



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:31 PM GMT

PDB ID : 4P59  
Title : HER3 extracellular domain in complex with Fab fragment of MOR09825  
Authors : Sprague, E.R.  
Deposited on : 2014-03-15  
Resolution : 3.40 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

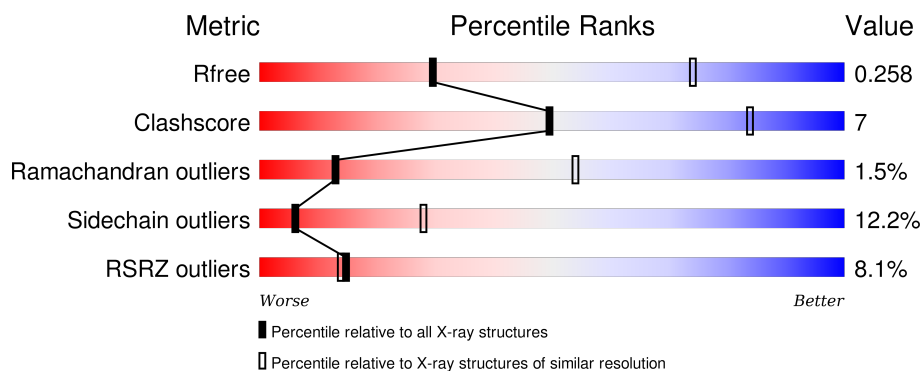
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	627	<div> <div>12%</div> <div>73%</div> <div>19%</div> <div>• 6%</div> </div>
2	H	238	<div> <div>%</div> <div>62%</div> <div>20%</div> <div>6%</div> <div>12%</div> </div>
3	L	214	<div> <div>3%</div> <div>71%</div> <div>24%</div> <div>• •</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7834 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 tyrosine-protein kinase erbB-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	592	Total	C	N	O	S	0	0	0
			4547	2813	823	852	59			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	641	GLU	HIS	cloning artifact	UNP P21860
A	642	PHE	LEU	cloning artifact	UNP P21860
A	643	ARG	THR	cloning artifact	UNP P21860
A	644	HIS	MET	cloning artifact	UNP P21860
A	645	ASP	ALA	cloning artifact	UNP P21860
A	646	SER	LEU	cloning artifact	UNP P21860

- Molecule 2 is a protein called MOR09825 Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	210	Total	C	N	O	S	0	0	0
			1568	990	263	309	6			

- Molecule 3 is a protein called MOR09825 Fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1618	1015	271	327	5			

- Molecule 4 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
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

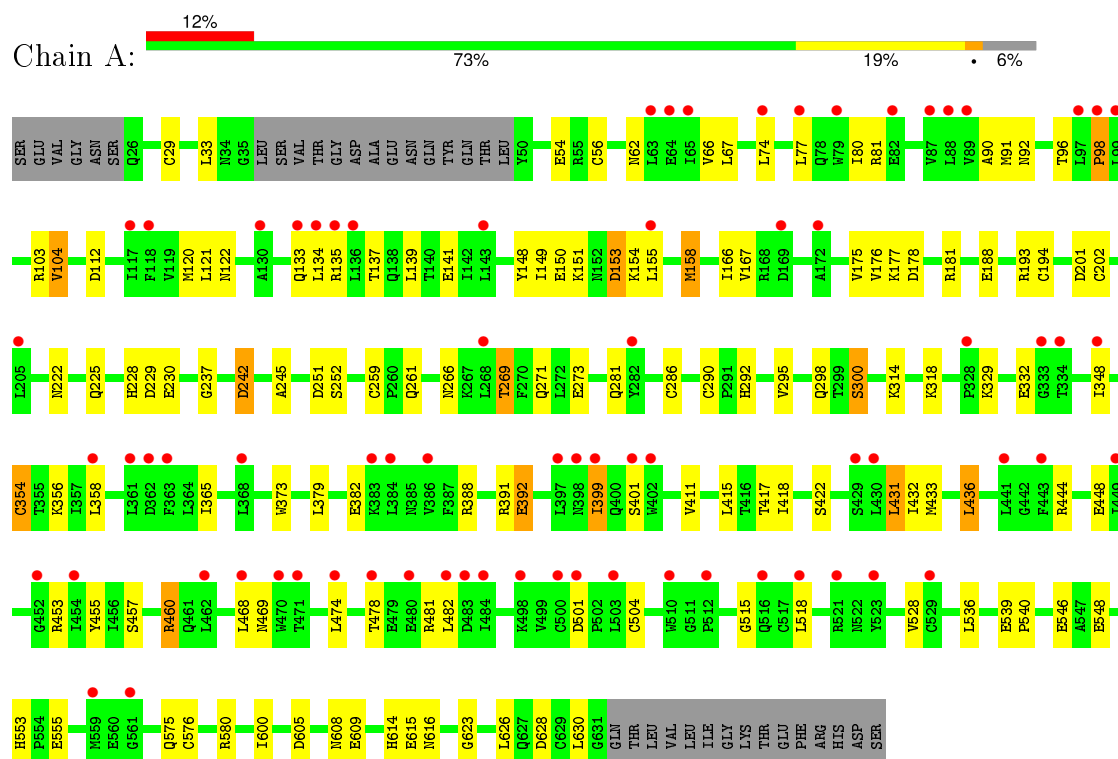
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	2	Total	O	0	0
			2	2		
5	L	1	Total	O	0	0
			1	1		

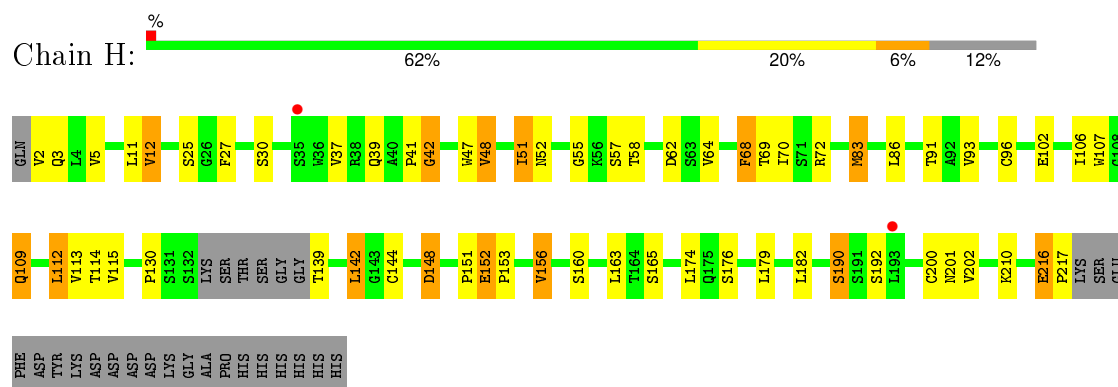
### 3 Residue-property plots

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.

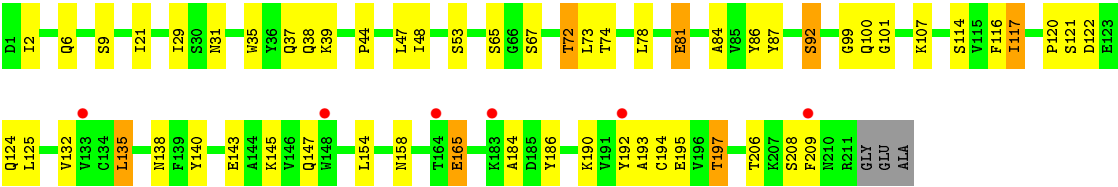
- Molecule 1: Receptor tyrosine-protein kinase erbB-3



- Molecule 2: MOR09825 Fab fragment heavy chain



- Molecule 3: MOR09825 Fab fragment light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.23Å 140.94Å 180.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	111.03 – 3.40 111.03 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (111.03-3.40) 99.9 (111.03-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 3.41Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, $R_{free}$	0.184 , 0.250 0.192 , 0.258	Depositor DCC
$R_{free}$ test set	1132 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.5	Xtriage
Anisotropy	0.778	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 81.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 22111 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7834	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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	0.44	0/4657	0.69	0/6317
2	H	0.49	0/1605	0.78	1/2186 (0.0%)
3	L	0.44	0/1654	0.72	0/2246
All	All	0.45	0/7916	0.72	1/10749 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	H	42	GLY	N-CA-C	-5.40	99.59	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	4547	0	4313	52	0
2	H	1568	0	1528	34	0
3	L	1618	0	1575	25	0
4	A	98	0	89	4	0
5	H	2	0	0	0	0
5	L	1	0	0	0	0
All	All	7834	0	7505	109	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 (109) 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:H:91:THR:HG22	2:H:115:VAL:H	1.38	0.89
2:H:48:VAL:HG22	2:H:64:VAL:HG21	1.61	0.81
3:L:6:GLN:HE22	3:L:87:TYR:HA	1.50	0.77
1:A:269:THR:HG23	1:A:271:GLN:HG2	1.66	0.76
3:L:145:LYS:HB2	3:L:197:THR:HG23	1.69	0.74
1:A:266:ASN:HB3	1:A:269:THR:HG22	1.73	0.70
2:H:216:GLU:HB3	2:H:217:PRO:HD3	1.73	0.70
4:A:702:NAG:H82	4:A:702:NAG:O3	1.94	0.68
1:A:623:GLY:H	1:A:628:ASP:HB3	1.57	0.67
2:H:51:ILE:HD12	2:H:58:THR:HG22	1.76	0.67
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.77	0.66
1:A:614:HIS:HD2	1:A:616:ASN:H	1.43	0.66
1:A:251:ASP:HA	1:A:286:CYS:HB2	1.79	0.64
2:H:5:VAL:HA	2:H:109:GLN:HE22	1.61	0.64
2:H:64:VAL:HG13	2:H:68:PHE:CG	2.34	0.62
3:L:147:GLN:HB2	3:L:195:GLU:HB3	1.81	0.61
2:H:37:VAL:HG22	2:H:47:TRP:HA	1.81	0.60
1:A:453:ARG:HG2	1:A:481:ARG:HB2	1.84	0.59
2:H:139:THR:N	2:H:190:SER:HG	2.00	0.58
3:L:116:PHE:HB2	3:L:135:LEU:HB3	1.86	0.58
1:A:158:MET:HB3	1:A:176:VAL:HG11	1.86	0.57
3:L:194:CYS:O	3:L:206:THR:HA	2.03	0.57
2:H:148:ASP:HB3	2:H:179:LEU:HD13	1.86	0.56
1:A:605:ASP:HB2	1:A:609:GLU:H	1.71	0.55
1:A:539:GLU:HB2	1:A:540:PRO:HD3	1.88	0.55
1:A:96:THR:HG22	1:A:133:GLN:HB2	1.88	0.55
3:L:86:TYR:O	3:L:101:GLY:HA2	2.07	0.54
2:H:91:THR:CG2	2:H:115:VAL:H	2.14	0.54
1:A:365:ILE:HD12	1:A:365:ILE:H	1.73	0.54
2:H:2:VAL:HG12	2:H:27:PHE:HB3	1.90	0.53
1:A:269:THR:CG2	1:A:271:GLN:HG2	2.37	0.53
1:A:431:LEU:HG	1:A:455:TYR:HB3	1.91	0.53
2:H:130:PRO:HG3	2:H:142:LEU:HB3	1.90	0.52
1:A:66:VAL:HG12	1:A:90:ALA:HB3	1.90	0.52
2:H:64:VAL:CG1	2:H:68:PHE:CG	2.93	0.52
2:H:12:VAL:HG21	2:H:86:LEU:HD13	1.92	0.52
2:H:93:VAL:HG22	2:H:112:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLY:H	1:A:242:ASP:HB3	1.76	0.51
1:A:104:VAL:HG11	1:A:245:ALA:HB2	1.92	0.50
1:A:417:THR:HG23	1:A:448:GLU:HB3	1.93	0.50
1:A:141:GLU:HA	1:A:166:ILE:HG23	1.94	0.50
3:L:117:ILE:HG12	3:L:209:PHE:HD2	1.77	0.49
1:A:281:GLN:HB2	1:A:300:SER:HB3	1.93	0.49
2:H:107:TRP:CE3	3:L:44:PRO:HD2	2.48	0.48
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.95	0.48
1:A:474:LEU:HD23	1:A:478:THR:HG22	1.95	0.48
1:A:222:ASN:HB2	1:A:225:GLN:HE21	1.77	0.48
1:A:98:PRO:HA	1:A:135:ARG:HB2	1.94	0.48
2:H:52:ASN:HB2	2:H:57:SER:O	2.14	0.47
1:A:134:LEU:HG	1:A:155:LEU:HD11	1.96	0.47
3:L:29:ILE:HG13	3:L:92:SER:HB3	1.95	0.47
1:A:614:HIS:CD2	1:A:616:ASN:H	2.28	0.47
3:L:81:GLU:HG3	3:L:81:GLU:H	1.54	0.47
3:L:39:LYS:HG2	3:L:84:ALA:HB2	1.97	0.46
2:H:64:VAL:HG13	2:H:68:PHE:CD2	2.51	0.46
2:H:139:THR:HA	2:H:190:SER:H	1.80	0.46
1:A:92:ASN:H	1:A:122:ASN:HA	1.81	0.46
2:H:152:GLU:OE1	2:H:153:PRO:HA	2.16	0.46
1:A:273:GLU:OE1	2:H:52:ASN:OD1	2.32	0.46
3:L:21:ILE:HD12	3:L:73:LEU:HD23	1.97	0.46
1:A:295:VAL:HG12	1:A:318:LYS:HB3	1.97	0.46
4:A:703:NAG:H61	4:A:704:NAG:C7	2.46	0.46
1:A:399:ILE:HD12	1:A:432:ILE:HG12	1.99	0.45
1:A:515:GLY:HA2	1:A:528:VAL:HA	1.98	0.45
1:A:269:THR:HG21	1:A:273:GLU:CG	2.47	0.45
1:A:149:ILE:HG21	1:A:158:MET:HG2	1.97	0.45
1:A:356:LYS:HG3	1:A:392:GLU:HB3	1.99	0.44
2:H:91:THR:HG22	2:H:115:VAL:N	2.19	0.44
3:L:107:LYS:HA	3:L:140:TYR:OH	2.18	0.44
1:A:433:MET:HA	1:A:457:SER:O	2.18	0.44
3:L:186:TYR:HA	3:L:192:TYR:OH	2.17	0.44
3:L:2:ILE:HD12	3:L:29:ILE:CD1	2.48	0.44
1:A:614:HIS:CD2	1:A:626:LEU:HD13	2.53	0.43
3:L:65:SER:HB3	3:L:72:THR:HG22	1.98	0.43
1:A:77:LEU:HA	1:A:80:ILE:HD12	2.00	0.43
1:A:415:LEU:HD21	1:A:418:ILE:HD11	2.00	0.43
1:A:120:MET:HG2	1:A:121:LEU:HG	2.00	0.43
2:H:51:ILE:HG13	2:H:52:ASN:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ARG:HG2	1:A:411:VAL:HA	1.99	0.43
2:H:39:GLN:HE22	3:L:38:GLN:HE22	1.67	0.43
2:H:68:PHE:N	2:H:68:PHE:CD1	2.87	0.43
1:A:615:GLU:HB3	3:L:31:ASN:ND2	2.34	0.42
3:L:193:ALA:HB2	3:L:208:SER:HB2	2.01	0.42
3:L:6:GLN:HE21	3:L:99:GLY:HA3	1.84	0.42
3:L:35:TRP:HB2	3:L:48:ILE:HB	2.01	0.42
1:A:553:HIS:HD2	1:A:555:GLU:H	1.67	0.42
3:L:122:ASP:HA	3:L:125:LEU:HD12	2.01	0.42
2:H:64:VAL:HG12	2:H:68:PHE:HB2	2.02	0.42
1:A:553:HIS:CD2	1:A:555:GLU:H	2.38	0.42
1:A:576:CYS:SG	1:A:580:ARG:HB2	2.59	0.42
2:H:64:VAL:CG1	2:H:68:PHE:HB2	2.49	0.41
1:A:436:LEU:HD21	4:A:702:NAG:H83	2.03	0.41
1:A:348:ILE:HD13	1:A:379:LEU:HD11	2.01	0.41
2:H:52:ASN:HB3	2:H:55:GLY:H	1.85	0.41
2:H:83:MET:HB2	2:H:86:LEU:HD21	2.02	0.41
2:H:11:LEU:HB2	2:H:151:PRO:HG3	2.03	0.41
1:A:148:TYR:CZ	1:A:150:GLU:HB2	2.55	0.41
1:A:194:CYS:HA	1:A:202:CYS:HA	2.02	0.41
2:H:11:LEU:HD12	2:H:114:THR:O	2.20	0.41
2:H:156:VAL:HB	2:H:202:VAL:HG22	2.02	0.41
1:A:228:HIS:CD2	1:A:230:GLU:H	2.38	0.41
1:A:329:LYS:HB3	1:A:354:CYS:HA	2.03	0.41
1:A:81:ARG:CZ	4:A:703:NAG:H2	2.51	0.41
1:A:222:ASN:H	1:A:225:GLN:HE21	1.67	0.41
1:A:74:LEU:HB3	1:A:77:LEU:HD12	2.03	0.41
2:H:41:PRO:HA	2:H:42:GLY:HA2	1.78	0.41
2:H:64:VAL:CG1	2:H:68:PHE:CD2	3.05	0.40
1:A:365:ILE:HG13	1:A:401:SER:HB2	2.01	0.40
3:L:165:GLU:CD	3:L:165:GLU:H	2.24	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	588/627 (94%)	520 (88%)	58 (10%)	10 (2%)	11	51
2	H	206/238 (87%)	190 (92%)	13 (6%)	3 (2%)	13	54
3	L	209/214 (98%)	190 (91%)	17 (8%)	2 (1%)	19	63
All	All	1003/1079 (93%)	900 (90%)	88 (9%)	15 (2%)	13	54

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	216	GLU
1	A	444	ARG
2	H	148	ASP
2	H	192	SER
3	L	138	ASN
1	A	153	ASP
1	A	298	GLN
1	A	139	LEU
1	A	167	VAL
1	A	188	GLU
1	A	242	ASP
3	L	184	ALA
1	A	460	ARG
1	A	608	ASN
1	A	98	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	512/543 (94%)	458 (90%)	54 (10%)	8	36
2	H	175/199 (88%)	143 (82%)	32 (18%)	2	10
3	L	185/186 (100%)	165 (89%)	20 (11%)	8	35
All	All	872/928 (94%)	766 (88%)	106 (12%)	6	28

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	CYS
1	A	33	LEU
1	A	54	GLU
1	A	56	CYS
1	A	62	ASN
1	A	67	LEU
1	A	91	MET
1	A	103	ARG
1	A	104	VAL
1	A	112	ASP
1	A	137	THR
1	A	151	LYS
1	A	153	ASP
1	A	154	LYS
1	A	158	MET
1	A	175	VAL
1	A	177	LYS
1	A	178	ASP
1	A	181	ARG
1	A	193	ARG
1	A	201	ASP
1	A	229	ASP
1	A	252	SER
1	A	259	CYS
1	A	261	GLN
1	A	269	THR
1	A	290	CYS
1	A	292	HIS
1	A	300	SER
1	A	314	LYS
1	A	332	GLU
1	A	354	CYS
1	A	358	LEU
1	A	373	TRP
1	A	382	GLU
1	A	391	ARG
1	A	392	GLU
1	A	399	ILE
1	A	422	SER
1	A	431	LEU
1	A	436	LEU
1	A	460	ARG

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Mol	Chain	Res	Type
1	A	468	LEU
1	A	469	ASN
1	A	482	LEU
1	A	501	ASP
1	A	504	CYS
1	A	518	LEU
1	A	536	LEU
1	A	546	GLU
1	A	548	GLU
1	A	575	GLN
1	A	600	ILE
1	A	630	LEU
2	H	3	GLN
2	H	12	VAL
2	H	25	SER
2	H	30	SER
2	H	48	VAL
2	H	51	ILE
2	H	62	ASP
2	H	68	PHE
2	H	69	THR
2	H	70	ILE
2	H	72	ARG
2	H	83	MET
2	H	96	CYS
2	H	102	GLU
2	H	106	ILE
2	H	109	GLN
2	H	112	LEU
2	H	113	VAL
2	H	142	LEU
2	H	144	CYS
2	H	152	GLU
2	H	156	VAL
2	H	160	SER
2	H	163	LEU
2	H	165	SER
2	H	174	LEU
2	H	176	SER
2	H	182	LEU
2	H	190	SER
2	H	200	CYS

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Mol	Chain	Res	Type
2	H	201	ASN
2	H	210	LYS
3	L	9	SER
3	L	53	SER
3	L	67	SER
3	L	72	THR
3	L	74	THR
3	L	78	LEU
3	L	81	GLU
3	L	92	SER
3	L	100	GLN
3	L	114	SER
3	L	117	ILE
3	L	121	SER
3	L	124	GLN
3	L	135	LEU
3	L	143	GLU
3	L	154	LEU
3	L	158	ASN
3	L	165	GLU
3	L	190	LYS
3	L	197	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	138	GLN
1	A	225	GLN
1	A	228	HIS
1	A	248	HIS
1	A	425	ASN
1	A	553	HIS
1	A	614	HIS
3	L	6	GLN
3	L	31	ASN
3	L	38	GLN
3	L	79	GLN
3	L	158	ASN

### 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 ⓘ

7 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$
4	NAG	A	701	1	14,14,15	0.36	0	15,19,21	0.60	0
4	NAG	A	702	1	14,14,15	0.75	0	15,19,21	2.78	3 (20%)
4	NAG	A	703	1,4	14,14,15	0.36	0	15,19,21	1.88	2 (13%)
4	NAG	A	704	4	14,14,15	0.38	0	15,19,21	2.50	2 (13%)
4	NAG	A	705	1,4	14,14,15	0.43	0	15,19,21	2.29	3 (20%)
4	NAG	A	706	4	14,14,15	0.45	0	15,19,21	0.63	0
4	NAG	A	707	1	14,14,15	0.23	0	15,19,21	0.57	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
4	NAG	A	701	1	-	0/6/23/26	0/1/1/1
4	NAG	A	702	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	703	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	704	4	-	0/6/23/26	0/1/1/1
4	NAG	A	705	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	706	4	-	0/6/23/26	0/1/1/1
4	NAG	A	707	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	702	NAG	C1-O5-C5	-9.28	100.47	112.25
4	A	705	NAG	C4-C3-C2	-2.06	108.03	111.23
4	A	702	NAG	C2-N2-C7	2.73	126.55	123.04
4	A	705	NAG	C2-N2-C7	3.06	126.97	123.04
4	A	703	NAG	C2-N2-C7	3.07	126.98	123.04
4	A	702	NAG	C6-C5-C4	3.15	120.77	113.02
4	A	704	NAG	C3-C4-C5	3.56	116.41	110.20
4	A	703	NAG	C1-O5-C5	5.91	119.75	112.25
4	A	705	NAG	C1-O5-C5	7.56	121.85	112.25
4	A	704	NAG	C1-O5-C5	8.74	123.34	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	702	NAG	2	0
4	A	703	NAG	2	0
4	A	704	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	592/627 (94%)	0.79	74 (12%) <b>5</b> <b>5</b>	42, 116, 172, 228	0
2	H	210/238 (88%)	0.47	2 (0%) <b>84</b> <b>79</b>	37, 60, 86, 119	0
3	L	211/214 (98%)	0.56	6 (2%) <b>56</b> <b>52</b>	42, 72, 113, 139	0
All	All	1013/1079 (93%)	0.68	82 (8%) <b>15</b> <b>14</b>	37, 88, 159, 228	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	LEU	6.6
1	A	98	PRO	6.0
1	A	430	LEU	5.8
1	A	363	PHE	5.7
1	A	135	ARG	5.7
1	A	134	LEU	5.7
1	A	470	TRP	5.5
1	A	521	ARG	4.6
1	A	397	LEU	4.1
1	A	97	LEU	4.1
1	A	130	ALA	4.0
1	A	503	LEU	4.0
1	A	518	LEU	3.9
1	A	77	LEU	3.8
1	A	516	GLN	3.8
1	A	484	ILE	3.6
1	A	118	PHE	3.5
1	A	449	ILE	3.5
1	A	133	GLN	3.5
1	A	510	TRP	3.4
1	A	483	ASP	3.4
1	A	529	CYS	3.4
1	A	333	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	89	VAL	3.3
1	A	512	PRO	3.3
1	A	443	PHE	3.2
1	A	468	LEU	3.2
1	A	480	GLU	3.2
1	A	399	ILE	3.1
1	A	498	LYS	3.0
1	A	87	VAL	3.0
1	A	361	LEU	3.0
1	A	482	LEU	2.9
1	A	478	THR	2.9
1	A	402	TRP	2.8
1	A	474	LEU	2.7
1	A	383	LYS	2.7
1	A	65	ILE	2.7
1	A	452	GLY	2.6
1	A	559	MET	2.6
1	A	136	LEU	2.6
1	A	82	GLU	2.5
1	A	155	LEU	2.5
1	A	362	ASP	2.5
1	A	386	VAL	2.5
1	A	88	LEU	2.5
1	A	328	PRO	2.5
1	A	348	ILE	2.5
1	A	117	ILE	2.4
1	A	282	TYR	2.4
1	A	401	SER	2.4
1	A	462	LEU	2.4
1	A	172	ALA	2.4
1	A	429	SER	2.4
1	A	501	ASP	2.4
1	A	143	LEU	2.3
1	A	268	LEU	2.3
1	A	441	LEU	2.3
1	A	454	ILE	2.3
1	A	64	GLU	2.3
1	A	358	LEU	2.3
3	L	192	TYR	2.3
1	A	99	LEU	2.3
3	L	164	THR	2.3
1	A	368	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	384	LEU	2.3
1	A	334	THR	2.3
1	A	205	LEU	2.2
1	A	561	GLY	2.2
3	L	209	PHE	2.2
1	A	398	ASN	2.2
3	L	183	LYS	2.1
1	A	523	TYR	2.1
1	A	500	CYS	2.1
1	A	471	THR	2.1
1	A	63	LEU	2.1
1	A	169	ASP	2.1
1	A	79	TRP	2.1
3	L	148	TRP	2.0
3	L	133	VAL	2.0
2	H	193	LEU	2.0
2	H	35	SER	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	NAG	A	702	14/15	0.79	0.29	0.65	106,111,120,120	0
4	NAG	A	703	14/15	0.92	0.25	-0.34	97,100,104,108	0
4	NAG	A	701	14/15	0.75	0.29	-0.50	114,116,120,121	0
4	NAG	A	705	14/15	0.84	0.26	-	147,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	704	14/15	0.79	0.23	-	107,111,112,113	0
4	NAG	A	706	14/15	0.88	0.19	-	148,151,151,151	0
4	NAG	A	707	14/15	0.55	0.36	-	168,171,174,174	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.