



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:11 PM GMT

PDB ID : 4ZS6  
Title : Receptor binding domain and Fab complex  
Authors : Yu, X.; Wang, X.  
Deposited on : 2015-05-13  
Resolution : 3.17 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

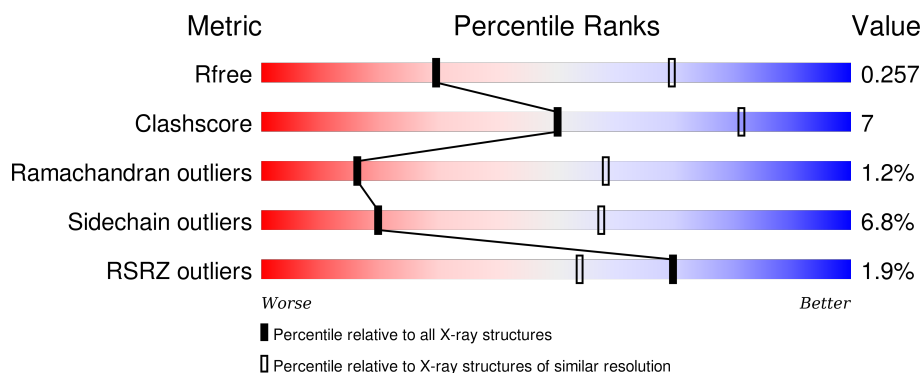
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.17 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	D	213	<div> <div>3%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>
1	L	213	<div> <div>75%</div> <div>22%</div> <div>..</div> </div>
2	C	227	<div> <div>4%</div> <div>74%</div> <div>22%</div> <div>..</div> </div>
2	H	227	<div> <div>%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>
3	A	229	<div> <div>70%</div> <div>18%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
3	B	229	

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
4	NAG	A	702	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9854 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 fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	210	Total	C	N	O	S	0	0	0
			1621	1016	276	324	5			
1	D	210	Total	C	N	O	S	0	0	0
			1621	1016	276	324	5			

- Molecule 2 is a protein called fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	2	0
			1678	1064	281	327	6			
2	C	221	Total	C	N	O	S	0	2	0
			1678	1064	281	327	6			

- Molecule 3 is a protein called S protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	207	Total	C	N	O	S	0	0	0
			1600	1020	255	314	11			
3	B	207	Total	C	N	O	S	0	0	0
			1600	1020	255	314	11			

There are 12 discrepancies between the modelled and reference sequences:

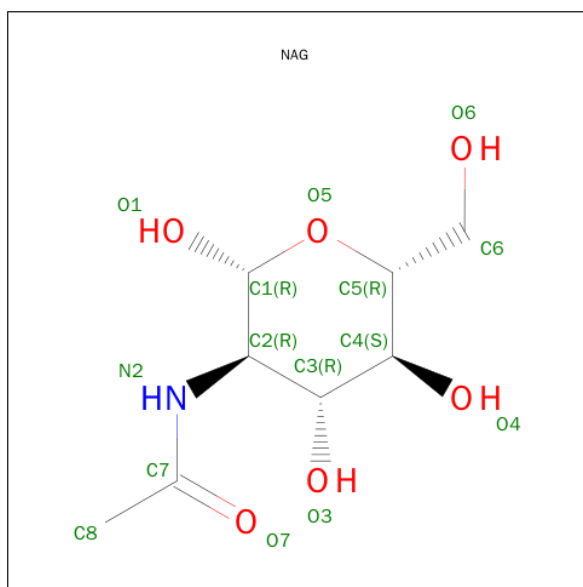
Chain	Residue	Modelled	Actual	Comment	Reference
A	590	HIS	-	expression tag	UNP W6A0A7
A	591	HIS	-	expression tag	UNP W6A0A7
A	592	HIS	-	expression tag	UNP W6A0A7
A	593	HIS	-	expression tag	UNP W6A0A7
A	594	HIS	-	expression tag	UNP W6A0A7
A	595	HIS	-	expression tag	UNP W6A0A7
B	590	HIS	-	expression tag	UNP W6A0A7
B	591	HIS	-	expression tag	UNP W6A0A7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	592	HIS	-	expression tag	UNP W6A0A7
B	593	HIS	-	expression tag	UNP W6A0A7
B	594	HIS	-	expression tag	UNP W6A0A7
B	595	HIS	-	expression tag	UNP W6A0A7

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

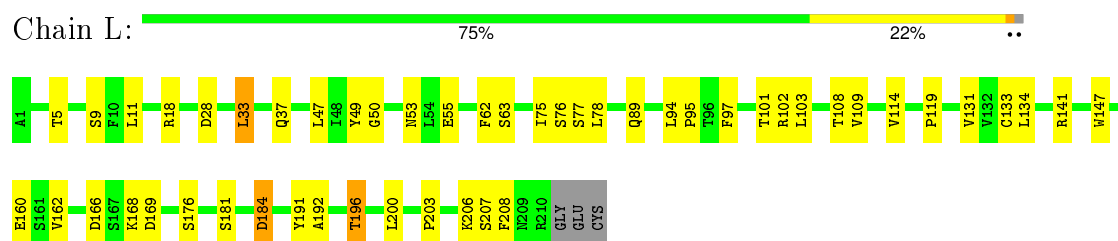


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

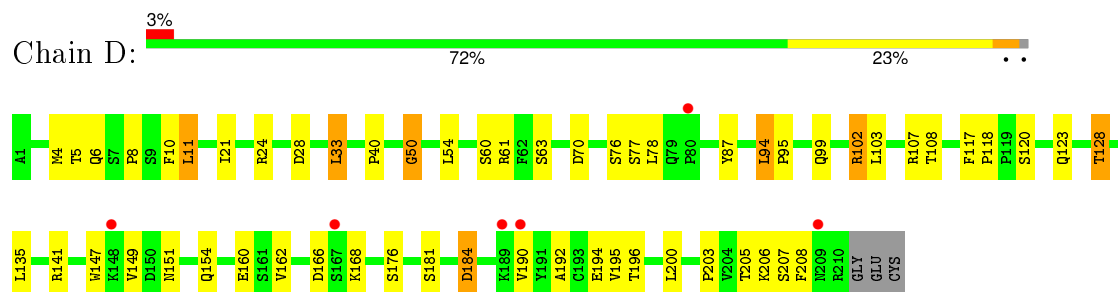
### 3 Residue-property plots

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.

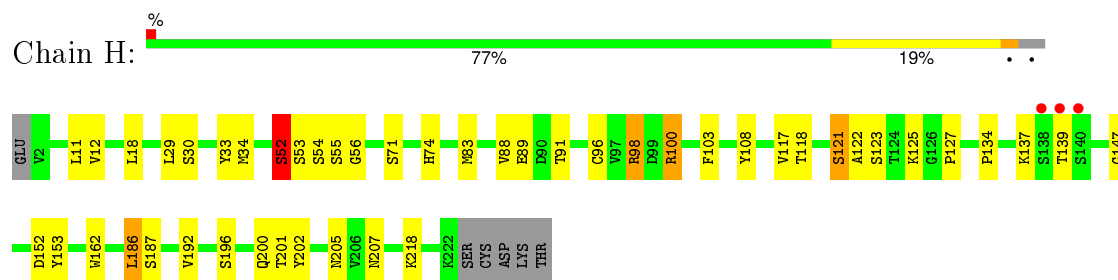
#### • Molecule 1: fab Light Chain



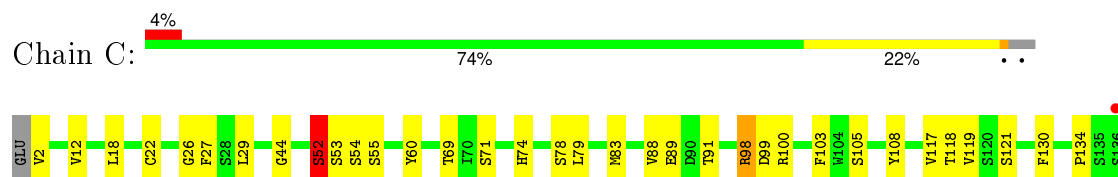
#### • Molecule 1: fab Light Chain

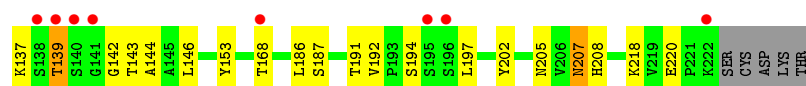


#### • Molecule 2: fab Heavy Chain

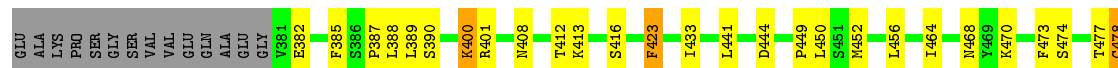


#### • Molecule 2: fab Heavy Chain





• Molecule 3: S protein



• Molecule 3: S protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.49Å 64.46Å 186.05Å 90.00° 100.43° 90.00°	Depositor
Resolution (Å)	36.95 – 3.17 36.95 – 3.17	Depositor EDS
% Data completeness (in resolution range)	94.7 (36.95-3.17) 94.7 (36.95-3.17)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.203 , 0.245 0.216 , 0.257	Depositor DCC
$R_{free}$ test set	1566 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.6	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 16.8	EDS
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 31133 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9854	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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

### 5.1 Standard geometry

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	D	0.54	0/1655	0.72	1/2246 (0.0%)
1	L	0.56	0/1655	0.71	0/2246
2	C	0.51	0/1727	0.69	0/2350
2	H	0.54	0/1727	0.70	1/2350 (0.0%)
3	A	0.64	0/1639	0.73	0/2238
3	B	0.49	0/1639	0.68	0/2238
All	All	0.55	0/10042	0.71	2/13668 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	50	GLY	N-CA-C	-5.18	100.16	113.10
2	H	56	GLY	N-CA-C	5.07	125.77	113.10

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	D	1621	0	1588	31	0
1	L	1621	0	1588	21	0
2	C	1678	0	1644	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1678	0	1644	21	0
3	A	1600	0	1561	23	1
3	B	1600	0	1561	20	1
4	A	28	0	26	1	0
4	B	28	0	26	0	0
All	All	9854	0	9638	136	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 7.

All (136) 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)
3:A:449:PRO:HG2	3:A:452:MET:HG3	1.57	0.86
3:B:449:PRO:HG2	3:B:452:MET:HG3	1.63	0.79
1:L:196:THR:HG22	1:L:203:PRO:HB3	1.69	0.73
2:H:83:MET:HE3	2:H:117:VAL:HG11	1.73	0.70
3:B:493:LYS:NZ	3:B:565:GLU:O	2.25	0.69
2:C:91:THR:HG23	2:C:118:THR:HA	1.75	0.68
3:B:464:ILE:HA	3:B:468:ASN:HD22	1.57	0.67
3:A:464:ILE:HA	3:A:468:ASN:HD22	1.61	0.66
2:H:91:THR:HG23	2:H:118:THR:HA	1.76	0.66
1:D:196:THR:HG22	1:D:203:PRO:HB3	1.80	0.64
1:D:107:ARG:HG2	1:D:108:THR:N	2.14	0.63
3:A:400:LYS:HE2	3:A:401:ARG:H	1.63	0.63
2:C:2:VAL:HA	2:C:26:GLY:HA3	1.81	0.62
3:A:505:ARG:HG2	3:A:554:LEU:HD12	1.81	0.61
3:A:441:LEU:HD12	3:A:575:VAL:HG12	1.83	0.60
3:B:388:LEU:HD11	3:B:571:PHE:HE1	1.67	0.60
2:H:201:THR:HG23	2:H:218:LYS:HZ2	1.66	0.60
3:A:456:LEU:HD23	3:A:481:LEU:HD21	1.84	0.60
2:H:103:PHE:HB3	3:A:540:TYR:HD2	1.67	0.59
1:D:78:LEU:HD21	1:D:103:LEU:HD11	1.83	0.59
3:A:401:ARG:HD2	3:A:444:ASP:OD1	2.04	0.57
3:B:456:LEU:HD23	3:B:481:LEU:HD21	1.86	0.57
3:B:388:LEU:HD11	3:B:571:PHE:CE1	2.40	0.56
1:D:166:ASP:OD1	1:D:168:LYS:HG2	2.05	0.56
1:D:192:ALA:HB2	1:D:207:SER:HB3	1.87	0.55
1:D:160:GLU:HA	1:D:176:SER:HA	1.89	0.54
1:L:160:GLU:HA	1:L:176:SER:HA	1.90	0.54
2:C:218:LYS:HE3	2:C:220:GLU:OE1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:401:ARG:HD2	3:B:444:ASP:OD1	2.09	0.53
2:C:153:TYR:OH	2:C:186:LEU:HD23	2.09	0.52
3:B:496:LYS:HD3	3:B:560:THR:HB	1.92	0.52
1:L:166:ASP:OD1	1:L:168:LYS:HG2	2.10	0.51
2:H:125:LYS:NZ	2:H:152:ASP:O	2.42	0.51
3:A:385:PHE:C	3:A:387:PRO:HD2	2.31	0.51
2:H:34:MET:SD	2:H:98:ARG:HB2	2.50	0.51
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.91	0.51
3:B:441:LEU:HD12	3:B:575:VAL:HG12	1.93	0.51
2:C:52:SER:OG	2:C:53:SER:N	2.45	0.50
1:D:10:PHE:HB2	1:D:102:ARG:HH11	1.77	0.50
3:A:584:VAL:O	3:A:584:VAL:HG12	2.11	0.50
1:D:194:GLU:HG3	1:D:205:THR:OG1	2.12	0.50
3:A:501:ASN:ND2	3:A:559:SER:OG	2.45	0.50
3:A:470:LYS:O	3:A:520:ALA:HA	2.11	0.50
3:B:457:SER:HA	3:B:479:LEU:HD23	1.92	0.49
1:L:141:ARG:CZ	1:L:162:VAL:HG11	2.43	0.49
2:C:27:PHE:CE2	2:C:29:LEU:HD23	2.47	0.49
3:B:504:SER:HB3	3:B:513:GLU:HG3	1.96	0.48
1:L:191:TYR:HB2	1:L:208:PHE:CE2	2.49	0.48
2:C:143:THR:HG23	2:C:191:THR:HB	1.96	0.48
1:L:49:TYR:O	1:L:53:ASN:HB2	2.14	0.47
2:H:11:LEU:HD12	2:H:12:VAL:N	2.28	0.47
2:C:137:LYS:HB3	2:C:137:LYS:HE2	1.38	0.47
3:A:416:SER:O	4:A:702:NAG:H3	2.14	0.47
3:A:473:PHE:H	3:A:473:PHE:HD2	1.63	0.47
2:C:60:TYR:OH	2:C:69:THR:HA	2.15	0.47
1:D:123:GLN:HG2	1:D:128:THR:O	2.14	0.47
1:D:54:LEU:HD21	1:D:60:SER:HA	1.97	0.47
3:A:388:LEU:HD11	3:A:571:PHE:CE1	2.49	0.46
2:H:18:LEU:HA	2:H:18:LEU:HD23	1.65	0.46
2:H:121:SER:OG	2:H:122:ALA:N	2.47	0.46
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.98	0.46
2:C:144:ALA:HB2	2:C:194:SER:HB3	1.98	0.46
1:D:87:TYR:OH	2:C:44:GLY:HA2	2.16	0.45
2:C:103:PHE:CE2	3:B:542:ARG:HD3	2.51	0.45
1:D:147:TRP:HB2	1:D:154:GLN:HB2	1.99	0.45
3:B:400:LYS:HG2	3:B:445:TYR:CZ	2.52	0.45
1:L:181:SER:OG	1:L:184:ASP:HB2	2.17	0.45
1:D:120:SER:OG	2:C:130:PHE:HB3	2.16	0.45
3:A:464:ILE:HA	3:A:468:ASN:ND2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:VAL:HB	1:D:154:GLN:HE21	1.82	0.44
3:A:509:ASP:O	3:A:510:ASP:HB2	2.17	0.44
2:H:147:GLY:HA2	2:H:162:TRP:CH2	2.52	0.44
2:H:192:VAL:HG11	2:H:202:TYR:CZ	2.51	0.44
3:B:478:CYS:HB2	3:B:573:ILE:HB	1.99	0.44
1:D:94:LEU:HA	1:D:95:PRO:HD3	1.77	0.44
1:L:89:GLN:HB2	1:L:97:PHE:CD2	2.53	0.44
1:D:206:LYS:HA	1:D:206:LYS:HD3	1.85	0.44
1:D:4:MET:O	1:D:99:GLN:NE2	2.50	0.44
1:D:135:LEU:HD11	1:D:195:VAL:HG21	1.99	0.44
3:B:479:LEU:HA	3:B:479:LEU:HD12	1.86	0.44
3:A:423:PHE:HE2	3:A:478:CYS:SG	2.41	0.44
1:D:33:LEU:O	1:D:50:GLY:O	2.36	0.43
2:C:139:THR:CG2	2:C:142:GLY:HA3	2.48	0.43
1:L:78:LEU:HD21	1:L:103:LEU:HD11	1.99	0.43
2:C:83:MET:HE1	2:C:117:VAL:HG11	2.00	0.43
1:D:61:ARG:HB2	1:D:76:SER:O	2.18	0.43
1:L:114:VAL:HA	1:L:134:LEU:O	2.17	0.43
1:L:9:SER:O	1:L:101:THR:HA	2.18	0.43
1:L:94:LEU:HA	1:L:95:PRO:HD3	1.86	0.43
2:H:53:SER:OG	2:H:54:SER:N	2.51	0.43
3:A:534:VAL:HG13	3:A:541:TYR:OH	2.19	0.43
2:C:22:CYS:O	2:C:78:SER:HA	2.18	0.43
1:D:168:LYS:HE2	1:D:168:LYS:HB3	1.83	0.43
1:L:33:LEU:O	1:L:50:GLY:O	2.36	0.43
1:L:192:ALA:HB2	1:L:207:SER:HB3	2.00	0.42
2:H:127:PRO:HB3	2:H:153:TYR:HB3	2.00	0.42
2:C:194:SER:HA	2:C:197:LEU:HG	2.00	0.42
1:D:8:PRO:HG2	1:D:11:LEU:HB3	2.01	0.42
2:C:12:VAL:HG13	2:C:119:VAL:HG22	2.01	0.42
2:H:33:TYR:CD1	2:H:52:SER:HA	2.54	0.42
2:H:53:SER:O	2:H:54:SER:C	2.58	0.42
3:B:502:LYS:HB3	3:B:557:SER:HB3	2.00	0.42
2:C:192:VAL:HG11	2:C:202:TYR:CE1	2.55	0.42
2:H:153:TYR:OH	2:H:186:LEU:HD23	2.20	0.42
2:H:137:LYS:HB3	2:H:137:LYS:HE2	1.46	0.42
3:B:505:ARG:HG2	3:B:554:LEU:HD12	2.00	0.42
1:D:141:ARG:CZ	1:D:162:VAL:HG11	2.50	0.42
1:L:133:CYS:HB2	1:L:147:TRP:CH2	2.55	0.42
1:D:107:ARG:NH1	1:D:108:THR:O	2.48	0.42
2:C:53:SER:OG	2:C:54:SER:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ARG:HD3	1:D:70:ASP:OD1	2.20	0.41
1:D:181:SER:OG	1:D:184:ASP:HB2	2.20	0.41
2:C:18:LEU:HA	2:C:18:LEU:HD23	1.82	0.41
3:B:530:VAL:HG22	3:B:541:TYR:CD2	2.56	0.41
1:L:18:ARG:HA	1:L:76:SER:HA	2.01	0.41
1:D:78:LEU:HD12	1:D:78:LEU:HA	1.88	0.41
2:H:196:SER:HB2	2:H:200:GLN:HG2	2.03	0.41
3:A:408:ASN:HA	3:A:585:CYS:O	2.21	0.41
2:C:99:ASP:OD1	2:C:105:SER:HB2	2.20	0.41
1:L:119:PRO:HD3	1:L:131:VAL:HG22	2.02	0.41
1:L:62:PHE:CE1	1:L:75:ILE:HG12	2.55	0.41
3:A:388:LEU:HD11	3:A:571:PHE:HE1	1.86	0.41
2:C:207:ASN:HD22	2:C:208:HIS:N	2.18	0.41
1:D:118:PRO:HB3	1:D:208:PHE:CE1	2.56	0.41
1:L:55:GLU:OE2	2:H:100:ARG:NH1	2.54	0.41
3:B:584:VAL:HG12	3:B:584:VAL:O	2.21	0.41
3:A:452:MET:HB3	3:A:452:MET:HE3	1.91	0.40
1:D:6:GLN:HE21	1:D:21:ILE:HG21	1.85	0.40
3:B:476:PRO:HB2	3:B:575:VAL:CG2	2.52	0.40
2:H:29:LEU:O	2:H:30:SER:OG	2.30	0.40
2:C:98:ARG:HD2	2:C:99:ASP:O	2.21	0.40
1:D:117:PHE:HA	1:D:118:PRO:HD2	1.90	0.40
1:D:190:VAL:HA	1:D:208:PHE:O	2.21	0.40
1:L:206:LYS:HA	1:L:206:LYS:HD3	1.54	0.40
3:A:566:GLN:HG2	3:A:566:GLN:H	1.73	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)
3:A:474:SER:O	3:B:427:GLN:NE2[2_7412]	2.02	0.18

## 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	D	208/213 (98%)	197 (95%)	9 (4%)	2 (1%)	19	63
1	L	208/213 (98%)	195 (94%)	11 (5%)	2 (1%)	19	63
2	C	221/227 (97%)	201 (91%)	15 (7%)	5 (2%)	8	42
2	H	221/227 (97%)	201 (91%)	14 (6%)	6 (3%)	6	37
3	A	205/229 (90%)	191 (93%)	14 (7%)	0	100	100
3	B	205/229 (90%)	192 (94%)	13 (6%)	0	100	100
All	All	1268/1338 (95%)	1177 (93%)	76 (6%)	15 (1%)	16	58

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	77	SER
2	C	139	THR
2	H	55	SER
2	H	121	SER
2	H	139	THR
1	D	77	SER
2	C	52	SER
2	C	55	SER
2	C	121	SER
2	H	134	PRO
2	H	52	SER
2	C	134	PRO
2	H	123	SER
1	L	169	ASP
1	D	40	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	D	183/185 (99%)	172 (94%)	11 (6%)	24	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	183/185 (99%)	172 (94%)	11 (6%)	24	63
2	C	189/193 (98%)	175 (93%)	14 (7%)	17	54
2	H	189/193 (98%)	175 (93%)	14 (7%)	17	54
3	A	189/207 (91%)	174 (92%)	15 (8%)	15	51
3	B	189/207 (91%)	176 (93%)	13 (7%)	19	57
All	All	1122/1170 (96%)	1044 (93%)	78 (7%)	20	57

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	11	LEU
1	L	28	ASP
1	L	33	LEU
1	L	63	SER
1	L	102	ARG
1	L	108	THR
1	L	109	VAL
1	L	184	ASP
1	L	196	THR
1	L	200	LEU
2	H	52	SER
2	H	71	SER
2	H	74	HIS
2	H	88	VAL
2	H	89	GLU
2	H	96	CYS
2	H	98	ARG
2	H	100	ARG
2	H	108	TYR
2	H	186	LEU
2	H	187[A]	SER
2	H	187[B]	SER
2	H	205	ASN
2	H	207	ASN
3	A	382	GLU
3	A	389	LEU
3	A	390	SER
3	A	400	LYS
3	A	412	THR

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Mol	Chain	Res	Type
3	A	413	LYS
3	A	423	PHE
3	A	433	ILE
3	A	450	LEU
3	A	477	THR
3	A	478	CYS
3	A	484	VAL
3	A	502	LYS
3	A	566	GLN
3	A	587	LYS
1	D	5	THR
1	D	11	LEU
1	D	28	ASP
1	D	33	LEU
1	D	63	SER
1	D	94	LEU
1	D	102	ARG
1	D	128	THR
1	D	151	ASN
1	D	184	ASP
1	D	200	LEU
2	C	52	SER
2	C	71	SER
2	C	74	HIS
2	C	88	VAL
2	C	89	GLU
2	C	98	ARG
2	C	100	ARG
2	C	108	TYR
2	C	146	LEU
2	C	168	THR
2	C	187[A]	SER
2	C	187[B]	SER
2	C	205	ASN
2	C	207	ASN
3	B	389	LEU
3	B	400	LYS
3	B	412	THR
3	B	413	LYS
3	B	423	PHE
3	B	433	ILE
3	B	477	THR

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Mol	Chain	Res	Type
3	B	478	CYS
3	B	484	VAL
3	B	501	ASN
3	B	502	LYS
3	B	566	GLN
3	B	587	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	$\# Z  > 2$
4	NAG	A	701	3	14,14,15	1.20	2 (14%)	15,19,21	0.72	1 (6%)
4	NAG	A	702	3	14,14,15	0.73	0	15,19,21	0.62	0
4	NAG	B	701	3	14,14,15	0.96	1 (7%)	15,19,21	1.13	1 (6%)
4	NAG	B	702	3	14,14,15	0.71	0	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
4	NAG	A	701	3	-	0/6/23/26	0/1/1/1
4	NAG	A	702	3	-	0/6/23/26	0/1/1/1
4	NAG	B	701	3	-	0/6/23/26	0/1/1/1
4	NAG	B	702	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	NAG	C1-C2	2.47	1.56	1.52
4	A	701	NAG	O5-C1	3.24	1.49	1.43
4	B	701	NAG	O5-C1	3.39	1.49	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	NAG	C1-O5-C5	2.45	115.75	112.14
4	B	701	NAG	C1-O5-C5	4.10	118.17	112.14

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
4	A	702	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	D	210/213 (98%)	-0.02	6 (2%) 55 39	64, 79, 93, 105	0
1	L	210/213 (98%)	-0.49	0 100 100	37, 52, 86, 94	0
2	C	221/227 (97%)	0.24	9 (4%) 41 25	66, 86, 118, 125	0
2	H	221/227 (97%)	-0.39	3 (1%) 78 64	36, 61, 95, 113	0
3	A	207/229 (90%)	-0.49	0 100 100	33, 47, 69, 93	0
3	B	207/229 (90%)	-0.05	6 (2%) 55 39	59, 73, 103, 127	0
All	All	1276/1338 (95%)	-0.20	24 (1%) 70 54	33, 70, 101, 127	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	508	SER	6.1
3	B	587	LYS	5.5
3	B	512	THR	5.4
2	C	136	SER	4.8
2	C	196	SER	4.3
2	H	140	SER	3.5
1	D	190	VAL	3.3
2	C	141	GLY	3.1
2	H	139	THR	3.0
2	C	139	THR	3.0
1	D	209	ASN	2.8
3	B	509	ASP	2.8
2	C	138	SER	2.5
1	D	80	PRO	2.5
2	C	222	LYS	2.4
3	B	507	LEU	2.4
1	D	148	LYS	2.4
2	C	140	SER	2.4
1	D	167	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	189	LYS	2.3
2	H	138	SER	2.3
3	B	511	ARG	2.2
2	C	195	SER	2.1
2	C	168	THR	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	0.31	5.56	78,79,81,84	0
4	NAG	B	701	14/15	0.87	0.27	-	92,96,101,101	0
4	NAG	A	701	14/15	0.88	0.39	-	74,78,80,81	0
4	NAG	B	702	14/15	0.84	0.31	-	106,111,114,118	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.