



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:31 PM GMT

PDB ID : 4Y61  
Title : Crystal structure of the complex between Slitrk2 LRR1 and PTP delta Ig1-Fn1  
Authors : Yamgata, A.; Sato, Y.; Goto-Ito, S.; Uemura, T.; Maeda, A.; Shiroshima, T.; Yoshida, T.; Fukai, S.  
Deposited on : 2015-02-12  
Resolution : 3.36 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

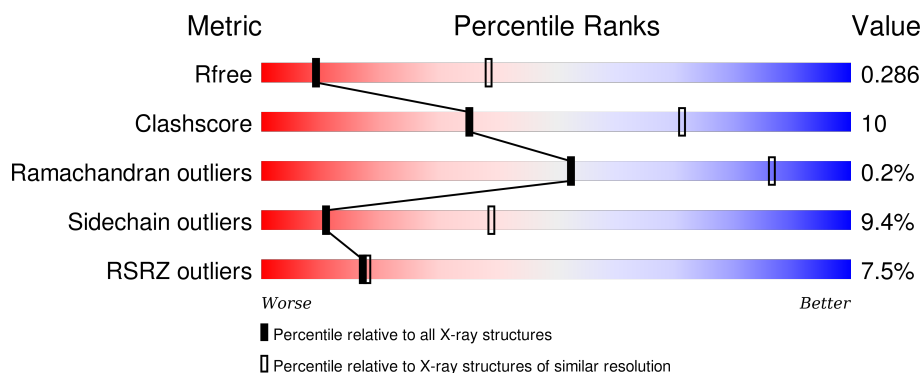
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.36 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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	398	<div> <div>12%</div> <div>78%</div> <div>18%</div> <div>• •</div> </div>
2	B	272	<div> <div>53%</div> <div>28%</div> <div>•</div> <div>14%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4947 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 Receptor-type tyrosine-protein phosphatase delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	391	3004	1876	525	590	13	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	LYS	-	expression tag	UNP Q64487
A	420	HIS	-	expression tag	UNP Q64487
A	421	HIS	-	expression tag	UNP Q64487
A	422	HIS	-	expression tag	UNP Q64487
A	423	HIS	-	expression tag	UNP Q64487
A	424	HIS	-	expression tag	UNP Q64487
A	425	HIS	-	expression tag	UNP Q64487

- Molecule 2 is a protein called SLIT and NTRK-like protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	235	1887	1211	322	344	10	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	267	HIS	-	expression tag	UNP Q810C0
B	268	HIS	-	expression tag	UNP Q810C0
B	269	HIS	-	expression tag	UNP Q810C0
B	270	HIS	-	expression tag	UNP Q810C0
B	271	HIS	-	expression tag	UNP Q810C0
B	272	HIS	-	expression tag	UNP Q810C0

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

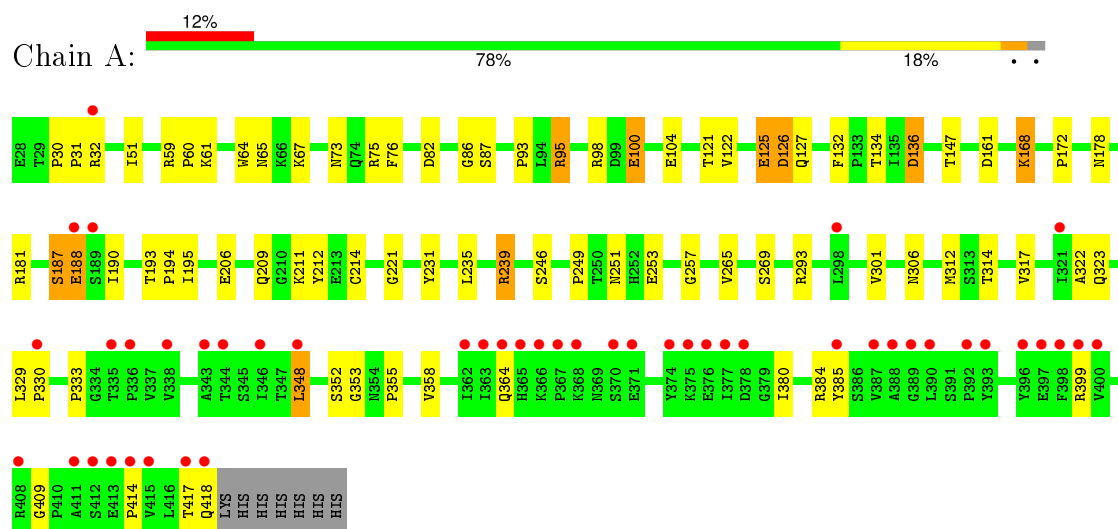


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

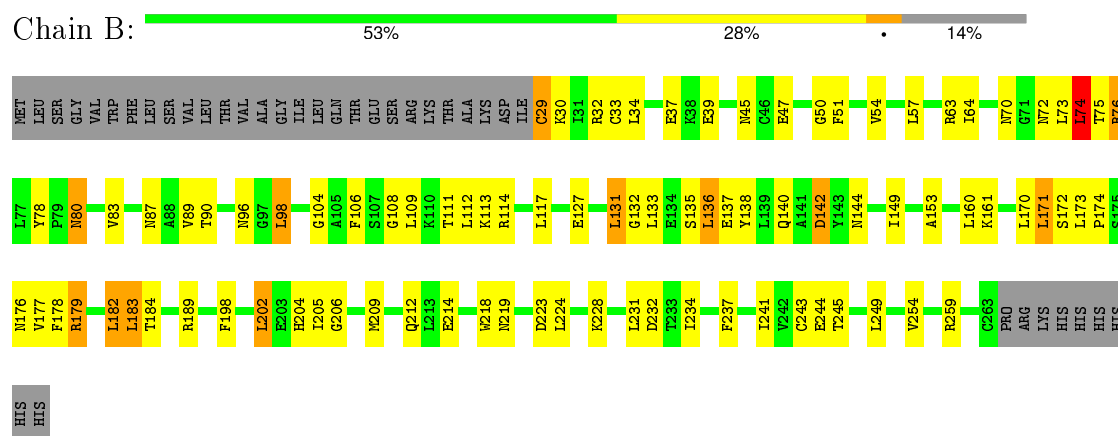
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Receptor-type tyrosine-protein phosphatase delta



- Molecule 2: SLIT and NTRK-like protein 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.23Å 91.31Å 123.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.65 – 3.36 45.65 – 3.36	Depositor EDS
% Data completeness (in resolution range)	99.1 (45.65-3.36) 99.1 (45.65-3.36)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.235 , 0.286 0.235 , 0.286	Depositor DCC
$R_{free}$ test set	727 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	96.3	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 50.1	EDS
Estimated twinning fraction	0.045 for k,h,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 14482 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4947	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.31	0/3069	0.57	1/4186 (0.0%)
2	B	0.26	0/1922	0.52	1/2607 (0.0%)
All	All	0.29	0/4991	0.55	2/6793 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	74	LEU	CA-CB-CG	5.75	128.52	115.30
1	A	86	GLY	N-CA-C	5.01	125.62	113.10

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	3004	0	2973	41	0
2	B	1887	0	1913	57	0
3	A	28	0	26	1	0
3	B	28	0	26	0	0
All	All	4947	0	4938	97	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 10.

All (97) 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:A:161:ASP:HB3	1:A:195:ILE:HD11	1.61	0.81
1:A:126:ASP:OD1	1:A:126:ASP:N	2.14	0.80
2:B:137:GLU:HA	2:B:160:LEU:HA	1.66	0.77
1:A:312:MET:HB3	1:A:317:VAL:HG22	1.67	0.76
1:A:31:PRO:O	1:A:32:ARG:NH1	2.18	0.72
2:B:113:LYS:HE3	2:B:135:SER:HB3	1.74	0.69
2:B:179:ARG:HB3	2:B:204:HIS:CE1	2.27	0.68
2:B:142:ASP:OD1	2:B:142:ASP:N	2.22	0.68
2:B:72:ASN:O	2:B:96:ASN:ND2	2.25	0.67
2:B:127:GLU:HA	2:B:153:ALA:HA	1.77	0.67
2:B:198:PHE:HA	2:B:202:LEU:HB2	1.77	0.67
2:B:34:LEU:HG	2:B:45:ASN:HB3	1.76	0.67
2:B:117:LEU:O	2:B:144:ASN:ND2	2.25	0.66
2:B:173:LEU:HD12	2:B:174:PRO:HD2	1.78	0.65
2:B:189:ARG:HG3	2:B:212:GLN:HB3	1.79	0.64
2:B:90:THR:HG22	2:B:114:ARG:HB3	1.79	0.64
1:A:231:TYR:OH	2:B:137:GLU:OE2	2.17	0.62
2:B:206:GLY:HA2	2:B:234:ILE:HD13	1.82	0.60
1:A:65:ASN:HB2	1:A:104:GLU:HG3	1.84	0.59
2:B:47:GLU:HG3	2:B:70:ASN:HB2	1.84	0.59
2:B:237:PHE:HZ	2:B:241:ILE:HD11	1.69	0.58
1:A:265:VAL:HG22	1:A:293:ARG:HG3	1.86	0.57
2:B:83:VAL:HA	2:B:108:GLY:HA3	1.87	0.57
1:A:333:PRO:HA	1:A:353:GLY:HA3	1.86	0.56
1:A:251:ASN:HB3	1:A:323:GLN:HB3	1.87	0.56
2:B:184:THR:HB	2:B:209:MET:HG2	1.89	0.54
2:B:109:LEU:HD13	2:B:112:LEU:HD22	1.89	0.54
2:B:114:ARG:HG3	2:B:138:TYR:CD2	2.45	0.52
2:B:29:CYS:O	2:B:33:CYS:HB3	2.11	0.51
1:A:51:ILE:HD13	1:A:172:PRO:HG3	1.92	0.51
2:B:89:VAL:HG12	2:B:90:THR:HG23	1.94	0.49
2:B:189:ARG:HG2	2:B:214:GLU:H	1.78	0.48
1:A:30:PRO:HB2	1:A:32:ARG:HH12	1.78	0.48
2:B:104:GLY:HA2	2:B:131:LEU:HB2	1.95	0.48
2:B:176:ASN:HA	2:B:204:HIS:HE1	1.79	0.48
2:B:140:GLN:HG2	2:B:142:ASP:OD1	2.14	0.47
2:B:106:PHE:HB3	2:B:109:LEU:HD12	1.95	0.47
1:A:187:SER:N	1:A:188:GLU:HA	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLN:HB2	1:A:399:ARG:HB2	1.95	0.47
1:A:249:PRO:HB2	1:A:322:ALA:HB2	1.97	0.47
2:B:113:LYS:HA	2:B:136:LEU:HA	1.97	0.46
1:A:352:SER:HB2	1:A:358:VAL:HG21	1.97	0.46
1:A:306:ASN:HD22	3:A:502:NAG:C7	2.27	0.46
2:B:114:ARG:HA	2:B:138:TYR:HB3	1.97	0.46
1:A:330:PRO:HB2	1:A:409:GLY:HA3	1.98	0.46
2:B:228:LYS:HD3	2:B:254:VAL:HG12	1.97	0.46
2:B:32:ARG:HB3	2:B:51:PHE:HZ	1.79	0.46
1:A:64:TRP:NE1	1:A:87:SER:OG	2.41	0.46
2:B:72:ASN:H	2:B:96:ASN:ND2	2.13	0.46
1:A:100:GLU:OE2	1:A:122:VAL:N	2.25	0.46
2:B:198:PHE:HA	2:B:202:LEU:CB	2.44	0.45
2:B:214:GLU:OE1	2:B:214:GLU:N	2.49	0.45
2:B:176:ASN:HA	2:B:204:HIS:CE1	2.52	0.45
2:B:237:PHE:CZ	2:B:241:ILE:HD11	2.50	0.45
2:B:106:PHE:O	2:B:132:GLY:HA3	2.16	0.45
2:B:171:LEU:HD12	2:B:172:SER:H	1.80	0.45
2:B:98:LEU:HA	2:B:98:LEU:HD23	1.79	0.45
1:A:168:LYS:HD3	1:A:212:TYR:CZ	2.51	0.45
2:B:149:ILE:O	2:B:174:PRO:HG3	2.17	0.44
1:A:75:ARG:NH1	1:A:93:PRO:O	2.47	0.44
1:A:73:ASN:HB3	1:A:76:PHE:CD1	2.52	0.44
1:A:209:GLN:HG3	1:A:231:TYR:HA	1.99	0.44
1:A:95:ARG:HB3	1:A:98:ARG:HD2	2.00	0.44
2:B:64:ILE:HD12	2:B:87:ASN:HB2	1.99	0.44
1:A:193:THR:HB	1:A:194:PRO:HD2	2.00	0.44
1:A:348:LEU:O	1:A:384:ARG:HA	2.18	0.44
2:B:178:PHE:CD2	2:B:205:ILE:HD11	2.53	0.44
2:B:80:ASN:ND2	2:B:80:ASN:O	2.41	0.43
1:A:100:GLU:HG3	1:A:121:THR:HA	1.99	0.43
2:B:87:ASN:HA	2:B:111:THR:OG1	2.19	0.43
2:B:202:LEU:HD13	2:B:202:LEU:HA	1.82	0.43
1:A:257:GLY:N	1:A:301:VAL:O	2.50	0.43
1:A:67:LYS:HD3	1:A:67:LYS:HA	1.61	0.43
1:A:59:ARG:HA	1:A:60:PRO:HD3	1.74	0.42
2:B:50:GLY:N	2:B:72:ASN:OD1	2.52	0.42
2:B:80:ASN:ND2	2:B:83:VAL:HB	2.35	0.42
1:A:211:LYS:HB2	1:A:211:LYS:HE3	1.80	0.42
1:A:125:GLU:OE2	1:A:125:GLU:N	2.49	0.42
1:A:136:ASP:N	1:A:136:ASP:OD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:SER:H	1:A:188:GLU:HA	1.83	0.42
2:B:219:ASN:HA	2:B:245:THR:HB	2.02	0.41
2:B:189:ARG:CG	2:B:212:GLN:HB3	2.49	0.41
2:B:218:TRP:CD1	2:B:241:ILE:HG23	2.55	0.41
1:A:399:ARG:NH1	1:A:414:PRO:HD3	2.36	0.41
1:A:246:SER:HB3	1:A:265:VAL:HG12	2.03	0.41
2:B:243:CYS:HB2	2:B:249:LEU:O	2.20	0.41
2:B:37:GLU:OE1	2:B:63:ARG:NH1	2.54	0.41
1:A:132:PHE:CE2	1:A:221:GLY:HA3	2.55	0.41
2:B:231:LEU:HA	2:B:234:ILE:HG22	2.03	0.41
1:A:380:ILE:HG21	1:A:385:TYR:HB2	2.03	0.41
2:B:74:LEU:HD22	2:B:96:ASN:HB3	2.02	0.41
2:B:161:LYS:HE2	2:B:182:LEU:HD13	2.02	0.41
1:A:239:ARG:HA	1:A:239:ARG:HD3	1.69	0.41
2:B:161:LYS:HA	2:B:183:LEU:HA	2.02	0.40
1:A:417:THR:OG1	1:A:418:GLN:N	2.54	0.40
2:B:76:ARG:HB2	2:B:78:TYR:HE2	1.85	0.40
1:A:95:ARG:HB3	1:A:98:ARG:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	389/398 (98%)	371 (95%)	17 (4%)	1 (0%)	46	82
2	B	233/272 (86%)	211 (91%)	22 (9%)	0	100	100
All	All	622/670 (93%)	582 (94%)	39 (6%)	1 (0%)	52	86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	PRO

### 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	338/345 (98%)	313 (93%)	25 (7%)	17	53
2	B	214/247 (87%)	187 (87%)	27 (13%)	5	24
All	All	552/592 (93%)	500 (91%)	52 (9%)	11	39

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	A	82	ASP
1	A	95	ARG
1	A	100	GLU
1	A	125	GLU
1	A	126	ASP
1	A	127	GLN
1	A	134	THR
1	A	136	ASP
1	A	147	THR
1	A	168	LYS
1	A	178	ASN
1	A	181	ARG
1	A	187	SER
1	A	188	GLU
1	A	190	ILE
1	A	206	GLU
1	A	214	CYS
1	A	235	LEU
1	A	239	ARG
1	A	253	GLU
1	A	269	SER
1	A	314	THR

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Mol	Chain	Res	Type
1	A	329	LEU
1	A	348	LEU
2	B	29	CYS
2	B	30	LYS
2	B	39	GLU
2	B	54	VAL
2	B	57	LEU
2	B	73	LEU
2	B	74	LEU
2	B	75	THR
2	B	76	ARG
2	B	80	ASN
2	B	98	LEU
2	B	131	LEU
2	B	133	LEU
2	B	136	LEU
2	B	142	ASP
2	B	170	LEU
2	B	171	LEU
2	B	177	VAL
2	B	179	ARG
2	B	182	LEU
2	B	183	LEU
2	B	202	LEU
2	B	223	ASP
2	B	224	LEU
2	B	232	ASP
2	B	244	GLU
2	B	259	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	GLN
2	B	61	GLN
2	B	204	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	501	1	14,14,15	0.25	0	15,19,21	0.63	1 (6%)
3	NAG	A	502	1	14,14,15	0.42	0	15,19,21	0.36	0
3	NAG	B	301	2	14,14,15	0.30	0	15,19,21	0.58	1 (6%)
3	NAG	B	302	2	14,14,15	0.36	0	15,19,21	0.25	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	501	1	-	0/6/23/26	0/1/1/1
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
3	NAG	B	301	2	-	0/6/23/26	0/1/1/1
3	NAG	B	302	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	NAG	C1-O5-C5	2.10	114.91	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAG	C1-O5-C5	2.22	115.06	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAG	1	0

## 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	391/398 (98%)	0.61	47 (12%) 6 5	54, 97, 224, 323	0
2	B	235/272 (86%)	0.06	0 100 100	48, 91, 129, 186	0
All	All	626/670 (93%)	0.40	47 (7%) 17 18	48, 94, 214, 323	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	ILE	12.3
1	A	398	PHE	9.2
1	A	365	HIS	8.7
1	A	411	ALA	6.3
1	A	393	TYR	6.0
1	A	397	GLU	5.7
1	A	364	GLN	5.5
1	A	392	PRO	5.0
1	A	414	PRO	5.0
1	A	415	VAL	4.8
1	A	188	GLU	4.5
1	A	375	LYS	4.4
1	A	389	GLY	4.4
1	A	388	ALA	4.3
1	A	390	LEU	4.0
1	A	366	LYS	4.0
1	A	338	VAL	3.9
1	A	374	TYR	3.8
1	A	400	VAL	3.8
1	A	377	ILE	3.8
1	A	348	LEU	3.6
1	A	408	ARG	3.5
1	A	387	VAL	3.3
1	A	412	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	399	ARG	3.2
1	A	385	TYR	3.2
1	A	378	ASP	3.2
1	A	367	PRO	2.9
1	A	368	LYS	2.8
1	A	413	GLU	2.8
1	A	371	GLU	2.7
1	A	417	THR	2.7
1	A	336	PRO	2.7
1	A	396	TYR	2.7
1	A	298	LEU	2.7
1	A	346	ILE	2.7
1	A	344	THR	2.6
1	A	362	ILE	2.4
1	A	376	GLU	2.4
1	A	330	PRO	2.4
1	A	32	ARG	2.4
1	A	370	SER	2.3
1	A	343	ALA	2.3
1	A	189	SER	2.2
1	A	418	GLN	2.1
1	A	335	THR	2.1
1	A	321	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( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	302	14/15	0.75	0.30	-	131,137,141,146	0
3	NAG	B	301	14/15	0.89	0.28	-	86,91,107,116	0
3	NAG	A	501	14/15	0.73	0.21	-	95,107,111,112	0
3	NAG	A	502	14/15	0.75	0.21	-	93,106,109,110	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.