



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:15 PM BST

PDB ID : 6JBU  
Title : High resolution crystal structure of human FLRT3 LRR domain in complex with mouse C1RL3 Olfactomedin like domain  
Authors : Liu, H.; Li, Z.; Xu, F.  
Deposited on : 2019-01-26  
Resolution : 1.85 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

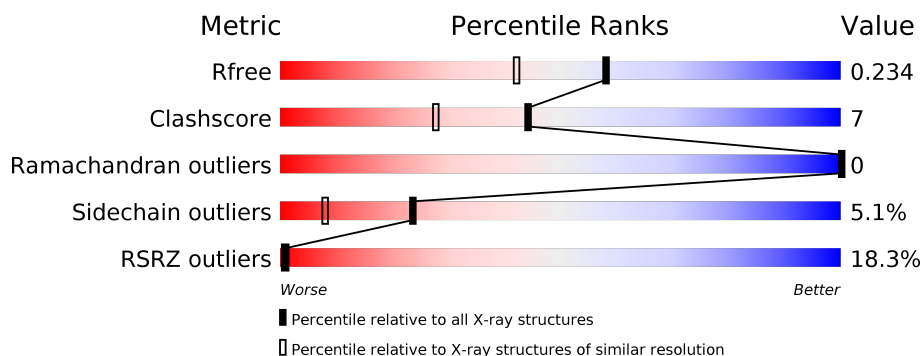
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 respectively. 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	276	<div> <div>2%</div> <div>85%</div> <div>10%</div> <div>5%</div> </div>
2	B	347	<div> <div>29%</div> <div>72%</div> <div>17%</div> <div>7%</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
6	NAG	B	402	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5137 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 Adhesion G protein-coupled receptor L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2124	1356	353	410	5			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	ALA	-	expression tag	UNP Q80TS3
A	197	PRO	-	expression tag	UNP Q80TS3
A	198	GLY	-	expression tag	UNP Q80TS3
A	199	ASP	-	expression tag	UNP Q80TS3
A	200	PRO	-	expression tag	UNP Q80TS3
A	201	ARG	-	expression tag	UNP Q80TS3
A	202	GLU	-	expression tag	UNP Q80TS3
A	462	ALA	-	expression tag	UNP Q80TS3
A	463	ALA	-	expression tag	UNP Q80TS3
A	464	ALA	-	expression tag	UNP Q80TS3
A	465	HIS	-	expression tag	UNP Q80TS3
A	466	HIS	-	expression tag	UNP Q80TS3
A	467	HIS	-	expression tag	UNP Q80TS3
A	468	HIS	-	expression tag	UNP Q80TS3
A	469	HIS	-	expression tag	UNP Q80TS3
A	470	HIS	-	expression tag	UNP Q80TS3
A	471	HIS	-	expression tag	UNP Q80TS3

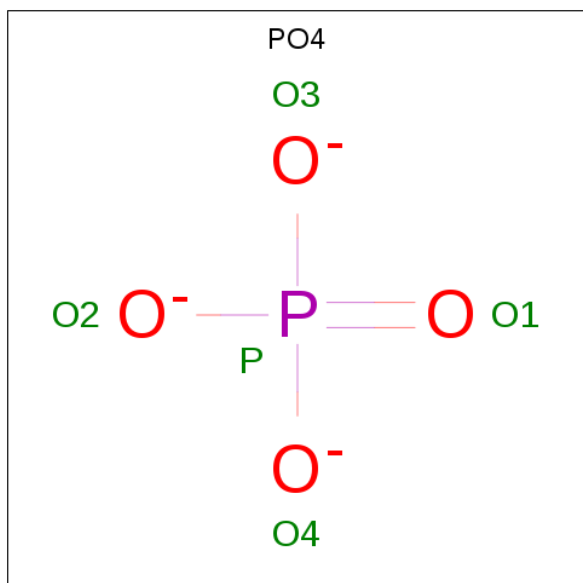
- Molecule 2 is a protein called Leucine-rich repeat transmembrane protein FLRT3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	322	Total	C	N	O	S	0	0	0
			2584	1634	456	483	11			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	ALA	-	expression tag	UNP Q9NZU0
B	23	PRO	-	expression tag	UNP Q9NZU0
B	24	GLY	-	expression tag	UNP Q9NZU0
B	25	ASP	-	expression tag	UNP Q9NZU0
B	26	PRO	-	expression tag	UNP Q9NZU0
B	27	ARG	-	expression tag	UNP Q9NZU0
B	28	GLU	-	expression tag	UNP Q9NZU0
B	359	ALA	-	expression tag	UNP Q9NZU0
B	360	ALA	-	expression tag	UNP Q9NZU0
B	361	ALA	-	expression tag	UNP Q9NZU0
B	362	HIS	-	expression tag	UNP Q9NZU0
B	363	HIS	-	expression tag	UNP Q9NZU0
B	364	HIS	-	expression tag	UNP Q9NZU0
B	365	HIS	-	expression tag	UNP Q9NZU0
B	366	HIS	-	expression tag	UNP Q9NZU0
B	367	HIS	-	expression tag	UNP Q9NZU0
B	368	HIS	-	expression tag	UNP Q9NZU0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

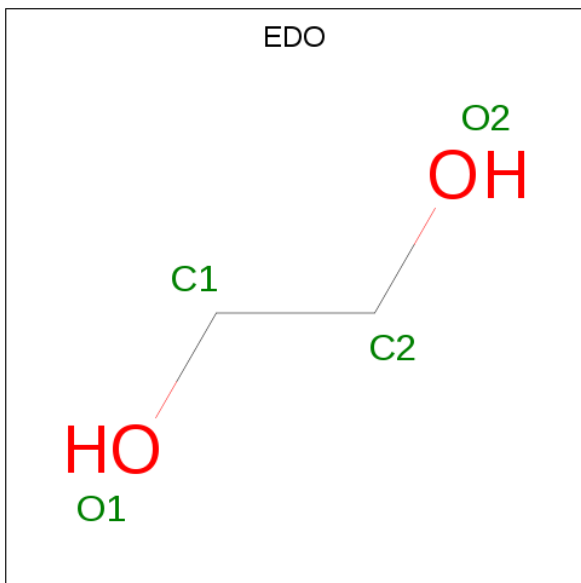


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

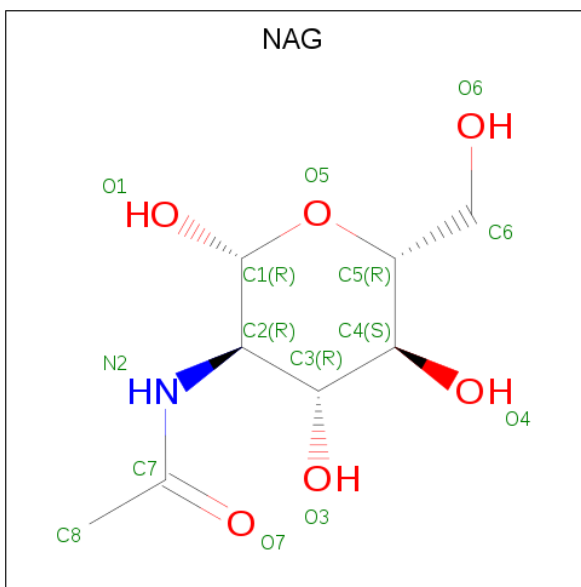
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Na	0	0
			3	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

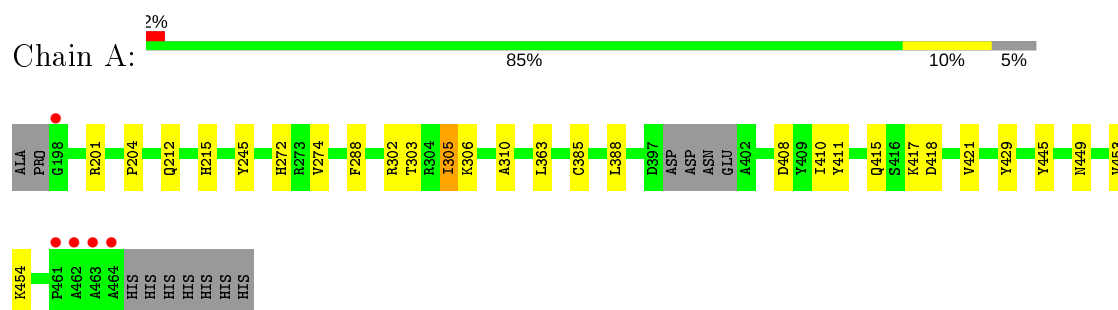
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	255	Total	O	0	0
			255	255		
7	B	117	Total	O	0	0
			117	117		

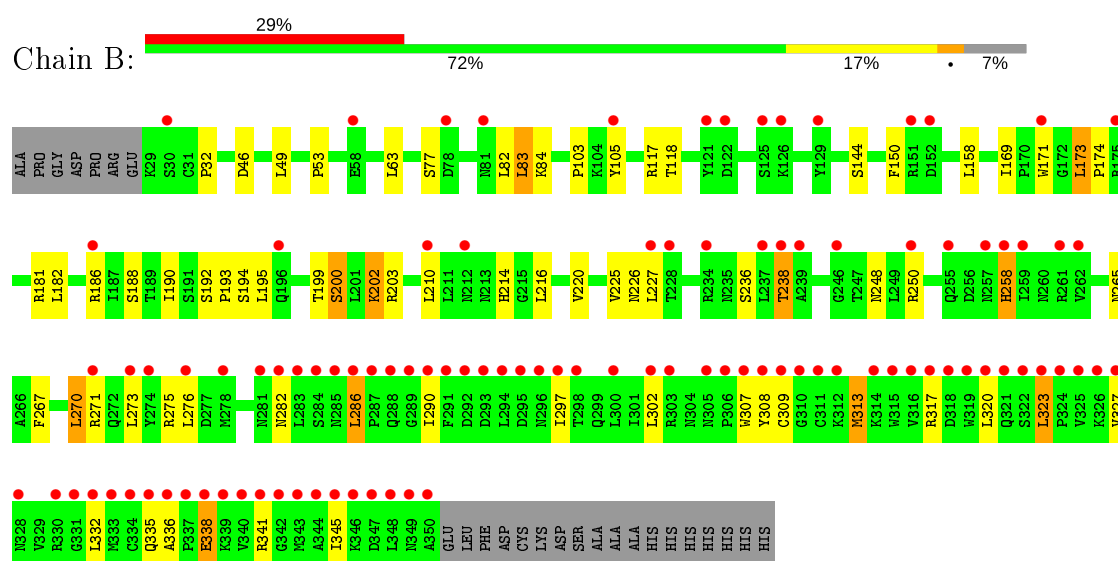
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Adhesion G protein-coupled receptor L3



- Molecule 2: Leucine-rich repeat transmembrane protein FLRT3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.14Å 121.14Å 83.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.40 – 1.85 44.40 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.40-1.85) 99.6 (44.40-1.85)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.14 _3260: ???)	Depositor
R, $R_{free}$	0.208 , 0.234 0.208 , 0.234	Depositor DCC
$R_{free}$ test set	2964 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 60.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5137	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PO4, NAG, EDO

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	0.57	0/2183	0.72	0/2974
2	B	0.40	0/2636	0.57	0/3585
All	All	0.48	0/4819	0.64	0/6559

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

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	2124	0	2014	18	0
2	B	2584	0	2590	44	0
3	A	10	0	0	0	0
4	A	3	0	0	0	0
5	A	16	0	24	3	0
6	B	28	0	26	0	0
7	A	255	0	0	3	0
7	B	117	0	0	6	0
All	All	5137	0	4654	62	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 7.

All (62) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:SER:HA	2:B:258:HIS:CE1	2.16	0.80
2:B:190:ILE:HG22	2:B:220:VAL:HG21	1.65	0.79
2:B:190:ILE:CG2	2:B:220:VAL:HG21	2.18	0.73
1:A:445:TYR:CE2	1:A:454:LYS:HE2	2.26	0.70
2:B:83:LEU:HG	2:B:105:TYR:HE1	1.59	0.68
2:B:273:LEU:HG	7:B:583:HOH:O	1.94	0.68
2:B:286:LEU:HG	2:B:290:ILE:HD11	1.76	0.67
1:A:306:LYS:HD3	5:A:507:EDO:H22	1.81	0.62
2:B:192:SER:N	2:B:193:PRO:HD2	2.14	0.62
2:B:302:LEU:HD12	2:B:332:LEU:HD11	1.80	0.62
2:B:238:THR:HB	7:B:559:HOH:O	1.99	0.61
1:A:305:ILE:HG13	5:A:506:EDO:H11	1.81	0.61
2:B:267:PHE:HA	2:B:270:LEU:HD22	1.84	0.60
2:B:199:THR:O	2:B:226:ASN:HB2	2.02	0.59
1:A:310:ALA:HB2	1:A:363:LEU:HB3	1.84	0.58
2:B:150:PHE:HB3	2:B:174:PRO:HG3	1.86	0.57
2:B:320:LEU:HD11	2:B:332:LEU:HD22	1.86	0.56
1:A:201:ARG:HD3	7:A:619:HOH:O	2.05	0.55
1:A:272:HIS:NE2	5:A:507:EDO:H21	2.21	0.55
2:B:273:LEU:HD21	2:B:276:LEU:HB2	1.89	0.55
2:B:286:LEU:HD13	2:B:307:TRP:HZ3	1.71	0.54
2:B:286:LEU:H	2:B:313:MET:HE1	1.72	0.54
2:B:297:ILE:CD1	7:B:583:HOH:O	2.58	0.51
1:A:204:PRO:HD2	1:A:385:CYS:SG	2.51	0.51
2:B:248:ASN:O	2:B:250:ARG:NH1	2.44	0.51
2:B:202:LYS:HA	2:B:227:LEU:HA	1.93	0.50
2:B:200:SER:O	2:B:202:LYS:HD2	2.12	0.50
1:A:215:HIS:HA	1:A:453:VAL:HG12	1.93	0.49
2:B:190:ILE:HG22	2:B:220:VAL:CG2	2.41	0.48
2:B:32:PRO:HB3	2:B:53:PRO:HB2	1.96	0.48
2:B:338:GLU:H	2:B:338:GLU:HG2	1.39	0.47
1:A:408:ASP:HA	1:A:421:VAL:O	2.16	0.46
1:A:201:ARG:HD2	7:A:631:HOH:O	2.16	0.46
2:B:297:ILE:HD13	7:B:583:HOH:O	2.14	0.45
2:B:265:ASN:N	2:B:265:ASN:OD1	2.44	0.45
2:B:117:ARG:O	2:B:144:SER:HB3	2.17	0.45
2:B:302:LEU:HB3	2:B:307:TRP:HZ2	1.82	0.45
2:B:323:LEU:HD12	2:B:327:VAL:HB	1.98	0.44
2:B:82:LEU:O	2:B:103:PRO:HB3	2.17	0.44
1:A:305:ILE:HD11	7:A:835:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ARG:HA	1:A:302:ARG:HD3	1.76	0.44
1:A:429:TYR:HB3	1:A:449:ASN:HB3	2.00	0.43
2:B:190:ILE:HG21	2:B:220:VAL:HG21	1.99	0.43
2:B:171:TRP:CD1	2:B:194:SER:HB3	2.53	0.43
1:A:274:VAL:HG22	1:A:288:PHE:CD2	2.54	0.43
2:B:169:ILE:HG12	2:B:182:LEU:HD13	2.01	0.43
2:B:275:ARG:NH2	7:B:508:HOH:O	2.46	0.42
2:B:181:ARG:HH21	2:B:203:ARG:HH22	1.66	0.42
2:B:195:LEU:HD12	2:B:220:VAL:HG22	2.00	0.42
2:B:286:LEU:N	2:B:313:MET:HE1	2.34	0.42
1:A:303:THR:OG1	1:A:305:ILE:HG22	2.20	0.42
2:B:335:GLN:HA	2:B:341:ARG:HG3	2.02	0.41
2:B:118:THR:HA	2:B:144:SER:HB3	2.02	0.41
2:B:236:SER:HA	2:B:258:HIS:NE2	2.36	0.41
1:A:388:LEU:O	1:A:410:ILE:HA	2.21	0.41
2:B:173:LEU:HA	2:B:173:LEU:HD12	1.86	0.41
2:B:188:SER:HA	2:B:210:LEU:O	2.20	0.41
2:B:309:CYS:SG	2:B:345:ILE:HG12	2.61	0.41
1:A:411:TYR:CD2	1:A:418:ASP:HB3	2.56	0.41
1:A:415:GLN:HE21	1:A:417:LYS:HB2	1.85	0.40
2:B:308:TYR:HD1	2:B:336:ALA:HB3	1.86	0.40
2:B:297:ILE:HD12	7:B:583:HOH:O	2.20	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	259/276 (94%)	255 (98%)	4 (2%)	0	100	100
2	B	320/347 (92%)	317 (99%)	3 (1%)	0	100	100
All	All	579/623 (93%)	572 (99%)	7 (1%)	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	228/240 (95%)	225 (99%)	3 (1%)	69	58
2	B	297/317 (94%)	273 (92%)	24 (8%)	11	2
All	All	525/557 (94%)	498 (95%)	27 (5%)	24	8

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	245	TYR
1	A	305	ILE
2	B	46	ASP
2	B	49	LEU
2	B	63	LEU
2	B	77	SER
2	B	83	LEU
2	B	84	LYS
2	B	158	LEU
2	B	173	LEU
2	B	186	ARG
2	B	200	SER
2	B	202	LYS
2	B	214	HIS
2	B	216	LEU
2	B	225	VAL
2	B	238	THR
2	B	258	HIS
2	B	270	LEU
2	B	271	ARG
2	B	282	ASN
2	B	286	LEU
2	B	313	MET
2	B	317	ARG

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Mol	Chain	Res	Type
2	B	323	LEU
2	B	338	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	272	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	PO4	A	502	-	4,4,4	0.96	0	6,6,6	0.77	0
5	EDO	A	505	-	3,3,3	0.72	0	2,2,2	0.54	0
3	PO4	A	501	-	4,4,4	0.87	0	6,6,6	0.43	0
5	EDO	A	506	-	3,3,3	0.48	0	2,2,2	0.28	0
5	EDO	A	508	-	3,3,3	0.52	0	2,2,2	0.25	0
5	EDO	A	507	-	3,3,3	0.50	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	B	401	2	14,14,15	0.42	0	17,19,21	0.39	0
6	NAG	B	402	2	14,14,15	0.42	0	17,19,21	0.43	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
6	NAG	B	401	2	-	4/6/23/26	0/1/1/1
5	EDO	A	505	-	-	0/1/1/1	-
5	EDO	A	506	-	-	0/1/1/1	-
5	EDO	A	508	-	-	1/1/1/1	-
5	EDO	A	507	-	-	0/1/1/1	-
6	NAG	B	402	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	401	NAG	O5-C5-C6-O6
6	B	401	NAG	C1-C2-N2-C7
5	A	508	EDO	O1-C1-C2-O2
6	B	401	NAG	C4-C5-C6-O6
6	B	401	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	506	EDO	1	0
5	A	507	EDO	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	263/276 (95%)	0.07	5 (1%) 66 65	22, 32, 52, 71	0
2	B	322/347 (92%)	1.84	102 (31%) 0 0	31, 59, 124, 153	0
All	All	585/623 (93%)	1.04	107 (18%) 1 1	22, 45, 104, 153	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	348	LEU	18.5
2	B	337	PRO	17.5
2	B	311	CYS	15.6
2	B	339	LYS	15.2
2	B	340	VAL	14.9
2	B	345	ILE	13.7
2	B	309	CYS	11.4
2	B	325	VAL	9.8
2	B	343	MET	9.5
2	B	259	ILE	8.9
2	B	258	HIS	8.8
2	B	336	ALA	8.8
2	B	323	LEU	8.7
2	B	310	GLY	8.6
2	B	289	GLY	8.5
2	B	341	ARG	8.5
2	B	315	TRP	8.4
2	B	335	GLN	8.2
2	B	349	ASN	7.7
2	B	308	TYR	7.4
2	B	324	PRO	7.0
2	B	322	SER	6.7
2	B	286	LEU	6.6
2	B	350	ALA	6.6

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Mol	Chain	Res	Type	RSRZ
2	B	317	ARG	6.5
2	B	319	TRP	6.4
1	A	463	ALA	5.9
2	B	285	ASN	5.9
2	B	342	GLY	5.8
2	B	288	GLN	5.7
2	B	312	LYS	5.6
2	B	274	TYR	5.4
2	B	307	TRP	5.3
2	B	318	ASP	5.3
2	B	334	CYS	5.1
2	B	344	ALA	5.1
2	B	320	LEU	4.7
2	B	314	LYS	4.7
2	B	300	LEU	4.6
2	B	333	MET	4.5
2	B	321	GLN	4.4
2	B	293	ASP	4.3
2	B	237	LEU	4.3
2	B	347	ASP	4.2
2	B	332	LEU	4.1
2	B	287	PRO	4.1
2	B	298	THR	4.1
2	B	295	ASP	4.0
2	B	346	LYS	4.0
2	B	327	VAL	4.0
2	B	283	LEU	3.9
2	B	290	ILE	3.9
2	B	316	VAL	3.8
1	A	464	ALA	3.7
2	B	306	PRO	3.6
2	B	196	GLN	3.5
2	B	126	LYS	3.5
2	B	328	ASN	3.4
2	B	171	TRP	3.3
2	B	186	ARG	3.2
2	B	129	TYR	3.2
2	B	151	ARG	3.1
2	B	261	ARG	3.1
2	B	210	LEU	3.1
2	B	338	GLU	3.1
2	B	291	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	271	ARG	3.0
2	B	284	SER	3.0
2	B	262	VAL	2.9
2	B	212	ASN	2.9
1	A	462	ALA	2.9
2	B	58	GLU	2.9
2	B	276	LEU	2.9
2	B	81	ASN	2.8
2	B	122	ASP	2.8
2	B	238	THR	2.7
2	B	326	LYS	2.7
2	B	125	SER	2.7
2	B	292	ASP	2.7
2	B	294	LEU	2.7
2	B	281	ASN	2.7
2	B	234	ARG	2.6
2	B	227	LEU	2.6
2	B	30	SER	2.6
2	B	152	ASP	2.6
2	B	121	TYR	2.5
2	B	78	ASP	2.5
1	A	461	PRO	2.5
2	B	175	ARG	2.5
2	B	273	LEU	2.5
2	B	257	ASN	2.4
2	B	105	TYR	2.4
2	B	297	ILE	2.3
2	B	282	ASN	2.3
2	B	302	LEU	2.3
2	B	303	ARG	2.3
2	B	239	ALA	2.3
2	B	255	GLN	2.2
2	B	228	THR	2.2
2	B	296	ASN	2.2
1	A	198	GLY	2.1
2	B	250	ARG	2.1
2	B	278	MET	2.1
2	B	305	ASN	2.1
2	B	246	GLY	2.1
2	B	331	GLY	2.1
2	B	330	ARG	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 monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	A	508	4/4	0.64	0.24	62,65,69,71	0
6	NAG	B	402	14/15	0.67	0.69	98,110,117,119	0
6	NAG	B	401	14/15	0.72	0.34	88,100,108,108	0
5	EDO	A	505	4/4	0.81	0.24	41,42,42,49	0
5	EDO	A	507	4/4	0.86	0.11	54,57,59,61	0
5	EDO	A	506	4/4	0.89	0.39	51,56,61,65	0
3	PO4	A	502	5/5	0.90	0.28	48,53,55,61	0
3	PO4	A	501	5/5	0.93	0.18	51,52,58,70	0
4	NA	A	504	1/1	0.97	0.09	36,36,36,36	0
4	NA	A	509	1/1	0.98	0.12	26,26,26,26	0
4	NA	A	503	1/1	1.00	0.12	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.