1	2.29	0.47
1:A:49:LEU:O	1:A:69:GLN:N	2.42	0.47
2:E:181:THR:HG23	2:E:201:LYS:HD3	1.95	0.47
2:G:148:LEU:HB3	2:G:192:ILE:HG12	1.96	0.47
1:A:50:THR:HG22	1:A:69:GLN:HB2	1.96	0.47
1:D:195:LEU:HB2	1:D:220:VAL:HG22	1.94	0.47
1:D:68:ASN:O	1:D:93:ASN:HA	2.15	0.47
1:A:239:ALA:HA	1:A:259:ILE:HG23	1.95	0.47
1:A:34:VAL:HG12	1:A:47:ARG:HD3	1.97	0.47
1:D:131:GLU:HA	1:D:156:LEU:HA	1.96	0.47
1:C:282:ASN:O	1:D:335:GLN:NE2	2.48	0.47
1:D:183:ASP:HB3	1:D:205:VAL:HG12	1.97	0.47
1:D:82:LEU:HB3	1:D:85:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:181:THR:HG22	2:G:201:LYS:HD3	1.97	0.47
2:G:163:LEU:HD22	2:G:215:ASP:HB2	1.97	0.47
1:A:298:THR:HG22	1:A:299:GLN:HG3	1.96	0.47
1:D:181:ARG:HA	1:D:205:VAL:HB	1.97	0.47
1:A:76:PRO:HG2	1:A:79:LEU:HB2	1.96	0.46
1:A:238:THR:HG22	1:B:304:ASN:ND2	2.30	0.46
1:D:45:ASN:HA	1:D:68:ASN:HD21	1.78	0.46
2:G:156:GLY:HA3	2:G:173:PRO:HA	1.97	0.46
2:G:287:ILE:HD13	2:G:320:LEU:HD22	1.97	0.46
1:D:274:TYR:HA	1:D:297:ILE:HA	1.97	0.46
1:C:238:THR:HG22	1:D:304:ASN:ND2	2.31	0.46
2:F:230:LYS:HD3	2:F:295:LEU:HD11	1.98	0.46
2:E:288:SER:HB3	2:E:297:ILE:HD12	1.97	0.46
2:F:312:ASN:ND2	2:F:366:ALA:HA	2.30	0.46
1:A:128:PRO:HG2	1:A:129:TYR:CE2	2.51	0.46
1:C:80:LYS:HZ3	1:C:101:ASN:HA	1.80	0.46
1:A:142:ALA:HB2	1:A:167:SER:OG	2.16	0.46
1:A:150:PHE:HB2	1:A:172:GLY:O	2.14	0.46
1:C:45:ASN:HB3	1:C:64:TYR:HB3	1.97	0.46
2:F:157:ALA:HB2	2:F:209:THR:HB	1.98	0.46
1:A:70:ILE:O	1:A:93:ASN:HB3	2.16	0.46
1:D:122:ASP:O	1:D:126:LYS:HG2	2.16	0.46
1:A:228:THR:O	1:A:249:LEU:HD12	2.16	0.46
1:B:136:ASP:O	1:B:138:ASN:ND2	2.49	0.46
1:B:182:LEU:HD12	1:B:206:LEU:HD21	1.97	0.46
1:C:121:TYR:HA	1:C:149:ALA:HA	1.98	0.46
2:E:276:TYR:HE2	2:E:278:THR:HG22	1.81	0.46
1:C:181:ARG:NH2	2:G:178:ARG:HG3	2.31	0.46
1:C:349:ASN:O	1:C:349:ASN:ND2	2.48	0.46
2:H:144:GLN:HG2	2:H:387:TYR:CE1	2.51	0.46
1:B:239:ALA:HA	1:B:259:ILE:HG23	1.98	0.45
1:C:136:ASP:HA	1:C:162:SER:O	2.15	0.45
2:F:228:ILE:HD11	2:F:263:ILE:HG21	1.98	0.45
1:B:232:LEU:HB2	1:B:254:LEU:HD23	1.97	0.45
1:A:136:ASP:OD1	2:E:224:ARG:NH2	2.49	0.45
2:E:248:ASN:HB3	2:E:252:THR:HB	1.98	0.45
2:F:252:THR:O	2:F:308:ARG:NH1	2.49	0.45
1:B:262:VAL:O	1:B:287:PRO:HG2	2.16	0.45
1:B:298:THR:HG22	1:B:299:GLN:HG3	1.98	0.45
1:B:64:TYR:CE1	2:F:252:THR:HA	2.52	0.45
2:H:251:ASP:N	2:H:262:ASP:OD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:182:LEU:HD22	2:F:218:LEU:HD22	1.97	0.45
2:E:238:LYS:HG2	2:E:240:GLY:H	1.82	0.45
2:E:226:ARG:HG3	2:E:243:ILE:HG23	1.99	0.45
1:A:136:ASP:HA	1:A:162:SER:O	2.16	0.45
1:D:136:ASP:OD1	1:D:136:ASP:N	2.46	0.45
1:B:196:GLN:NE2	1:D:147:GLU:HB2	2.32	0.45
2:F:249:TYR:HA	2:F:262:ASP:CB	2.46	0.45
1:D:115:ASN:OD1	1:D:117:ARG:NH1	2.50	0.45
2:F:226:ARG:HG3	2:F:243:ILE:HG23	1.98	0.45
2:F:359:ASN:OD1	2:F:359:ASN:N	2.50	0.45
1:B:169:ILE:HD12	1:B:190:ILE:HG23	1.98	0.45
1:C:175:ARG:HG2	1:C:197:GLY:O	2.17	0.45
1:D:121:TYR:HD1	1:D:148:GLY:O	2.00	0.45
2:E:258:GLY:O	2:E:261:SER:OG	2.25	0.45
2:F:181:THR:HG22	2:F:201:LYS:HD3	1.98	0.45
1:D:229:GLU:HG2	1:D:251:LYS:HB2	1.99	0.45
2:F:147:HIS:HE2	2:F:383:HIS:CD2	2.34	0.44
1:A:312:LYS:CB	1:B:338:GLU:HG3	2.47	0.44
1:D:192:SER:HB2	1:D:193:PRO:HD3	1.99	0.44
1:D:209:ASN:O	1:D:235:ASN:HA	2.18	0.44
1:D:207:ASP:HB3	1:D:234:ARG:NH1	2.33	0.44
2:E:339:ILE:O	2:E:353:VAL:HG23	2.17	0.44
2:F:155:SER:HB2	2:F:174:TRP:CE3	2.52	0.44
2:F:255:TYR:CE2	2:F:312:ASN:HA	2.52	0.44
2:H:182:LEU:HD22	2:H:218:LEU:HD22	1.99	0.44
1:D:166:LEU:HB3	1:D:187:ILE:HD11	1.99	0.44
2:E:338:LYS:HD3	2:E:355:VAL:O	2.17	0.44
1:B:154:ASN:O	1:B:176:THR:HG21	2.17	0.44
1:D:134:HIS:HA	1:D:160:PHE:HB2	2.00	0.44
2:H:376:LEU:HG	2:H:389:LEU:HD21	1.99	0.44
1:A:154:ASN:O	1:A:176:THR:HG21	2.17	0.44
1:B:164:ASN:HB3	1:B:165:HIS:H	1.70	0.44
1:B:111:LEU:HB2	1:B:135:LEU:HD23	1.99	0.44
1:C:154:ASN:O	1:C:176:THR:HG21	2.17	0.44
2:F:163:LEU:HD22	2:F:215:ASP:HB2	1.99	0.44
2:G:136:PRO:HD2	2:G:317:CYS:SG	2.58	0.44
2:H:254:PRO:HD2	2:H:308:ARG:NH1	2.32	0.44
1:A:321:GLN:NE2	1:A:346:LYS:O	2.51	0.44
1:A:71:ASN:HB3	1:A:94:SER:OG	2.17	0.44
1:A:317:ARG:NH2	1:A:318:ASP:OD1	2.51	0.44
1:A:98:PHE:HA	1:A:99:PRO:HD3	1.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ASN:O	1:B:47:ARG:NH1	2.51	0.44
1:C:143:VAL:HG21	2:H:227:ASN:ND2	2.31	0.44
1:B:193:PRO:HB2	1:D:171:TRP:CE3	2.53	0.44
1:D:287:PRO:HD2	1:D:290:ILE:HD13	2.00	0.44
1:D:335:GLN:HA	1:D:341:ARG:HG3	2.00	0.44
2:F:242:ALA:HB2	2:F:295:LEU:HB3	2.00	0.44
2:H:291:ASN:HB2	2:H:298:GLU:CD	2.38	0.44
1:B:159:LEU:HB3	1:B:180:LEU:HD12	2.00	0.44
1:C:111:LEU:HB2	1:C:135:LEU:HD23	1.99	0.44
2:E:177:TYR:HA	2:E:223:GLU:OE2	2.17	0.44
2:H:155:SER:HB2	2:H:174:TRP:CE3	2.53	0.44
2:H:268:ASP:OD1	2:H:273:TRP:NE1	2.51	0.44
1:C:161:LEU:HB2	1:C:182:LEU:HD23	2.00	0.43
2:H:377:TYR:CE2	2:H:386:LYS:HE2	2.51	0.43
1:D:112:GLN:H	1:D:112:GLN:CD	2.21	0.43
1:B:177:ILE:HG22	1:B:201:LEU:HD13	2.00	0.43
2:G:153:HIS:O	2:G:382:TYR:HA	2.18	0.43
2:G:284:LYS:HD3	2:G:304:ALA:HA	1.99	0.43
2:E:316:ILE:HB	2:E:321:TYR:CE2	2.45	0.43
1:A:195:LEU:HD12	1:A:220:VAL:HG22	2.00	0.43
1:C:264:PRO:HA	1:C:290:ILE:HG22	2.00	0.43
1:A:267:PHE:HB3	1:A:294:LEU:HD21	1.99	0.43
1:D:64:TYR:CE1	2:H:252:THR:HA	2.53	0.43
2:G:257:TRP:HB2	2:G:363:TYR:CZ	2.53	0.43
2:E:184:GLU:HB3	2:E:198:THR:HG22	2.01	0.43
2:E:325:SER:OG	2:E:364:ILE:HD12	2.19	0.43
1:A:190:ILE:HD11	1:A:211:LEU:HD11	1.99	0.43
2:G:170:TYR:HB3	2:G:182:LEU:HD11	2.01	0.43
1:A:259:ILE:HG22	1:A:283:LEU:HD21	2.00	0.43
1:C:103:PRO:O	1:C:106:VAL:HG23	2.18	0.43
1:C:271:ARG:HG2	1:C:293:ASP:O	2.19	0.43
1:A:64:TYR:CE1	2:E:252:THR:HA	2.53	0.43
2:F:301:TRP:HD1	2:F:348:SER:HG	1.64	0.43
2:H:228:ILE:HD12	2:H:265:LEU:HD11	2.01	0.43
1:B:238:THR:HA	1:B:258:HIS:O	2.19	0.43
1:B:45:ASN:ND2	1:B:46:ASP:OD1	2.44	0.43
1:C:142:ALA:HB2	1:C:167:SER:OG	2.19	0.43
1:C:195:LEU:HD12	1:C:220:VAL:HG22	2.00	0.43
2:F:226:ARG:HB3	2:F:249:TYR:CD1	2.54	0.43
2:H:253:SER:O	2:H:307:LYS:HD3	2.18	0.43
1:A:263:PRO:HG2	1:A:266:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LYS:HD3	1:A:84:LYS:HA	1.80	0.42
1:A:94:SER:OG	1:A:94:SER:O	2.27	0.42
1:D:265:ASN:ND2	2:E:297:ILE:O	2.52	0.42
1:A:179:GLU:HG2	1:A:180:LEU:N	2.34	0.42
1:D:256:ASP:OD2	1:D:256:ASP:N	2.51	0.42
2:E:276:TYR:CE2	2:E:278:THR:HG22	2.54	0.42
2:G:312:ASN:ND2	2:G:366:ALA:HA	2.33	0.42
1:C:71:ASN:HB3	1:C:94:SER:O	2.20	0.42
2:H:339:ILE:O	2:H:353:VAL:HG23	2.19	0.42
1:A:252:LEU:HD23	1:A:276:LEU:HD13	2.02	0.42
1:B:134:HIS:HA	1:B:160:PHE:HB2	2.00	0.42
1:A:92:HIS:HA	1:A:113:GLU:O	2.20	0.42
1:B:72:ASN:ND2	1:B:97:GLU:HG2	2.34	0.42
1:D:154:ASN:O	1:D:176:THR:HG21	2.19	0.42
1:D:262:VAL:O	1:D:287:PRO:HG2	2.19	0.42
2:F:170:TYR:CE2	2:F:213:VAL:HG11	2.54	0.42
1:A:112:GLN:CD	1:A:112:GLN:H	2.23	0.42
1:A:48:PHE:HA	1:A:69:GLN:OE1	2.19	0.42
1:B:110:HIS:CE1	1:B:134:HIS:CD2	3.07	0.42
1:C:112:GLN:HA	1:C:136:ASP:O	2.20	0.42
1:C:150:PHE:HB3	1:C:174:PRO:HD3	2.01	0.42
1:D:150:PHE:HB3	1:D:174:PRO:HD3	2.02	0.42
1:D:271:ARG:NH2	1:D:293:ASP:OD2	2.53	0.42
2:F:339:ILE:O	2:F:353:VAL:HG23	2.20	0.42
2:H:207:ASP:CG	2:H:223:GLU:HA	2.40	0.42
1:A:278:MET:O	1:A:281:ASN:ND2	2.52	0.42
1:B:151:ARG:NH1	1:D:175:ARG:HD2	2.33	0.42
1:C:317:ARG:O	1:C:321:GLN:HG2	2.19	0.42
1:D:170:PRO:HB2	1:D:173:LEU:HD13	2.01	0.42
2:E:144:GLN:HG3	2:E:145:SER:N	2.33	0.42
1:B:112:GLN:HG3	2:F:224:ARG:HD3	2.02	0.42
1:A:112:GLN:HA	1:A:136:ASP:O	2.20	0.42
1:A:308:TYR:HB2	1:B:336:ALA:HB1	2.00	0.42
1:B:98:PHE:HA	1:B:99:PRO:HD3	1.80	0.42
1:D:207:ASP:OD1	1:D:231:SER:OG	2.29	0.42
2:G:226:ARG:HD3	2:G:244:ILE:O	2.19	0.42
2:G:261:SER:O	2:G:307:LYS:NZ	2.38	0.42
2:G:324:LYS:O	2:G:337:ASN:HB2	2.20	0.42
1:A:110:HIS:HB3	1:A:112:GLN:NE2	2.35	0.41
1:A:170:PRO:HB2	1:A:173:LEU:HD13	2.01	0.41
1:B:300:LEU:HB3	1:B:329:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:TYR:HE1	2:E:249:TYR:CE2	2.37	0.41
2:F:344:ASN:O	2:F:348:SER:N	2.53	0.41
2:G:316:ILE:HB	2:G:321:TYR:CE2	2.53	0.41
1:A:201:LEU:HD23	1:A:224:LEU:HD13	2.02	0.41
1:C:181:ARG:HG2	1:C:205:VAL:HG21	2.02	0.41
1:C:246:GLY:HA3	1:C:269:TYR:O	2.19	0.41
1:D:98:PHE:HA	1:D:99:PRO:HD3	1.69	0.41
2:F:303:THR:HG22	2:F:343:TYR:CD2	2.56	0.41
1:C:242:VAL:HG12	1:C:266:ALA:HA	2.02	0.41
1:C:316:VAL:O	1:C:320:LEU:HG	2.21	0.41
2:F:254:PRO:HD2	2:F:308:ARG:NH1	2.36	0.41
2:F:230:LYS:HB2	2:F:295:LEU:HD21	2.02	0.41
2:H:207:ASP:N	2:H:221:ASN:O	2.43	0.41
1:A:188:SER:HA	1:A:210:LEU:O	2.20	0.41
1:A:182:LEU:HD12	1:A:206:LEU:HD21	2.02	0.41
1:D:126:LYS:HD3	1:D:126:LYS:HA	1.80	0.41
2:G:370:ASN:OD1	2:G:372:ARG:HB3	2.21	0.41
2:H:226:ARG:HD3	2:H:244:ILE:O	2.19	0.41
1:A:212:ASN:O	1:A:216:LEU:HD13	2.21	0.41
1:C:98:PHE:HA	1:C:99:PRO:HD3	1.83	0.41
1:D:205:VAL:HA	1:D:231:SER:HB3	2.02	0.41
1:C:282:ASN:ND2	1:D:306:PRO:HD3	2.35	0.41
1:A:150:PHE:CB	1:A:174:PRO:HD3	2.50	0.41
1:C:136:ASP:O	1:C:138:ASN:ND2	2.52	0.41
1:D:263:PRO:HA	1:D:264:PRO:HD2	1.81	0.41
1:D:45:ASN:HB2	1:D:66:GLN:HG2	2.03	0.41
2:E:135:CYS:HA	2:E:136:PRO:HD3	1.89	0.41
1:C:174:PRO:HG2	1:C:177:ILE:HG12	2.02	0.41
1:A:262:VAL:HA	1:A:263:PRO:HD2	1.93	0.41
1:C:262:VAL:O	1:C:287:PRO:HG2	2.21	0.41
1:A:251:LYS:HD2	1:A:253:TYR:OH	2.21	0.41
1:B:320:LEU:HD13	1:B:346:LYS:HB3	2.02	0.41
1:C:190:ILE:HD11	1:C:211:LEU:HD11	2.03	0.41
2:F:210:GLY:CA	2:F:264:ASP:HA	2.48	0.41
2:G:170:TYR:CD2	2:G:213:VAL:HG21	2.56	0.41
2:H:150:GLU:HG3	2:H:383:HIS:CD2	2.55	0.41
1:B:112:GLN:HA	1:B:138:ASN:HD21	1.85	0.41
1:C:166:LEU:HD12	1:C:185:ASN:ND2	2.36	0.41
2:F:154:GLN:HB2	2:F:382:TYR:CZ	2.56	0.41
2:G:134:LEU:HD23	2:G:134:LEU:HA	1.93	0.41
2:G:357:PHE:HA	2:G:358:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:156:GLY:HA3	2:H:173:PRO:HA	2.02	0.41
1:D:135:LEU:O	1:D:138:ASN:ND2	2.54	0.41
2:F:142:VAL:O	2:F:358:PRO:HD3	2.21	0.41
2:F:241:GLU:N	2:F:295:LEU:HD13	2.36	0.41
2:F:287:ILE:HG13	2:F:301:TRP:HB2	2.03	0.41
1:A:82:LEU:HB3	1:A:85:VAL:HG23	2.02	0.40
1:B:118:THR:HA	1:B:144:SER:O	2.20	0.40
1:C:91:TYR:HB2	1:C:112:GLN:HG2	2.03	0.40
2:H:203:PRO:HG3	2:H:238:LYS:HB2	2.01	0.40
1:D:64:TYR:OH	2:H:251:ASP:O	2.30	0.40
2:H:142:VAL:O	2:H:358:PRO:HD3	2.21	0.40
1:B:150:PHE:HB2	1:B:172:GLY:O	2.22	0.40
1:D:207:ASP:HA	1:D:233:VAL:O	2.21	0.40
2:G:375:LEU:HD13	2:G:386:LYS:HD3	2.03	0.40
1:C:333:MET:HG2	1:C:344:ALA:HA	2.03	0.40
1:C:90:LEU:O	1:C:93:ASN:ND2	2.52	0.40
2:E:168:LYS:HA	2:E:185:TYR:O	2.22	0.40
2:G:154:GLN:O	2:G:379:TRP:NE1	2.53	0.40
1:D:206:LEU:HB2	1:D:232:LEU:HD23	2.03	0.40
2:F:380:ASN:O	2:F:383:HIS:HB2	2.20	0.40
1:A:126:LYS:HD3	1:A:126:LYS:HA	1.88	0.40
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.93	0.40
1:C:47:ARG:HB2	1:C:49:LEU:HD13	2.04	0.40
2:G:251:ASP:N	2:G:262:ASP:OD1	2.52	0.40
2:H:363:TYR:HB2	2:H:381:ASN:ND2	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:TYR:OH	1:C:147:GLU:O[4_565]	2.12	0.08

## 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	319/333 (96%)	296 (93%)	23 (7%)	0	100	100
1	B	319/333 (96%)	298 (93%)	21 (7%)	0	100	100
1	C	319/333 (96%)	295 (92%)	24 (8%)	0	100	100
1	D	319/333 (96%)	294 (92%)	25 (8%)	0	100	100
2	E	243/261 (93%)	229 (94%)	14 (6%)	0	100	100
2	F	243/261 (93%)	228 (94%)	15 (6%)	0	100	100
2	G	243/261 (93%)	227 (93%)	16 (7%)	0	100	100
2	H	243/261 (93%)	228 (94%)	15 (6%)	0	100	100
All	All	2248/2376 (95%)	2095 (93%)	153 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 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	296/306 (97%)	291 (98%)	5 (2%)	66	88
1	B	296/306 (97%)	291 (98%)	5 (2%)	66	88
1	C	296/306 (97%)	290 (98%)	6 (2%)	60	85
1	D	296/306 (97%)	290 (98%)	6 (2%)	60	85
2	E	219/230 (95%)	215 (98%)	4 (2%)	64	87
2	F	219/230 (95%)	215 (98%)	4 (2%)	64	87
2	G	219/230 (95%)	218 (100%)	1 (0%)	91	97
2	H	219/230 (95%)	215 (98%)	4 (2%)	64	87
All	All	2060/2144 (96%)	2025 (98%)	35 (2%)	66	88

All (35) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	31	CYS
1	A	46	ASP
1	A	152	ASP
1	A	173	LEU
1	A	274	TYR
1	B	136	ASP
1	B	152	ASP
1	B	173	LEU
1	B	199	THR
1	B	274	TYR
1	C	46	ASP
1	C	69	GLN
1	C	71	ASN
1	C	136	ASP
1	C	173	LEU
1	C	274	TYR
1	D	46	ASP
1	D	136	ASP
1	D	152	ASP
1	D	173	LEU
1	D	199	THR
1	D	274	TYR
2	E	181	THR
2	E	211	PHE
2	E	287	ILE
2	E	359	ASN
2	F	144	GLN
2	F	212	VAL
2	F	359	ASN
2	F	383	HIS
2	G	359	ASN
2	H	144	GLN
2	H	179	THR
2	H	211	PHE
2	H	359	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	HIS
1	D	72	ASN
1	D	138	ASN
2	F	144	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](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	NAG	A	901	1	14,14,15	0.50	0	15,19,21	0.52	0
3	NAG	B	901	1	14,14,15	0.52	0	15,19,21	0.44	0
3	NAG	C	901	1	14,14,15	0.75	1 (7%)	15,19,21	0.74	0
3	NAG	D	901	1	14,14,15	0.91	1 (7%)	15,19,21	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	901	1	-	0/6/23/26	0/1/1/1
3	NAG	B	901	1	-	0/6/23/26	0/1/1/1
3	NAG	C	901	1	-	0/6/23/26	0/1/1/1
3	NAG	D	901	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	NAG	C1-C2	2.26	1.55	1.52
3	D	901	NAG	C1-C2	3.03	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	321/333 (96%)	0.46	13 (4%) 39 28	52, 119, 208, 276	0
1	B	321/333 (96%)	0.32	6 (1%) 67 53	61, 111, 175, 250	0
1	C	321/333 (96%)	0.73	31 (9%) 8 7	50, 134, 211, 263	0
1	D	321/333 (96%)	0.42	9 (2%) 53 40	47, 110, 184, 261	0
2	E	247/261 (94%)	0.38	6 (2%) 59 45	59, 102, 162, 219	0
2	F	247/261 (94%)	0.54	17 (6%) 18 13	67, 116, 178, 307	0
2	G	247/261 (94%)	0.42	9 (3%) 43 32	56, 112, 177, 224	0
2	H	247/261 (94%)	0.73	28 (11%) 6 5	67, 116, 183, 262	0
All	All	2272/2376 (95%)	0.50	119 (5%) 28 20	47, 114, 189, 307	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	356	PRO	6.9
2	H	359	ASN	6.1
1	A	288	GLN	6.0
1	C	40	GLY	5.3
1	C	54	THR	4.9
2	F	359	ASN	4.9
1	C	336	ALA	4.9
1	C	262	VAL	4.8
1	C	276	LEU	4.7
1	A	345	ILE	4.7
2	H	366	ALA	4.6
1	C	261	ARG	4.5
2	G	141	GLY	4.4
2	G	349	LYS	4.2
1	D	285	ASN	4.1
1	A	276	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	287	PRO	4.1
2	F	183	THR	4.0
2	F	351	SER	3.9
2	E	181	THR	3.8
1	C	345	ILE	3.8
2	H	352	LEU	3.7
1	A	287	PRO	3.7
2	H	214	TYR	3.6
1	C	285	ASN	3.5
2	G	142	VAL	3.5
1	D	345	ILE	3.5
2	H	365	ALA	3.4
2	F	352	LEU	3.4
1	C	221	PHE	3.3
2	F	314	PHE	3.3
1	D	129	TYR	3.2
1	C	252	LEU	3.1
1	C	299	GLN	3.1
2	H	209	THR	3.0
1	C	62	THR	3.0
2	H	351	SER	3.0
1	A	221	PHE	3.0
1	D	331	GLY	3.0
1	C	300	LEU	2.9
1	A	186	ARG	2.9
1	B	275	ARG	2.9
2	F	139	LEU	2.9
2	H	357	PHE	2.9
1	C	329	VAL	2.9
2	F	180	ASP	2.9
1	C	348	LEU	2.8
2	H	150	GLU	2.8
1	A	301	ILE	2.8
2	H	353	VAL	2.8
2	H	342	ILE	2.8
2	F	184	GLU	2.7
1	C	87	ARG	2.7
1	C	61	THR	2.7
2	H	385	VAL	2.7
2	H	244	ILE	2.7
1	D	107	LYS	2.6
2	F	323	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	258	GLY	2.6
2	E	356	PRO	2.6
2	F	322	VAL	2.6
1	C	337	PRO	2.5
2	H	142	VAL	2.5
2	F	174	TRP	2.5
2	F	285	ILE	2.5
2	H	256	ARG	2.5
1	A	278	MET	2.5
2	G	321	TYR	2.4
2	F	263	ILE	2.4
1	D	273	LEU	2.4
1	B	58	GLU	2.4
1	A	267	PHE	2.4
2	H	355	VAL	2.4
1	D	86	GLU	2.4
1	C	325	VAL	2.4
1	B	250	ARG	2.3
2	F	341	TYR	2.3
2	H	311	SER	2.3
2	F	385	VAL	2.3
1	C	286	LEU	2.3
1	C	275	ARG	2.3
1	C	284	SER	2.3
2	E	157	ALA	2.3
2	G	389	LEU	2.3
2	H	243	ILE	2.3
2	H	358	PRO	2.3
1	C	335	GLN	2.3
2	G	342	ILE	2.3
2	G	373	ASP	2.3
2	H	151	SER	2.3
1	A	88	ILE	2.2
1	C	260	ASN	2.2
1	B	108	GLU	2.2
1	A	289	GLY	2.2
1	C	251	LYS	2.2
1	B	276	LEU	2.2
2	H	257	TRP	2.2
1	D	159	LEU	2.2
2	H	267	VAL	2.1
1	C	129	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	142	VAL	2.1
2	H	320	LEU	2.1
2	F	209	THR	2.1
2	F	365	ALA	2.1
2	H	168	LYS	2.1
1	C	312	LYS	2.1
2	G	343	TYR	2.1
1	C	30	SER	2.1
2	E	355	VAL	2.1
1	C	42	ILE	2.1
2	H	387	TYR	2.1
1	A	232	LEU	2.1
1	C	76	PRO	2.0
2	E	158	TRP	2.0
2	G	378	VAL	2.0
1	B	229	GLU	2.0
1	A	256	ASP	2.0
2	H	386	LYS	2.0
1	D	42	ILE	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](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(Å <sup>2</sup> )	Q<0.9
4	CA	F	401	1/1	0.98	0.07	-1.96	124,124,124,124	0
4	CA	G	401	1/1	0.93	0.09	-1.99	98,98,98,98	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	E	401	1/1	0.95	0.14	-2.52	133,133,133,133	0
4	CA	H	401	1/1	0.97	0.10	-2.73	188,188,188,188	0
3	NAG	A	901	14/15	0.83	0.26	-	135,141,145,146	0
3	NAG	C	901	14/15	0.86	0.19	-	88,103,107,107	0
3	NAG	B	901	14/15	0.84	0.24	-	103,120,123,125	0
3	NAG	D	901	14/15	0.86	0.24	-	85,101,110,110	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.