



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2016 – 05:20 PM EDT

PDB ID : 5JPM  
Title : Structure of the complex of human complement C4 with MASP-2 rebuilt using iMDFF  
Authors : Croll, T.I.; Andersen, G.R.  
Deposited on : 2016-05-03  
Resolution : 3.75 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-20027939  
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-20027939



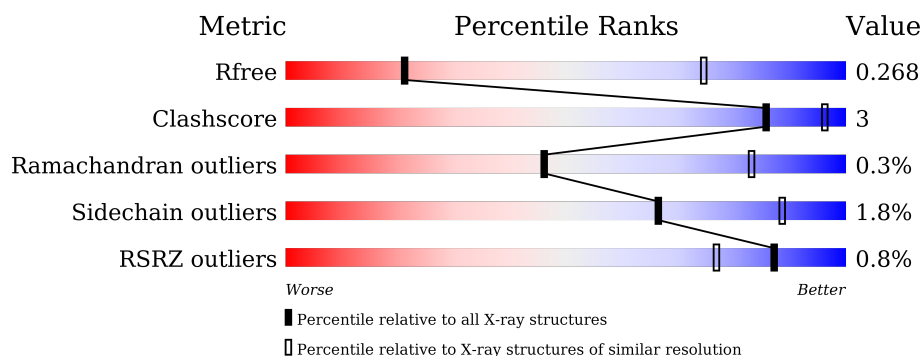
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.75 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	1268 (4.02-3.50)
Clashscore	102246	1407 (4.02-3.50)
Ramachandran outliers	100387	1346 (4.02-3.50)
Sidechain outliers	100360	1342 (4.02-3.50)
RSRZ outliers	91569	1276 (4.02-3.50)

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	656	<div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	D	656	<div> <div>87%</div> <div>11%</div> <div>..</div> </div>
2	B	767	<div> <div>%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>
2	E	767	<div> <div>%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
3	C	291	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
3	F	291	<div> <div>%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	154	<div><div>%</div><div><div></div><div></div><div></div></div><div>90%5%6%</div></div>
4	I	154	<div><div>3%</div><div><div></div><div></div><div></div></div><div>90%5%6%</div></div>
5	H	242	<div><div>2%</div><div><div></div><div></div><div></div></div><div>89%11%</div></div>
5	J	242	<div><div>%</div><div><div></div><div></div><div></div></div><div>95%.</div></div>



## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 32214 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 Complement C4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	0	0
			5012	3185	872	939	16			
1	D	651	Total	C	N	O	S	0	0	0
			5012	3185	872	939	16			

- Molecule 2 is a protein called Complement C4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	740	Total	C	N	O	S	0	0	0
			5718	3588	1002	1102	26			
2	E	740	Total	C	N	O	S	0	0	0
			5718	3588	1002	1102	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1201	SER	THR	variant	UNP P0C0L4
E	1201	SER	THR	variant	UNP P0C0L4

- Molecule 3 is a protein called Complement C4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	287	Total	C	N	O	S	0	0	0
			2290	1437	407	429	17			
3	F	287	Total	C	N	O	S	0	0	0
			2290	1437	407	429	17			

- Molecule 4 is a protein called Mannan-binding lectin serine protease 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	145	Total	C	N	O	S	0	0	0
			1103	701	177	213	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	145	Total	C	N	O	S	0	0	0
			1103	701	177	213	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	298	HIS	GLN	engineered mutation	UNP O00187
G	299	ALA	PRO	engineered mutation	UNP O00187
I	298	HIS	GLN	engineered mutation	UNP O00187
I	299	ALA	PRO	engineered mutation	UNP O00187

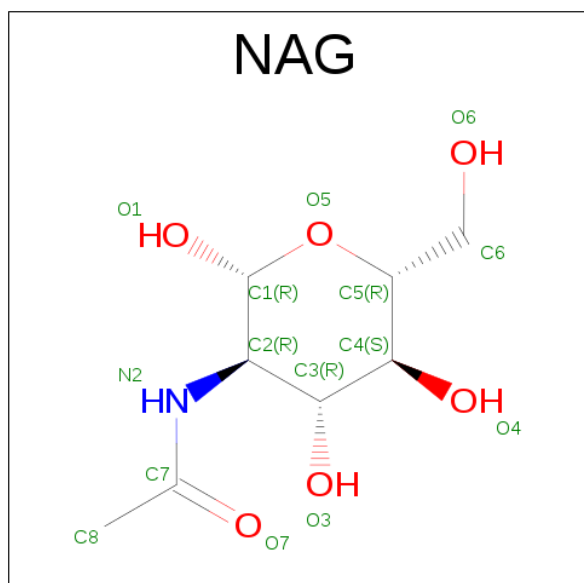
- Molecule 5 is a protein called Mannan-binding lectin serine protease 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	242	Total	C	N	O	S	0	0	0
			1867	1190	317	350	10			
5	J	242	Total	C	N	O	S	0	0	0
			1867	1190	317	350	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	633	ALA	SER	engineered mutation	UNP O00187
J	633	ALA	SER	engineered mutation	UNP O00187

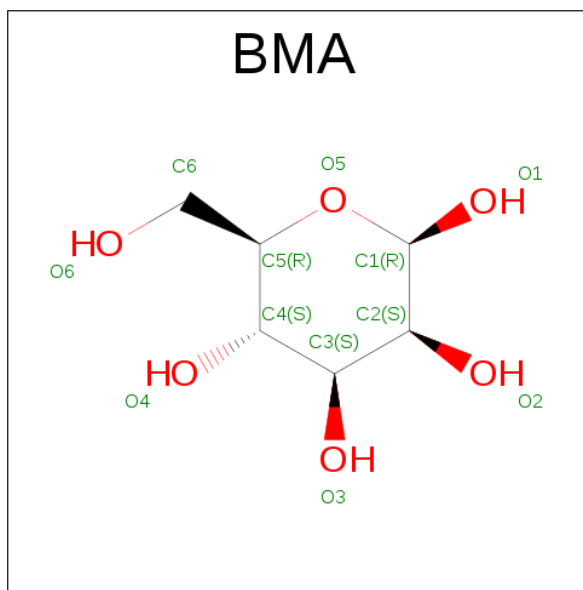
- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





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

- Molecule 7 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).





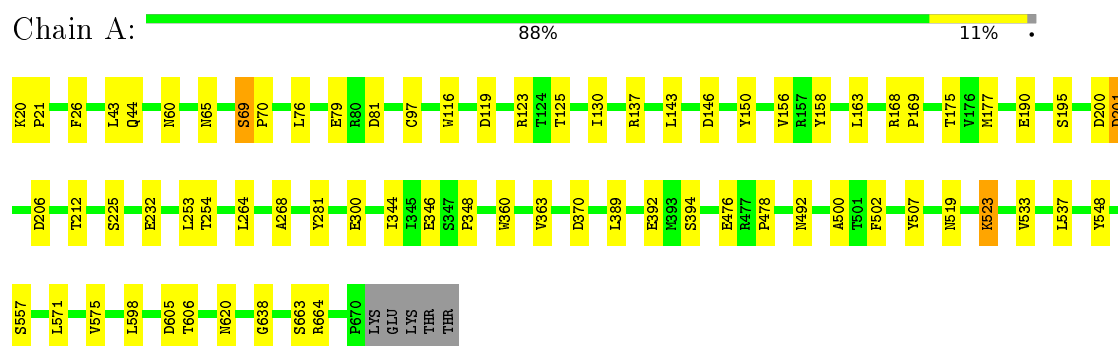
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		



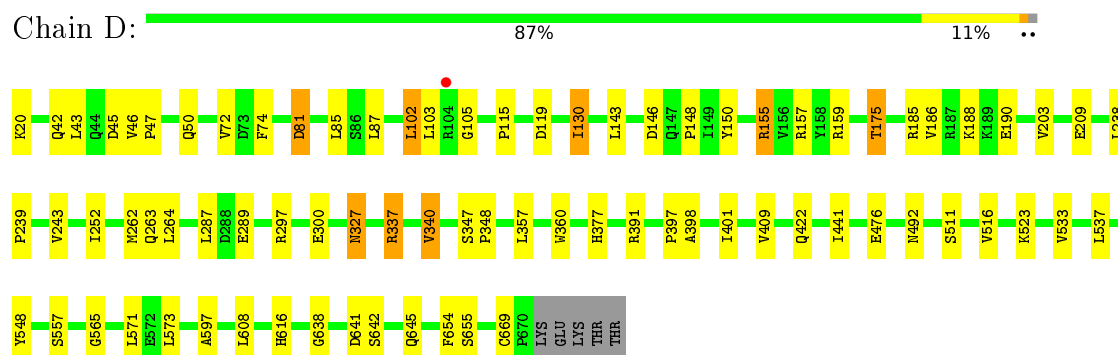
### 3 Residue-property plots

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.

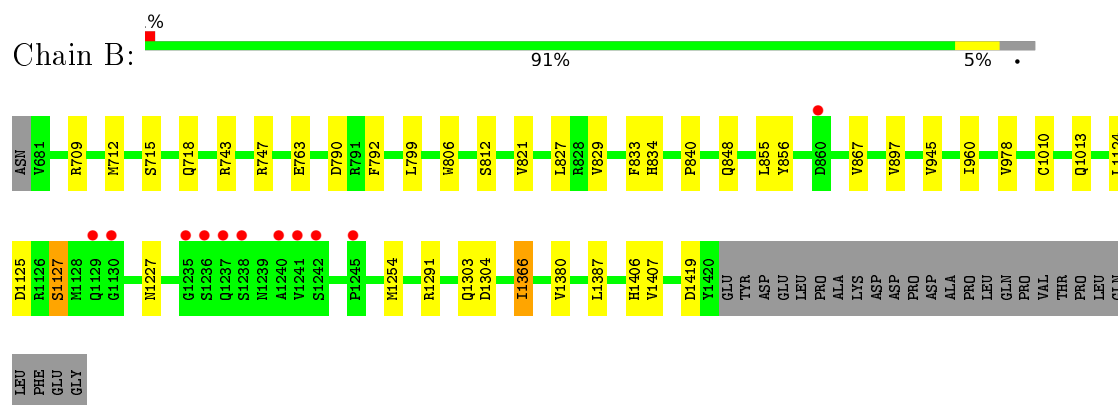
#### • Molecule 1: Complement C4-A



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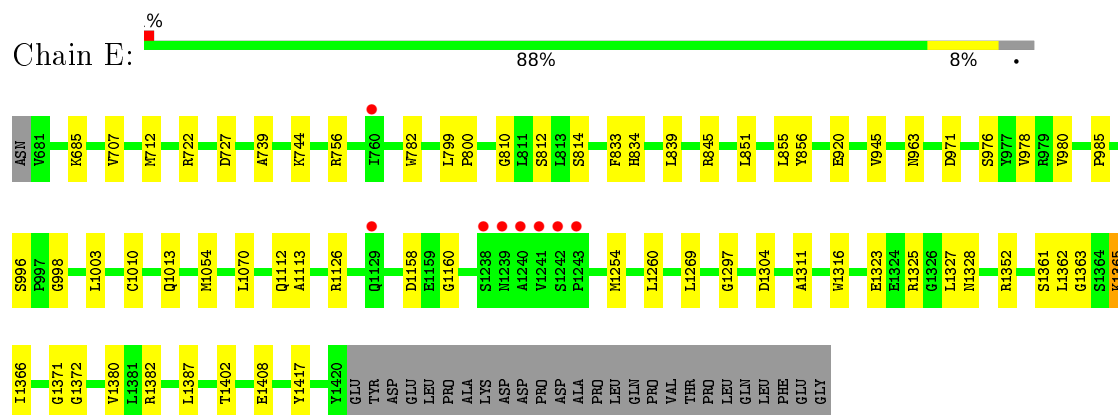


#### • Molecule 2: Complement C4-A

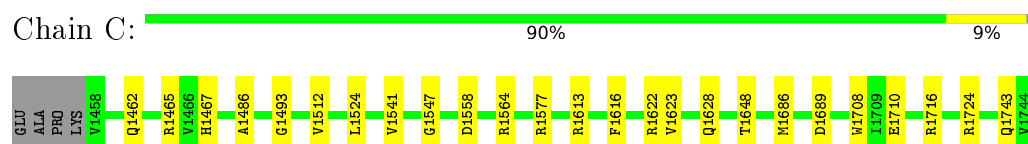




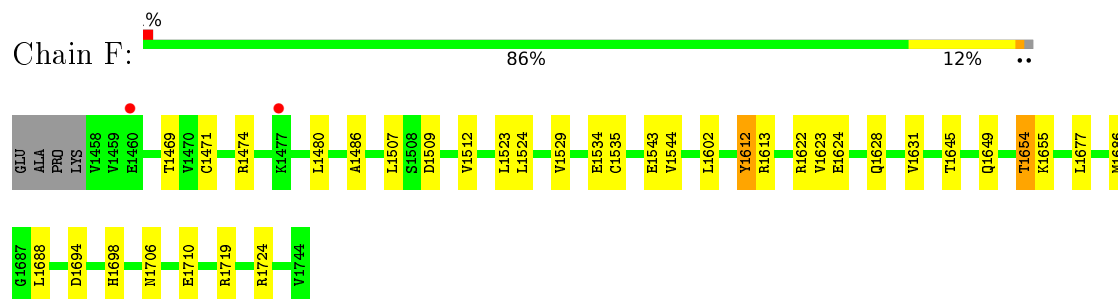
## • Molecule 2: Complement C4-A



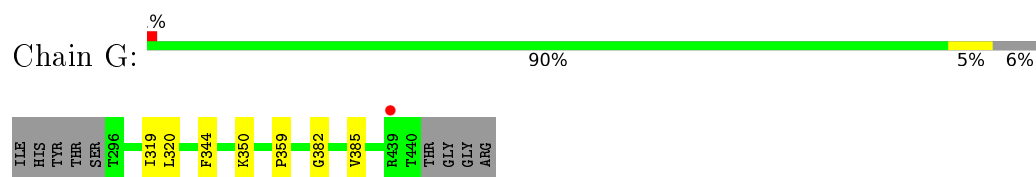
## • Molecule 3: Complement C4-A



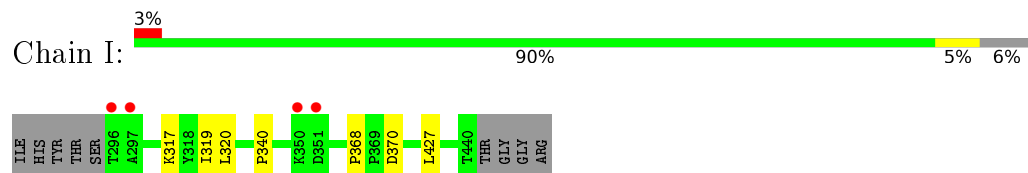
## • Molecule 3: Complement C4-A



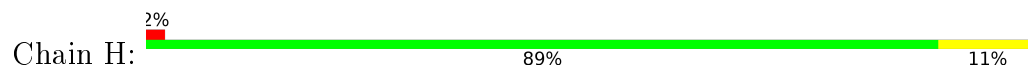
## • Molecule 4: Mannan-binding lectin serine protease 2



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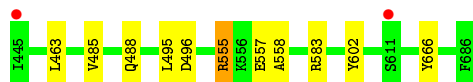
## • Molecule 5: Mannan-binding lectin serine protease 2







- Molecule 5: Mannan-binding lectin serine protease 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.01Å 215.01Å 142.86Å 90.00° 110.11° 90.00°	Depositor
Resolution (Å)	48.97 – 3.75 48.97 – 3.75	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.97-3.75) 98.6 (48.97-3.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 3.77Å)	Xtriage
Refinement program	PHENIX (dev_2376: ???)	Depositor
R, $R_{free}$	0.212 , 0.268 0.211 , 0.268	Depositor DCC
$R_{free}$ test set	1726 reflections (3.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	118.2	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 63.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.083 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32214	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: BMA, NAG, TYS

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	0.25	0/5128	0.44	0/6961
1	D	0.25	0/5128	0.44	0/6961
2	B	0.23	0/5799	0.42	0/7875
2	E	0.23	0/5799	0.41	0/7875
3	C	0.24	0/2337	0.43	0/3158
3	F	0.24	0/2337	0.45	0/3158
4	G	0.24	0/1136	0.46	0/1549
4	I	0.24	0/1136	0.45	0/1549
5	H	0.24	0/1915	0.43	0/2604
5	J	0.24	0/1915	0.42	0/2604
All	All	0.24	0/32630	0.43	0/44294

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	5012	0	5025	35	0
1	D	5012	0	5025	37	0
2	B	5718	0	5645	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	5718	0	5647	40	0
3	C	2290	0	2228	13	0
3	F	2290	0	2228	20	0
4	G	1103	0	1051	4	0
4	I	1103	0	1051	5	0
5	H	1867	0	1803	16	0
5	J	1867	0	1803	7	0
6	A	28	0	24	0	0
6	B	56	0	48	0	0
6	D	28	0	24	0	0
6	E	56	0	48	0	0
7	A	11	0	10	0	0
7	B	22	0	20	0	0
7	D	11	0	10	0	0
7	E	22	0	20	0	0
All	All	32214	0	31710	177	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 3.

All (177) 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)
5:H:485:VAL:HG13	5:H:495:LEU:HD11	1.75	0.68
1:D:185:ARG:HD3	1:D:188:LYS:HB2	1.75	0.67
5:H:602:TYR:OH	5:H:666:TYR:O	2.14	0.65
1:A:346:GLU:HG2	1:A:348:PRO:HD2	1.79	0.65
5:H:491:ASP:HB3	5:H:494:ALA:HB2	1.79	0.63
2:E:845:ARG:NH2	2:E:971:ASP:O	2.28	0.61
1:A:571:LEU:HD22	2:B:812:SER:HB2	1.82	0.61
1:D:557:SER:OG	1:D:638:GLY:O	2.19	0.60
2:B:945:VAL:HG23	2:B:1254:MET:HB3	1.84	0.60
2:B:1227:ASN:OD1	2:B:1291:ARG:NH1	2.34	0.59
1:D:476:GLU:HB3	1:D:492:ASN:HB2	1.84	0.59
1:A:557:SER:OG	1:A:638:GLY:O	2.21	0.58
1:D:81:ASP:N	1:D:81:ASP:OD2	2.36	0.58
3:F:1543:GLU:HG3	3:F:1544:VAL:HG23	1.85	0.58
1:D:642:SER:HB3	1:D:645:GLN:HG2	1.85	0.58
2:E:978:VAL:HG22	2:E:1380:VAL:HG12	1.85	0.57
1:A:212:THR:HG22	1:A:232:GLU:HG2	1.84	0.57
2:E:1126:ARG:HD3	2:E:1260:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASP:OD1	1:A:150:TYR:OH	2.16	0.57
2:E:980:VAL:O	2:E:1352:ARG:NH2	2.37	0.57
2:E:1361:SER:O	2:E:1363:GLY:N	2.34	0.57
2:B:1013:GLN:N	2:B:1013:GLN:OE1	2.39	0.56
2:E:1327:LEU:HA	2:E:1372:GLY:HA3	1.88	0.56
1:A:281:TYR:OH	1:A:300:GLU:OE1	2.19	0.56
5:J:602:TYR:OH	5:J:666:TYR:O	2.21	0.56
2:B:834:HIS:HB3	2:B:856:TYR:HB2	1.88	0.55
3:C:1462:GLN:HG2	5:J:488:GLN:HG2	1.89	0.54
2:E:722:ARG:NH2	3:F:1534:GLU:OE1	2.37	0.54
1:D:571:LEU:HD22	2:E:812:SER:HB2	1.88	0.54
1:D:391:ARG:HA	1:D:397:PRO:HA	1.89	0.54
3:F:1471:CYS:HA	3:F:1535:CYS:HA	1.88	0.54
1:D:209:GLU:HB2	2:E:1070:LEU:HD21	1.89	0.54
1:A:175:THR:HG22	1:A:190:GLU:HG2	1.90	0.54
1:D:409:VAL:HG13	1:D:441:ILE:HD13	1.88	0.54
5:H:671:LYS:HE2	5:H:673:ILE:HD11	1.89	0.53
3:F:1486:ALA:HB3	3:F:1524:LEU:HB2	1.90	0.53
2:E:744:LYS:NZ	2:E:1417:TYR:O3	2.39	0.53
1:A:500:ALA:HB3	1:A:502:PHE:HD1	1.74	0.53
2:E:1013:GLN:OE1	2:E:1013:GLN:N	2.38	0.53
2:E:945:VAL:HG23	2:E:1254:MET:HB3	1.90	0.52
3:F:1654:THR:HG23	3:F:1655:LYS:H	1.75	0.52
3:F:1613:ARG:NH1	3:F:1710:GLU:OE2	2.38	0.52
5:H:487:GLU:HG3	5:H:488:GLN:HG2	1.92	0.52
3:C:1613:ARG:NH1	3:C:1710:GLU:OE1	2.35	0.52
2:B:799:LEU:HD21	2:B:829:VAL:HB	1.91	0.52
2:B:1125:ASP:O	2:B:1127:SER:N	2.42	0.51
3:F:1631:VAL:HA	3:F:1645:THR:HG22	1.92	0.51
1:D:47:PRO:HG2	1:D:50:GLN:HB2	1.91	0.51
3:F:1688:LEU:HD13	3:F:1706:ASN:HB3	1.91	0.51
1:D:42:GLN:NE2	1:D:43:LEU:O	2.45	0.50
4:I:319:ILE:HG22	4:I:320:LEU:H	1.76	0.50
2:B:960:ILE:HB	2:B:1366:ILE:HG23	1.94	0.50
1:A:123:ARG:HG3	1:A:125:THR:H	1.75	0.50
1:A:20:LYS:HB2	1:A:21:PRO:HD3	1.94	0.50
2:E:839:LEU:HA	3:F:1544:VAL:HG21	1.93	0.50
1:A:370:ASP:HB3	1:A:389:LEU:HB3	1.94	0.50
3:C:1716:ARG:HG2	4:I:368:PRO:HG3	1.94	0.49
5:H:471:ALA:HB2	5:H:636:ALA:HB2	1.94	0.49
5:J:463:LEU:HB2	5:J:496:ASP:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:597:ALA:HB2	2:E:814:SER:HB2	1.95	0.49
2:E:851:LEU:HD23	2:E:851:LEU:H	1.77	0.49
2:E:996:SER:OG	2:E:998:GLY:O	2.25	0.49
5:H:673:ILE:HA	5:H:676:ILE:HG12	1.95	0.49
2:B:833:PHE:HZ	2:B:855:LEU:HD22	1.79	0.48
3:C:1465:ARG:HG2	3:C:1541:VAL:HG22	1.94	0.48
2:E:1269:LEU:HD12	2:E:1311:ALA:HB1	1.95	0.48
1:D:340:VAL:HG23	1:D:357:LEU:HB3	1.95	0.48
3:F:1623:VAL:HG11	3:F:1686:MET:HB3	1.96	0.48
1:D:115:PRO:O	1:D:119:ASP:N	2.45	0.48
4:G:320:LEU:HD22	4:G:350:LYS:HA	1.96	0.48
4:G:319:ILE:HG22	4:G:320:LEU:H	1.77	0.48
3:C:1486:ALA:HB3	3:C:1524:LEU:HB2	1.96	0.47
1:D:533:VAL:HA	1:D:537:LEU:HD22	1.96	0.47
3:F:1612:TYR:HD2	3:F:1612:TYR:H	1.61	0.47
1:D:148:PRO:HG2	1:D:608:LEU:HD13	1.97	0.47
2:B:840:PRO:HB3	3:C:1493:GLY:HA2	1.95	0.47
2:B:978:VAL:HG22	2:B:1380:VAL:HG12	1.96	0.47
5:J:555:ARG:HG2	5:J:558:ALA:HB2	1.97	0.47
1:A:268:ALA:HB2	1:A:344:ILE:HD13	1.97	0.47
5:H:605:PRO:O	5:H:609:ARG:NH2	2.47	0.46
2:E:833:PHE:HZ	2:E:855:LEU:HD22	1.81	0.46
3:F:1624:GLU:HB3	3:F:1654:THR:HG21	1.98	0.46
5:J:557:GLU:OE1	5:J:557:GLU:N	2.45	0.46
1:D:377:HIS:CD2	1:D:641:ASP:HB2	2.51	0.46
5:H:447:GLY:HA2	5:H:577:GLN:HB3	1.98	0.46
2:B:848:GLN:O	3:C:1547:GLY:N	2.38	0.46
3:C:1558:ASP:OD1	3:C:1564:ARG:NH2	2.46	0.46
3:F:1507:LEU:O	3:F:1509:ASP:N	2.48	0.45
1:D:146:ASP:OD1	1:D:150:TYR:OH	2.19	0.45
5:H:445:ILE:HB	5:H:586:MET:HB2	1.98	0.45
1:A:392:GLU:O	1:A:394:SER:N	2.43	0.45
1:A:60:ASN:O	1:A:65:ASN:HA	2.16	0.45
2:E:1323:GLU:HG2	2:E:1325:ARG:HG3	1.97	0.45
2:E:727:ASP:OD1	2:E:727:ASP:N	2.50	0.45
1:A:620:ASN:HA	2:B:821:VAL:HG11	1.98	0.45
2:B:867:VAL:HG21	2:B:897:VAL:HG11	1.98	0.45
1:D:300:GLU:OE2	2:E:685:LYS:NZ	2.42	0.45
1:A:43:LEU:HD22	1:A:76:LEU:HD13	1.99	0.45
1:D:74:PHE:HB3	1:D:85:LEU:HD11	1.98	0.45
1:D:297:ARG:HA	1:D:297:ARG:HE	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:ASN:N	1:D:327:ASN:OD1	2.51	0.44
4:I:370:ASP:HB2	4:I:427:LEU:HD21	1.98	0.44
1:D:155:ARG:HA	1:D:203:VAL:HA	2.00	0.44
4:I:317:LYS:HE2	4:I:319:ILE:HD11	1.99	0.44
1:D:238:LEU:HD12	1:D:239:PRO:HD2	2.00	0.44
3:C:1686:MET:HG3	3:C:1708:TRP:HB3	2.00	0.44
2:E:1158:ASP:O	2:E:1160:GLY:N	2.43	0.43
5:H:563:ARG:H	5:H:563:ARG:HG2	1.59	0.43
1:D:511:SER:HB3	1:D:516:VAL:HG21	2.00	0.43
2:B:1419:ASP:O	5:J:583:ARG:NH1	2.52	0.43
1:A:116:TRP:HA	1:A:119:ASP:HB3	1.99	0.43
1:A:605:ASP:OD1	1:A:606:THR:N	2.51	0.43
1:D:289:GLU:HA	1:D:337:ARG:HH11	1.84	0.43
2:B:790:ASP:O	2:B:792:PHE:N	2.51	0.43
1:D:43:LEU:HD12	1:D:46:VAL:HG11	2.00	0.43
1:D:72:VAL:HG12	1:D:87:LEU:HD13	2.01	0.43
2:E:985:PRO:HB3	2:E:1316:TRP:CD2	2.53	0.43
2:E:1408:GLU:CD	5:H:498:ARG:HH22	2.22	0.43
3:F:1628:GLN:HB3	3:F:1649:GLN:HB2	2.01	0.43
4:G:382:GLY:O	4:G:385:VAL:HG12	2.18	0.43
1:D:186:VAL:HB	2:E:1054:MET:HG3	2.00	0.43
1:D:20:LYS:HB3	1:D:45:ASP:OD2	2.19	0.43
2:E:834:HIS:HB3	2:E:856:TYR:HB2	2.00	0.43
5:H:497:ILE:HD11	5:H:536:ILE:HG21	2.01	0.43
1:A:81:ASP:N	1:A:81:ASP:OD2	2.51	0.43
2:B:715:SER:HB2	2:B:718:GLN:HB3	2.01	0.43
1:D:573:LEU:HD11	2:E:810:GLY:HA3	2.00	0.43
2:E:963:ASN:HB2	2:E:1382:ARG:HD2	2.00	0.43
2:B:743:ARG:HD2	2:B:763:GLU:HB3	2.00	0.43
1:D:130:ILE:HG23	1:D:655:SER:HB3	2.01	0.43
1:A:476:GLU:HB2	1:A:492:ASN:HB2	2.01	0.42
1:A:69:SER:HB2	1:A:70:PRO:HD3	2.01	0.42
3:C:1616:PHE:CE1	3:C:1708:TRP:HB2	2.54	0.42
2:E:1112:GLN:HG3	2:E:1113:ALA:H	1.82	0.42
2:E:707:VAL:HG12	2:E:739:ALA:HB2	2.02	0.42
3:F:1507:LEU:C	3:F:1509:ASP:H	2.21	0.42
1:A:253:LEU:HD23	1:A:363:VAL:HG23	2.02	0.42
1:A:507:TYR:CZ	1:A:519:ASN:HB3	2.54	0.42
1:A:201:ASP:N	1:A:201:ASP:OD2	2.52	0.42
1:D:252:ILE:HD13	1:D:262:MET:HG2	2.02	0.42
3:F:1612:TYR:CD2	3:F:1612:TYR:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:VAL:HA	1:A:537:LEU:HD22	2.02	0.42
1:A:195:SER:HB3	1:A:598:LEU:HD11	2.02	0.41
3:C:1628:GLN:O	3:C:1648:THR:OG1	2.33	0.41
2:E:1402:THR:HG23	3:F:1469:THR:HB	2.02	0.41
1:D:398:ALA:HB1	1:D:401:ILE:HD13	2.02	0.41
1:A:163:LEU:HD23	1:A:169:PRO:HA	2.02	0.41
2:E:1365:LYS:HG3	2:E:1365:LYS:H	1.65	0.41
2:E:799:LEU:HD12	2:E:800:PRO:HD2	2.01	0.41
5:J:485:VAL:HG13	5:J:495:LEU:HD11	2.01	0.41
1:A:137:ARG:HA	1:A:225:SER:HB2	2.02	0.41
2:E:1328:ASN:N	2:E:1371:GLY:O	2.39	0.41
2:E:1408:GLU:OE1	5:H:498:ARG:NH2	2.51	0.41
2:B:1406:HIS:HA	3:C:1467:HIS:CD2	2.56	0.41
1:D:175:THR:HB	1:D:190:GLU:HG2	2.03	0.41
1:D:347:SER:HB2	1:D:348:PRO:HD3	2.03	0.41
2:E:1003:LEU:HB3	2:E:1297:GLY:HA3	2.03	0.41
1:A:523:LYS:HE3	1:A:523:LYS:HB3	1.91	0.41
2:E:782:TRP:CD1	2:E:800:PRO:HG2	2.56	0.41
4:G:344:PHE:CZ	4:G:359:PRO:HD3	2.56	0.41
5:H:465:GLY:HA3	5:H:487:GLU:HG2	2.03	0.41
2:E:756:ARG:HG2	5:H:655:TRP:HA	2.02	0.41
1:A:158:TYR:CZ	1:A:200:ASP:HB3	2.56	0.41
1:A:206:ASP:OD2	1:A:206:ASP:N	2.48	0.41
3:F:1474:ARG:NH1	3:F:1529:VAL:O	2.54	0.41
1:A:168:ARG:HA	1:A:168:ARG:HD3	1.85	0.40
2:E:1323:GLU:OE2	2:E:1325:ARG:NE	2.32	0.40
3:F:1719:ARG:O	3:F:1724:ARG:NH2	2.54	0.40
3:C:1724:ARG:HG2	4:I:340:PRO:HD3	2.04	0.40
1:A:79:GLU:OE1	1:A:79:GLU:N	2.53	0.40
2:B:1124:LEU:HD21	2:B:1303:GLN:HG3	2.03	0.40
1:D:102:LEU:HD23	1:D:103:LEU:H	1.85	0.40
3:F:1694:ASP:OD1	3:F:1698:HIS:N	2.54	0.40
2:B:1406:HIS:CD2	2:B:1407:VAL:HG13	2.57	0.40
1:A:575:VAL:HG21	2:B:827:LEU:HD11	2.03	0.40
1:A:500:ALA:HB3	1:A:502:PHE:CD1	2.56	0.40
2:E:976:SER:HB3	2:E:1362:LEU:HA	2.02	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	649/656 (99%)	618 (95%)	28 (4%)	3 (0%)	34	77
1	D	649/656 (99%)	619 (95%)	26 (4%)	4 (1%)	30	75
2	B	737/767 (96%)	708 (96%)	28 (4%)	1 (0%)	56	90
2	E	737/767 (96%)	714 (97%)	23 (3%)	0	100	100
3	C	285/291 (98%)	270 (95%)	14 (5%)	1 (0%)	39	80
3	F	285/291 (98%)	270 (95%)	13 (5%)	2 (1%)	26	72
4	G	143/154 (93%)	134 (94%)	9 (6%)	0	100	100
4	I	143/154 (93%)	134 (94%)	9 (6%)	0	100	100
5	H	240/242 (99%)	228 (95%)	12 (5%)	0	100	100
5	J	240/242 (99%)	231 (96%)	9 (4%)	0	100	100
All	All	4108/4220 (97%)	3926 (96%)	171 (4%)	11 (0%)	46	83

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1127	SER
1	D	616	HIS
1	A	69	SER
1	A	663	SER
3	C	1622	ARG
3	F	1622	ARG
3	F	1677	LEU
1	D	565	GLY
1	A	478	PRO
1	D	105	GLY
1	D	669	CYS



### 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	557/562 (99%)	543 (98%)	14 (2%)	55	83
1	D	557/562 (99%)	537 (96%)	20 (4%)	42	77
2	B	615/639 (96%)	607 (99%)	8 (1%)	76	91
2	E	615/639 (96%)	608 (99%)	7 (1%)	80	92
3	C	246/249 (99%)	241 (98%)	5 (2%)	63	87
3	F	246/249 (99%)	240 (98%)	6 (2%)	57	84
4	G	124/131 (95%)	124 (100%)	0	100	100
4	I	124/131 (95%)	124 (100%)	0	100	100
5	H	193/193 (100%)	190 (98%)	3 (2%)	70	90
5	J	193/193 (100%)	192 (100%)	1 (0%)	92	97
All	All	3470/3548 (98%)	3406 (98%)	64 (2%)	66	88

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	PHE
1	A	44	GLN
1	A	97	CYS
1	A	130	ILE
1	A	143	LEU
1	A	156	VAL
1	A	177	MET
1	A	201	ASP
1	A	254	THR
1	A	264	LEU
1	A	360	TRP
1	A	523	LYS
1	A	548	TYR
1	A	664	ARG
2	B	709	ARG
2	B	712	MET

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Mol	Chain	Res	Type
2	B	747	ARG
2	B	806	TRP
2	B	1010	CYS
2	B	1304	ASP
2	B	1366	ILE
2	B	1387	LEU
3	C	1512	VAL
3	C	1577	ARG
3	C	1623	VAL
3	C	1689	ASP
3	C	1743	GLN
1	D	81	ASP
1	D	102	LEU
1	D	130	ILE
1	D	143	LEU
1	D	155	ARG
1	D	157	ARG
1	D	159	ARG
1	D	175	THR
1	D	243	VAL
1	D	263	GLN
1	D	264	LEU
1	D	287	LEU
1	D	327	ASN
1	D	337	ARG
1	D	340	VAL
1	D	360	TRP
1	D	422	GLN
1	D	523	LYS
1	D	548	TYR
1	D	654	PHE
2	E	712	MET
2	E	920	GLU
2	E	1010	CYS
2	E	1304	ASP
2	E	1365	LYS
2	E	1366	ILE
2	E	1387	LEU
3	F	1480	LEU
3	F	1512	VAL
3	F	1523	LEU
3	F	1602	LEU

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Mol	Chain	Res	Type
3	F	1612	TYR
3	F	1654	THR
5	H	463	LEU
5	H	563	ARG
5	H	583	ARG
5	J	555	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	535	HIS
1	D	536	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
2	TYS	B	1417	2	14,16,17	0.90	0	16,22,24	1.09	2 (12%)
2	TYS	B	1420	2	14,16,17	0.90	0	16,22,24	1.12	3 (18%)
2	TYS	E	1417	2	14,16,17	0.91	0	16,22,24	1.01	2 (12%)
2	TYS	E	1420	2	14,16,17	0.89	0	16,22,24	1.05	3 (18%)

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
2	TYS	B	1417	2	-	0/9/11/13	0/1/1/1
2	TYS	B	1420	2	-	0/9/11/13	0/1/1/1
2	TYS	E	1417	2	-	0/9/11/13	0/1/1/1
2	TYS	E	1420	2	-	0/9/11/13	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( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	1417	TYS	O2-S-O1	-2.44	100.97	112.29
2	B	1420	TYS	O2-S-O1	-2.40	101.20	112.29
2	B	1420	TYS	CG-CB-CA	-2.33	108.74	114.12
2	B	1417	TYS	O-C-CA	-2.26	119.65	125.72
2	E	1417	TYS	O-C-CA	-2.25	119.70	125.72
2	E	1420	TYS	CG-CB-CA	-2.20	109.06	114.12
2	B	1420	TYS	O-C-CA	-2.15	119.97	125.72
2	E	1420	TYS	O-C-CA	-2.09	120.13	125.72
2	E	1417	TYS	O3-S-O1	-2.06	101.04	108.89
2	E	1420	TYS	O3-S-O2	-2.03	101.13	108.89

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
2	E	1417	TYS	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

18 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	$\# Z  > 2$
6	NAG	A	701	1,6	14,14,15	0.24	0	15,19,21	0.36	0
6	NAG	A	702	7,6	14,14,15	0.23	0	15,19,21	0.33	0
7	BMA	A	703	6	11,11,12	0.58	0	15,15,17	0.70	0
6	NAG	B	1501	2,6	14,14,15	0.19	0	15,19,21	0.32	0
6	NAG	B	1502	7,6	14,14,15	0.25	0	15,19,21	0.42	0
7	BMA	B	1503	6	11,11,12	0.59	0	15,15,17	0.68	0
6	NAG	B	1504	2,6	14,14,15	0.29	0	15,19,21	0.34	0
6	NAG	B	1505	7,6	14,14,15	0.27	0	15,19,21	0.50	0
7	BMA	B	1506	6	11,11,12	0.54	0	15,15,17	0.81	0
6	NAG	D	701	1,6	14,14,15	0.24	0	15,19,21	0.32	0
6	NAG	D	702	7,6	14,14,15	0.23	0	15,19,21	0.31	0
7	BMA	D	703	6	11,11,12	0.56	0	15,15,17	0.68	0
6	NAG	E	1501	2,6	14,14,15	0.25	0	15,19,21	0.36	0
6	NAG	E	1502	7,6	14,14,15	0.22	0	15,19,21	0.31	0
7	BMA	E	1503	6	11,11,12	0.54	0	15,15,17	0.73	0
6	NAG	E	1504	2,6	14,14,15	0.27	0	15,19,21	0.39	0
6	NAG	E	1505	7,6	14,14,15	0.18	0	15,19,21	0.38	0
7	BMA	E	1506	6	11,11,12	0.62	0	15,15,17	0.78	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	A	701	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	702	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	703	6	-	0/2/19/22	0/1/1/1
6	NAG	B	1501	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1502	7,6	-	0/6/23/26	0/1/1/1
7	BMA	B	1503	6	-	0/2/19/22	0/1/1/1
6	NAG	B	1504	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1505	7,6	-	0/6/23/26	0/1/1/1
7	BMA	B	1506	6	-	0/2/19/22	0/1/1/1
6	NAG	D	701	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	702	7,6	-	0/6/23/26	0/1/1/1
7	BMA	D	703	6	-	0/2/19/22	0/1/1/1
6	NAG	E	1501	2,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1502	7,6	-	0/6/23/26	0/1/1/1
7	BMA	E	1503	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	E	1504	2,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1505	7,6	-	0/6/23/26	0/1/1/1
7	BMA	E	1506	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	651/656 (99%)	-0.26	0 100 100	86, 135, 179, 201	0
1	D	651/656 (99%)	-0.30	1 (0%) 95 91	82, 122, 170, 205	0
2	B	738/767 (96%)	-0.17	11 (1%) 76 62	85, 131, 178, 239	0
2	E	738/767 (96%)	-0.17	8 (1%) 82 69	91, 135, 199, 257	0
3	C	287/291 (98%)	-0.32	0 100 100	74, 111, 154, 186	0
3	F	287/291 (98%)	-0.23	2 (0%) 89 80	74, 115, 161, 218	0
4	G	145/154 (94%)	-0.41	1 (0%) 89 80	117, 143, 178, 213	0
4	I	145/154 (94%)	-0.21	4 (2%) 56 40	121, 146, 199, 232	0
5	H	242/242 (100%)	0.12	6 (2%) 61 44	160, 205, 245, 258	0
5	J	242/242 (100%)	-0.06	2 (0%) 87 77	104, 154, 202, 234	0
All	All	4126/4220 (97%)	-0.21	35 (0%) 87 77	74, 133, 202, 258	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1236	SER	6.7
2	E	1242	SER	5.1
2	B	1242	SER	4.8
2	B	1237	GLN	4.3
2	B	1235	GLY	3.5
5	J	611	SER	3.4
2	B	1129	GLN	3.1
5	H	567	ILE	3.0
5	H	445	ILE	2.9
2	E	1241	VAL	2.9
5	J	445	ILE	2.8
4	G	439	ARG	2.8
2	B	1240	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	1241	VAL	2.8
2	E	760	ILE	2.7
2	B	1245	PRO	2.7
5	H	453	PRO	2.6
2	E	1240	ALA	2.5
5	H	465	GLY	2.5
2	B	1130	GLY	2.5
1	D	104	ARG	2.5
2	E	1238	SER	2.4
2	B	860	ASP	2.4
2	E	1243	PRO	2.4
5	H	626	LYS	2.3
3	F	1460	GLU	2.3
4	I	297	ALA	2.3
2	B	1238	SER	2.2
3	F	1477	LYS	2.2
4	I	296	THR	2.2
4	I	351	ASP	2.2
5	H	499	MET	2.1
4	I	350	LYS	2.1
2	E	1239	ASN	2.1
2	E	1129	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
2	TYS	B	1417	16/17	0.76	0.34	-	197,209,219,226	0
2	TYS	E	1420	16/17	0.40	0.49	-	241,269,310,311	0
2	TYS	B	1420	16/17	0.48	0.39	-	236,247,264,264	0
2	TYS	E	1417	16/17	0.66	0.36	-	218,242,263,264	0

## 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
6	NAG	E	1504	14/15	0.90	0.20	-0.76	210,217,220,221	0
6	NAG	B	1504	14/15	0.88	0.12	-1.00	220,227,232,233	0
6	NAG	A	701	14/15	0.94	0.19	-	143,148,158,160	0
7	BMA	E	1503	11/12	0.75	0.29	-	239,249,265,267	0
6	NAG	E	1502	14/15	0.87	0.29	-	201,211,226,232	0
7	BMA	B	1503	11/12	0.64	0.43	-	302,309,311,313	0
6	NAG	D	702	14/15	0.90	0.17	-	169,179,189,193	0
7	BMA	D	703	11/12	0.72	0.28	-	197,212,219,225	0
6	NAG	E	1501	14/15	0.90	0.33	-	189,195,200,203	0
7	BMA	B	1506	11/12	0.66	0.33	-	232,237,241,242	0
6	NAG	E	1505	14/15	0.77	0.24	-	202,205,207,208	0
6	NAG	B	1502	14/15	0.62	0.38	-	300,306,310,312	0
7	BMA	E	1506	11/12	0.59	0.25	-	202,204,206,206	0
6	NAG	A	702	14/15	0.93	0.12	-	162,171,180,181	0
6	NAG	B	1501	14/15	0.87	0.31	-	309,315,319,319	0
6	NAG	D	701	14/15	0.93	0.16	-	143,151,162,165	0
6	NAG	B	1505	14/15	0.74	0.31	-	224,232,239,240	0
7	BMA	A	703	11/12	0.68	0.22	-	187,197,203,210	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.