



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:13 am GMT

PDB ID : 3NID  
Title : The Closed Headpiece of Integrin  $\alpha$ IIB  $\beta$ 3 and its Complex with an  $\alpha$ IIB  $\beta$ 3 -Specific Antagonist That Does Not Induce Opening  
Authors : Zhu, J.H.; Zhu, J.Q.; Springer, T.A.  
Deposited on : 2010-06-15  
Resolution : 2.30 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28683  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

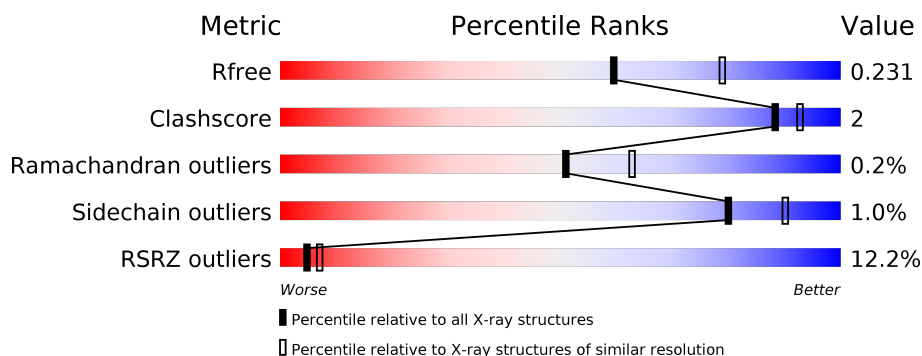
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	457	<div> <div></div> <div>94% 5% .</div> </div>
1	C	457	<div> <div></div> <div>94% 5% .</div> </div>
2	B	471	<div> <div>14%</div> <div>91% 7% .</div> </div>
2	D	471	<div> <div>9%</div> <div>95% 5%</div> </div>
3	E	221	<div> <div>34%</div> <div>87% 10% .</div> </div>
3	H	221	<div> <div>16%</div> <div>86% 12% .</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	214	
4	L	214	

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
10	MAN	B	3322	X	-	-	-
12	MAN	D	3322	X	-	-	-
6	GOL	A	460	-	-	-	X
6	GOL	A	463	-	-	-	X
6	GOL	C	458	-	-	-	X
7	SO4	A	464	-	-	-	X
7	SO4	B	473	-	-	-	X
7	SO4	C	460	-	-	-	X
7	SO4	C	461	-	-	-	X
7	SO4	D	472	-	-	-	X
7	SO4	D	473	-	-	-	X
7	SO4	H	222	-	-	-	X
7	SO4	L	215	-	-	-	X
8	MG	D	2001	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 22131 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 Integrin alpha-IIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	5	0
			3504	2229	602	665	8			
1	C	453	Total	C	N	O	S	0	2	0
			3484	2214	600	662	8			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	4	2	0
			3601	2243	615	710	33			
2	D	471	Total	C	N	O	S	3	1	0
			3634	2265	620	715	34			

- Molecule 3 is a protein called Monoclonal antibody 10E5 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1631	1035	264	326	6			
3	H	216	Total	C	N	O	S	0	0	0
			1642	1041	266	329	6			

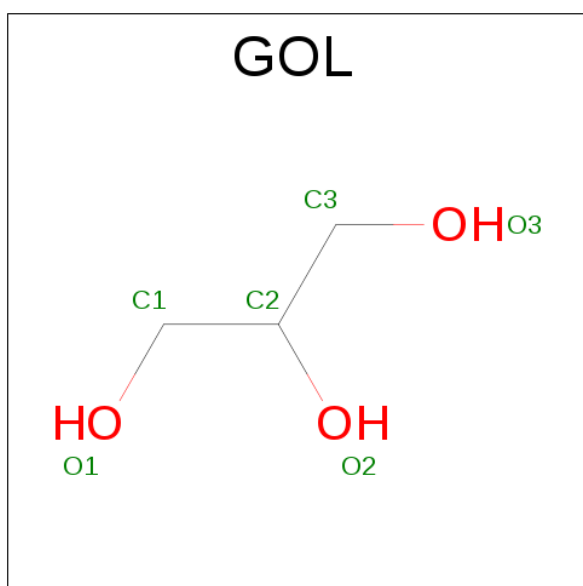
- Molecule 4 is a protein called Monoclonal antibody 10E5 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			
4	L	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Ca 2 2	0	0
5	A	4	Total Ca 4 4	0	0
5	D	2	Total Ca 2 2	0	0
5	C	4	Total Ca 4 4	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

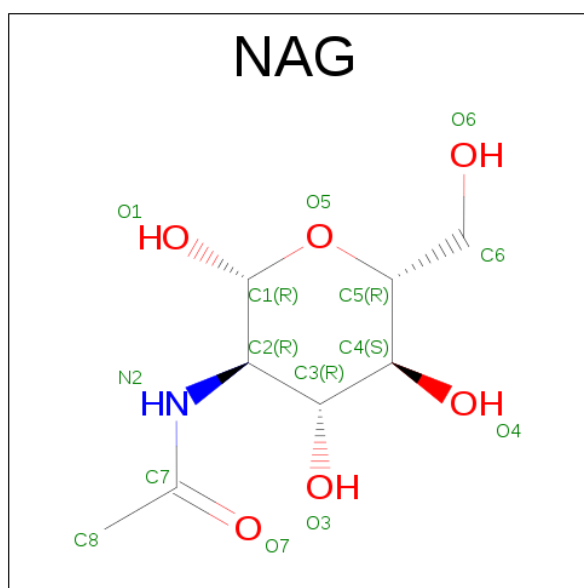


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		

- Molecule 9 is SUGAR (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
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 12 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	386	Total	O	0	0
			386	386		
13	B	192	Total	O	0	0
			192	192		
13	C	205	Total	O	0	0
			205	205		
13	D	182	Total	O	0	0
			182	182		
13	E	12	Total	O	0	0
			12	12		
13	F	12	Total	O	0	0
			12	12		
13	H	32	Total	O	0	0
			32	32		
13	L	38	Total	O	0	0
			38	38		



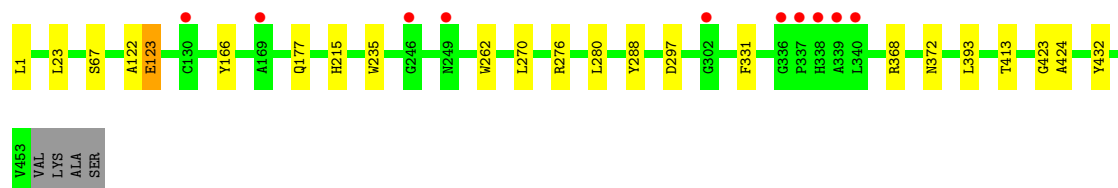
### 3 Residue-property plots [i](#)

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

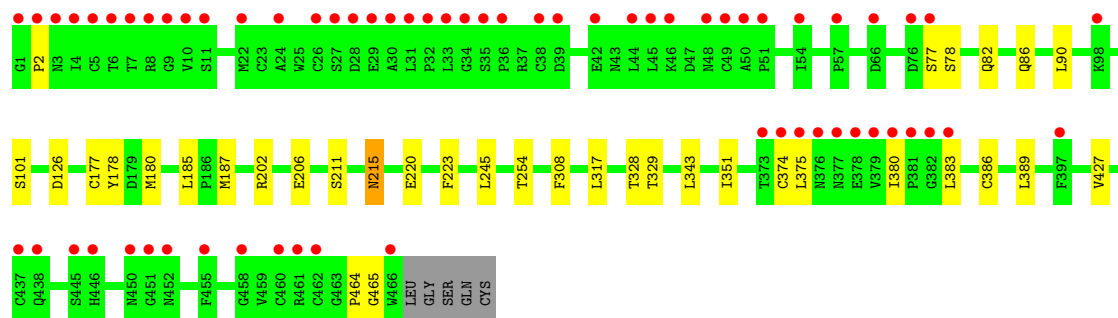
#### • Molecule 1: Integrin alpha-IIb



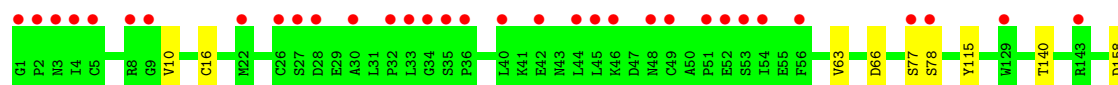
#### • Molecule 1: Integrin alpha-IIb



#### • Molecule 2: Integrin beta-3

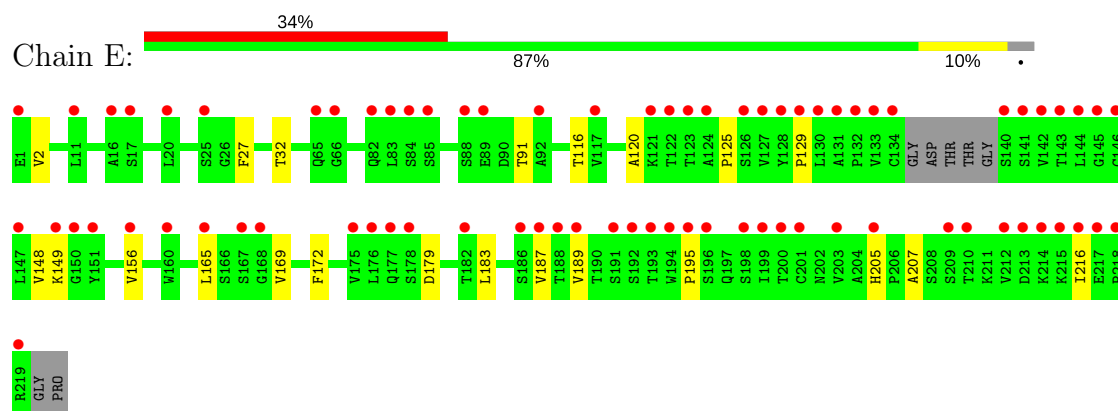


#### • Molecule 2: Integrin beta-3

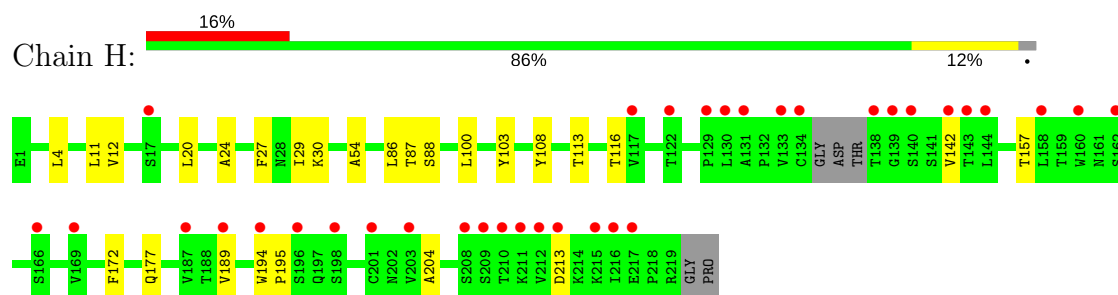




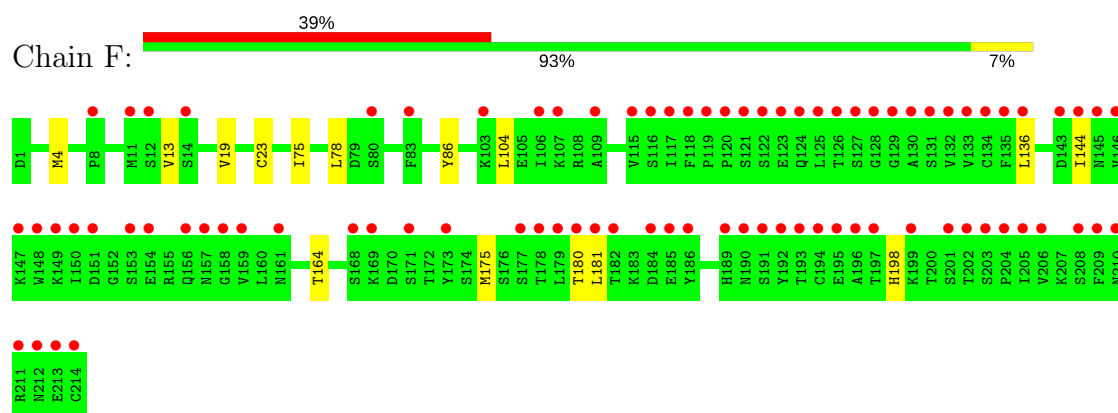
- Molecule 3: Monoclonal antibody 10E5 heavy chain



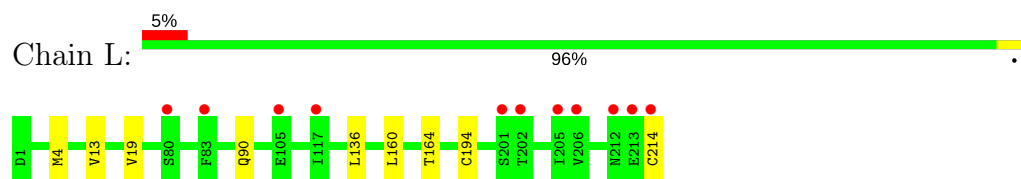
- Molecule 3: Monoclonal antibody 10E5 heavy chain



- Molecule 4: Monoclonal antibody 10E5 light chain



- Molecule 4: Monoclonal antibody 10E5 light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	258.97Å 144.49Å 104.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.21 – 2.30 48.21 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.21-2.30) 97.8 (48.21-2.30)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	0.01	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.179 , 0.215 0.192 , 0.231	Depositor DCC
$R_{free}$ test set	1029 reflections (0.61%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22131	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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: GOL, MG, NAG, CA, SO4, MAN

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	0/3616	0.61	0/4929
1	C	0.38	0/3587	0.57	0/4888
2	B	0.38	0/3674	0.56	0/4982
2	D	0.37	0/3706	0.53	0/5026
3	E	0.31	0/1673	0.46	0/2290
3	H	0.32	0/1684	0.49	0/2305
4	F	0.32	0/1673	0.46	0/2269
4	L	0.33	0/1673	0.51	0/2269
All	All	0.37	0/21286	0.54	0/28958

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	B	1	0
12	D	1	0
All	All	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	3322	MAN	C1
12	D	3322	MAN	C1

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	3504	0	3351	14	0
1	C	3484	0	3320	11	0
2	B	3601	0	3525	19	0
2	D	3634	0	3551	14	0
3	E	1631	0	1590	14	0
3	H	1642	0	1600	16	0
4	F	1637	0	1553	10	0
4	L	1637	0	1553	6	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	4	0	0	0	0
5	D	2	0	0	0	0
6	A	36	0	48	1	0
6	B	6	0	8	0	0
6	C	12	0	16	0	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	20	0	0	0	0
7	D	10	0	0	0	0
7	H	5	0	0	0	0
7	L	5	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	B	14	0	13	0	0
9	D	14	0	13	0	0
10	B	61	0	52	0	0
11	B	28	0	25	0	0
11	D	28	0	25	1	0
12	D	39	0	34	0	0
13	A	386	0	0	1	0
13	B	192	0	0	1	0
13	C	205	0	0	1	0
13	D	182	0	0	1	0
13	E	12	0	0	0	0
13	F	12	0	0	0	0
13	H	32	0	0	0	0
13	L	38	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22131	0	20277	93	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 2.

All (93) 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)
4:L:13:VAL:HG11	4:L:19:VAL:HG11	1.73	0.70
3:E:165:LEU:HD23	3:E:187:VAL:HG21	1.74	0.69
2:B:90:LEU:HD13	2:B:427:VAL:HG13	1.78	0.64
3:E:169:VAL:HG22	3:E:187:VAL:HG23	1.80	0.61
1:A:276:ARG:NH1	13:A:931:HOH:O	2.34	0.61
3:E:120:ALA:HB2	3:E:179:ASP:O	2.01	0.60
3:E:129:PRO:HB2	3:E:216:ILE:HD13	1.83	0.60
3:E:205:HIS:CE1	3:E:207:ALA:HB3	2.36	0.60
3:E:129:PRO:CB	3:E:216:ILE:HD13	2.31	0.60
2:D:63:VAL:HG11	2:D:66:ASP:HB2	1.83	0.60
1:C:235:TRP:CZ2	1:C:270:LEU:HD11	2.42	0.55
3:E:2:VAL:HG13	3:E:27:PHE:CE1	2.42	0.55
1:A:280:LEU:CD1	1:A:306:LEU:HD23	2.37	0.54
2:B:380:ILE:HG21	2:B:383:LEU:HD22	1.89	0.53
2:B:245:LEU:HD22	2:B:351:ILE:HD13	1.90	0.52
1:A:285:MET:HE1	2:B:317:LEU:HD12	1.92	0.52
4:F:86:TYR:CE1	4:F:104:LEU:HD22	2.45	0.52
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.91	0.52
2:D:235:LYS:HE3	2:D:276:GLY:O	2.10	0.52
2:D:249:THR:HG22	2:D:309:ALA:HB3	1.92	0.51
2:D:158:ASP:HB3	2:D:187:MET:CE	2.41	0.51
3:H:4:LEU:N	3:H:4:LEU:HD12	2.26	0.51
3:H:177:GLN:HB2	4:L:160:LEU:HD21	1.92	0.51
1:A:345:LEU:HD21	1:A:347:LEU:HD21	1.93	0.51
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.43	0.50
1:A:189:TYR:O	1:A:192:LEU:HD13	2.12	0.49
1:C:413:THR:HG23	13:C:731:HOH:O	2.12	0.49
1:A:122:ALA:O	1:A:123:GLU:HB2	2.13	0.49
1:C:1:LEU:HB2	1:C:393:LEU:HD11	1.94	0.48
1:A:8:LEU:HD21	1:A:448:TYR:CE2	2.49	0.48
4:F:13:VAL:HG11	4:F:19:VAL:HG11	1.96	0.48
1:A:401:SER:H	6:A:458:GOL:H2	1.78	0.48
2:B:329:THR:HG23	13:B:503:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:LEU:HD23	1:C:276:ARG:HA	1.96	0.47
3:E:149:LYS:NZ	4:F:180:THR:HG21	2.30	0.47
2:B:185:LEU:HG	2:B:211:SER:OG	2.15	0.47
2:D:202:ARG:NH1	13:D:515:HOH:O	2.40	0.47
4:F:136:LEU:N	4:F:136:LEU:HD12	2.30	0.47
2:B:308:PHE:CE2	2:B:328:THR:HG21	2.50	0.47
2:D:306:LEU:HB3	2:D:328:THR:HG22	1.96	0.47
2:D:400:GLU:HB2	11:D:3371:NAG:H83	1.97	0.47
3:H:30:LYS:HG3	3:H:54:ALA:HB2	1.97	0.46
2:B:223:PHE:CZ	2:B:254:THR:HG21	2.49	0.46
2:B:386:CYS:HB3	2:B:389:LEU:HD11	1.98	0.46
4:L:4:MET:HE2	4:L:90:GLN:HB3	1.98	0.46
1:C:262:TRP:HB3	2:D:317:LEU:HD13	1.96	0.46
1:C:122:ALA:O	1:C:123:GLU:HB2	2.16	0.45
2:D:10:VAL:HG21	2:D:16:CYS:HB2	1.99	0.45
3:H:11:LEU:HD12	3:H:116:THR:HB	1.99	0.45
4:F:75:ILE:HG21	4:F:78:LEU:HD23	1.98	0.45
2:B:77:SER:N	2:B:78:SER:HA	2.32	0.45
4:L:136:LEU:N	4:L:136:LEU:HD12	2.32	0.45
3:H:172:PHE:CD1	4:L:164:THR:HG23	2.52	0.45
3:H:24:ALA:HB1	3:H:27:PHE:CZ	2.52	0.44
2:D:249:THR:HA	2:D:309:ALA:O	2.17	0.44
1:A:262:TRP:HB3	2:B:317:LEU:HD13	1.98	0.44
2:B:177:CYS:HB3	2:B:180:MET:HE2	2.00	0.44
2:B:90:LEU:HD13	2:B:427:VAL:CG1	2.45	0.44
1:C:215:HIS:CD2	3:E:32:THR:HG22	2.53	0.44
4:F:144:ILE:HG23	4:F:198:HIS:CD2	2.52	0.44
3:E:165:LEU:HD21	3:E:189:VAL:CG1	2.48	0.43
2:B:220:GLU:OE1	2:B:220:GLU:HA	2.18	0.43
3:H:100:LEU:HD13	3:H:108:TYR:OH	2.18	0.43
3:H:142:VAL:HG12	3:H:189:VAL:O	2.17	0.43
2:D:77:SER:HA	2:D:78:SER:HA	1.62	0.43
1:A:280:LEU:HD11	1:A:306:LEU:HD23	1.99	0.43
4:F:144:ILE:HD13	4:F:175:MET:SD	2.58	0.43
1:A:213:LEU:HD13	3:H:103:TYR:CD2	2.54	0.43
2:B:464:PRO:HA	2:B:465:GLY:HA2	1.73	0.43
4:F:4:MET:CE	4:F:23:CYS:SG	3.06	0.43
1:C:368:ARG:HD3	1:C:432:TYR:CE2	2.54	0.43
3:H:20:LEU:HD22	3:H:113:THR:HG21	2.01	0.42
3:E:172:PHE:CD1	4:F:164:THR:HG23	2.54	0.42
3:H:24:ALA:HB2	3:H:29:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:TYR:CZ	2:D:236:ILE:HD12	2.55	0.42
3:E:125:PRO:HB2	3:E:148:VAL:HG13	2.01	0.42
3:H:177:GLN:CB	4:L:160:LEU:HD21	2.50	0.42
2:D:218:ALA:HB3	2:D:219:PRO:HD3	2.01	0.42
3:E:91:THR:HG23	3:E:116:THR:HA	2.02	0.42
3:H:157:THR:OG1	3:H:204:ALA:HB3	2.19	0.41
2:B:187:MET:CE	2:B:215:ASN:HB3	2.49	0.41
1:C:297:ASP:O	1:C:372:ASN:HB2	2.21	0.41
1:A:158:ASN:HA	2:D:140:THR:HG21	2.02	0.41
3:E:156:VAL:CG2	3:E:183:LEU:HD13	2.51	0.41
3:H:194:TRP:CG	3:H:195:PRO:HA	2.56	0.41
3:H:87:THR:HG22	3:H:88:SER:N	2.35	0.41
1:A:8:LEU:HD21	1:A:448:TYR:CD2	2.56	0.41
4:F:4:MET:HE1	4:F:23:CYS:SG	2.61	0.40
1:A:9:THR:HB	1:A:447:VAL:HB	2.02	0.40
2:B:343:LEU:C	2:B:343:LEU:HD23	2.42	0.40
2:B:126:ASP:N	2:B:126:ASP:OD1	2.55	0.40
1:C:280:LEU:HD13	1:C:331:PHE:CE1	2.56	0.40
1:C:423:GLY:O	1:C:424:ALA:HB3	2.20	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	457/457 (100%)	444 (97%)	12 (3%)	1 (0%)	51 63
1	C	453/457 (99%)	440 (97%)	12 (3%)	1 (0%)	51 63
2	B	466/471 (99%)	451 (97%)	13 (3%)	2 (0%)	38 47
2	D	470/471 (100%)	457 (97%)	13 (3%)	0	100 100
3	E	210/221 (95%)	200 (95%)	9 (4%)	1 (0%)	32 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	212/221 (96%)	203 (96%)	9 (4%)	0	100	100
4	F	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
4	L	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
All	All	2692/2726 (99%)	2608 (97%)	79 (3%)	5 (0%)	51	63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	375	LEU
1	C	123	GLU
2	B	2	PRO
3	E	195	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	367/364 (101%)	362 (99%)	5 (1%)	71	85
1	C	363/364 (100%)	358 (99%)	5 (1%)	71	85
2	B	414/416 (100%)	408 (99%)	6 (1%)	71	85
2	D	417/416 (100%)	413 (99%)	4 (1%)	80	90
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	186 (100%)	1 (0%)	91	96
4	F	188/188 (100%)	187 (100%)	1 (0%)	91	96
4	L	188/188 (100%)	186 (99%)	2 (1%)	78	89
All	All	2310/2316 (100%)	2286 (99%)	24 (1%)	80	90

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU

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Mol	Chain	Res	Type
1	A	166	TYR
1	A	190	TYR
1	A	270	LEU
1	A	288	TYR
2	B	82	GLN
2	B	86	GLN
2	B	101	SER
2	B	178	TYR
2	B	215	ASN
2	B	374	CYS
1	C	23	LEU
1	C	67	SER
1	C	166	TYR
1	C	177	GLN
1	C	288	TYR
2	D	178	TYR
2	D	202	ARG
2	D	215	ASN
2	D	462	CYS
4	F	181	LEU
3	H	213	ASP
4	L	194	CYS
4	L	214	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	301	GLN
1	C	15	ASN
1	C	177	GLN
4	F	124	GLN
3	H	170	HIS
4	L	138	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 ⓘ

12 carbohydrates 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	$\# Z  > 2$
10	NAG	B	3320	10,2	14,14,15	0.49	0	15,19,21	1.11	2 (13%)
10	NAG	B	3321	10	14,14,15	0.57	0	15,19,21	1.18	2 (13%)
10	MAN	B	3322	10	11,11,12	0.57	0	13,15,17	1.47	2 (15%)
10	MAN	B	3323	10	11,11,12	0.55	0	13,15,17	0.65	0
10	MAN	B	3324	10	11,11,12	0.63	0	13,15,17	1.24	2 (15%)
11	NAG	B	3371	11,2	14,14,15	0.58	0	15,19,21	0.76	0
11	NAG	B	3372	11	14,14,15	0.48	0	15,19,21	1.06	1 (6%)
12	NAG	D	3320	12,2	14,14,15	0.48	0	15,19,21	1.29	2 (13%)
12	NAG	D	3321	12	14,14,15	0.56	0	15,19,21	0.83	0
12	MAN	D	3322	12	11,11,12	0.47	0	13,15,17	1.55	1 (7%)
11	NAG	D	3371	11,2	14,14,15	0.55	0	15,19,21	0.84	0
11	NAG	D	3372	11	14,14,15	0.49	0	15,19,21	0.83	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
10	NAG	B	3320	10,2	-	0/6/23/26	0/1/1/1
10	NAG	B	3321	10	-	0/6/23/26	0/1/1/1
10	MAN	B	3322	10	1/1/4/5	0/2/19/22	0/1/1/1
10	MAN	B	3323	10	-	0/2/19/22	0/1/1/1
10	MAN	B	3324	10	-	0/2/19/22	0/1/1/1
11	NAG	B	3371	11,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	B	3372	11	-	0/6/23/26	0/1/1/1
12	NAG	D	3320	12,2	-	0/6/23/26	0/1/1/1
12	NAG	D	3321	12	-	0/6/23/26	0/1/1/1
12	MAN	D	3322	12	1/1/4/5	0/2/19/22	1/1/1/1
11	NAG	D	3371	11,2	-	0/6/23/26	0/1/1/1
11	NAG	D	3372	11	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	3324	MAN	O5-C1-C2	-2.89	106.26	110.79
10	B	3320	NAG	O5-C1-C2	-2.66	107.77	111.47
12	D	3320	NAG	O5-C1-C2	-2.60	107.86	111.47
11	B	3372	NAG	O5-C1-C2	-2.29	108.29	111.47
10	B	3322	MAN	O5-C1-C2	-2.13	107.45	110.79
10	B	3324	MAN	C1-O5-C5	2.03	114.96	112.17
10	B	3320	NAG	C1-O5-C5	2.46	115.55	112.17
10	B	3321	NAG	C3-C4-C5	2.68	114.94	110.22
10	B	3321	NAG	C4-C3-C2	2.93	115.31	111.02
10	B	3322	MAN	C3-C4-C5	3.38	116.18	110.22
12	D	3320	NAG	C1-O5-C5	3.47	116.95	112.17
12	D	3322	MAN	C1-O5-C5	5.13	119.24	112.17

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	3322	MAN	C1
12	D	3322	MAN	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	D	3322	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	3371	NAG	1	0

## 5.6 Ligand geometry

Of 35 ligands modelled in this entry, 14 are monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
6	GOL	A	458	-	5,5,5	0.35	0	5,5,5	0.29	0
6	GOL	A	459	-	5,5,5	0.38	0	5,5,5	0.22	0
6	GOL	A	460	-	5,5,5	0.33	0	5,5,5	0.45	0
6	GOL	A	461	-	5,5,5	0.22	0	5,5,5	0.38	0
6	GOL	A	462	-	5,5,5	0.34	0	5,5,5	0.16	0
6	GOL	A	463	-	5,5,5	0.34	0	5,5,5	0.21	0
7	SO4	A	464	-	4,4,4	0.18	0	6,6,6	0.05	0
9	NAG	B	3099	2	14,14,15	0.57	0	15,19,21	0.90	1 (6%)
6	GOL	B	472	-	5,5,5	0.30	0	5,5,5	0.25	0
7	SO4	B	473	-	4,4,4	0.16	0	6,6,6	0.17	0
6	GOL	C	458	-	5,5,5	0.23	0	5,5,5	0.35	0
6	GOL	C	459	-	5,5,5	0.38	0	5,5,5	0.22	0
7	SO4	C	460	-	4,4,4	0.17	0	6,6,6	0.26	0
7	SO4	C	461	-	4,4,4	0.16	0	6,6,6	0.25	0
7	SO4	C	462	-	4,4,4	0.17	0	6,6,6	0.10	0
7	SO4	C	463	-	4,4,4	0.15	0	6,6,6	0.12	0
9	NAG	D	3099	2	14,14,15	0.59	0	15,19,21	0.87	0
7	SO4	D	472	-	4,4,4	0.18	0	6,6,6	0.13	0
7	SO4	D	473	-	4,4,4	0.15	0	6,6,6	0.10	0
7	SO4	H	222	-	4,4,4	0.16	0	6,6,6	0.06	0
7	SO4	L	215	-	4,4,4	0.15	0	6,6,6	0.11	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	GOL	A	458	-	-	0/4/4/4	0/0/0/0
6	GOL	A	459	-	-	0/4/4/4	0/0/0/0
6	GOL	A	460	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	461	-	-	0/4/4/4	0/0/0/0
6	GOL	A	462	-	-	0/4/4/4	0/0/0/0
6	GOL	A	463	-	-	0/4/4/4	0/0/0/0
7	SO4	A	464	-	-	0/0/0/0	0/0/0/0
9	NAG	B	3099	2	-	0/6/23/26	0/1/1/1
6	GOL	B	472	-	-	0/4/4/4	0/0/0/0
7	SO4	B	473	-	-	0/0/0/0	0/0/0/0
6	GOL	C	458	-	-	0/4/4/4	0/0/0/0
6	GOL	C	459	-	-	0/4/4/4	0/0/0/0
7	SO4	C	460	-	-	0/0/0/0	0/0/0/0
7	SO4	C	461	-	-	0/0/0/0	0/0/0/0
7	SO4	C	462	-	-	0/0/0/0	0/0/0/0
7	SO4	C	463	-	-	0/0/0/0	0/0/0/0
9	NAG	D	3099	2	-	0/6/23/26	0/1/1/1
7	SO4	D	472	-	-	0/0/0/0	0/0/0/0
7	SO4	D	473	-	-	0/0/0/0	0/0/0/0
7	SO4	H	222	-	-	0/0/0/0	0/0/0/0
7	SO4	L	215	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	3099	NAG	C1-O5-C5	2.18	115.17	112.17

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
6	A	458	GOL	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	454/457 (99%)	0.38	6 (1%) 77 81	9, 20, 49, 89	0
1	C	453/457 (99%)	0.24	10 (2%) 62 69	15, 32, 63, 106	0
2	B	466/471 (98%)	0.86	65 (13%) 3 5	10, 44, 127, 170	1 (0%)
2	D	471/471 (100%)	0.54	43 (9%) 10 14	16, 41, 101, 142	1 (0%)
3	E	214/221 (96%)	1.88	76 (35%) 0 0	41, 96, 147, 161	0
3	H	216/221 (97%)	0.66	35 (16%) 2 3	24, 73, 143, 176	0
4	F	214/214 (100%)	1.85	84 (39%) 0 0	41, 91, 143, 170	1 (0%)
4	L	214/214 (100%)	0.30	11 (5%) 29 36	26, 57, 104, 194	1 (0%)
All	All	2702/2726 (99%)	0.72	330 (12%) 5 7	9, 44, 128, 194	4 (0%)

All (330) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	212	VAL	13.5
4	F	214	CYS	12.6
3	E	133	VAL	11.8
2	B	33	LEU	11.3
3	E	201	CYS	11.0
4	F	181	LEU	9.1
3	E	216	ILE	8.7
3	E	131	ALA	8.6
2	B	77	SER	8.4
3	E	134	CYS	8.4
2	D	469	SER	8.1
4	F	126	THR	8.1
3	E	219	ARG	8.0
4	L	214	CYS	7.9
2	B	44	LEU	7.9
3	E	194	TRP	7.8

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Mol	Chain	Res	Type	RSRZ
2	B	30	ALA	7.8
2	D	471	CYS	7.4
1	A	337	PRO	7.4
2	B	36	PRO	7.4
4	F	212	ASN	7.4
4	F	125	LEU	7.2
4	F	122	SER	7.1
4	F	148	TRP	7.0
4	F	193	THR	6.8
4	F	130	ALA	6.7
3	H	133	VAL	6.4
3	H	134	CYS	6.4
4	F	179	LEU	6.4
3	E	142	VAL	6.3
3	E	144	LEU	6.3
3	E	129	PRO	6.2
2	B	375	LEU	6.2
3	E	200	THR	6.1
2	B	10	VAL	6.1
3	E	215	LYS	6.0
2	B	76	ASP	6.0
4	F	180	THR	5.7
3	E	147	LEU	5.6
2	B	34	GLY	5.6
4	F	210	ASN	5.5
3	E	192	SER	5.5
2	B	4	ILE	5.4
4	F	129	GLY	5.4
3	E	196	SER	5.4
2	D	470	GLN	5.4
3	E	210	THR	5.3
3	E	217	GLU	5.2
2	B	2	PRO	5.2
4	F	213	GLU	5.2
4	F	135	PHE	5.2
2	B	450	ASN	5.1
4	F	150	ILE	5.1
3	E	127	VAL	5.1
4	F	184	ASP	5.1
3	E	203	VAL	5.1
4	F	118	PHE	5.0
4	F	158	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
3	E	198	SER	5.0
3	E	218	PRO	4.9
2	D	51	PRO	4.9
2	B	46	LYS	4.8
2	B	374	CYS	4.8
3	E	130	LEU	4.8
3	E	165	LEU	4.8
4	F	119	PRO	4.8
2	B	446	HIS	4.8
2	B	28	ASP	4.7
2	D	44	LEU	4.7
4	F	147	LYS	4.6
3	E	117	VAL	4.6
2	B	32	PRO	4.6
2	B	45	LEU	4.6
3	E	199	ILE	4.6
3	E	132	PRO	4.6
2	B	7	THR	4.6
3	E	150	GLY	4.5
2	B	466	TRP	4.5
2	B	1	GLY	4.5
4	F	182	THR	4.5
4	F	136	LEU	4.5
4	F	127	SER	4.4
4	F	208	SER	4.4
2	D	2	PRO	4.4
3	E	126	SER	4.4
4	F	131	SER	4.3
2	B	8	ARG	4.3
2	D	33	LEU	4.3
3	E	195	PRO	4.2
2	B	31	LEU	4.2
1	A	339	ALA	4.2
2	B	39	ASP	4.2
4	F	120	PRO	4.2
2	D	9	GLY	4.2
3	E	128	TYR	4.2
3	H	187	VAL	4.1
2	D	1	GLY	4.1
4	F	196	ALA	4.1
4	F	116	SER	4.1
2	B	29	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
3	E	186	SER	4.1
4	F	115	VAL	4.1
4	F	154	GLU	4.1
4	F	195	GLU	4.0
3	E	160	TRP	4.0
2	B	376	ASN	4.0
4	F	134	CYS	4.0
2	B	42	GLU	4.0
3	E	213	ASP	4.0
3	H	189	VAL	4.0
2	B	35	SER	3.9
2	B	22	MET	3.9
3	E	83	LEU	3.9
3	E	143	THR	3.9
3	E	145	GLY	3.9
2	D	54	ILE	3.9
3	E	141	SER	3.9
4	F	132	VAL	3.9
4	F	186	TYR	3.8
2	B	3	ASN	3.8
3	E	123	THR	3.8
2	B	460	CYS	3.8
2	D	376	ASN	3.8
2	D	36	PRO	3.8
2	D	8	ARG	3.7
3	E	146	CYS	3.7
2	D	46	LYS	3.7
4	F	157	ASN	3.7
2	B	379	VAL	3.7
2	D	45	LEU	3.7
2	B	51	PRO	3.7
3	E	178	SER	3.6
2	B	383	LEU	3.6
3	E	167	SER	3.6
3	H	217	GLU	3.6
3	H	196	SER	3.6
2	D	4	ILE	3.6
2	B	452	ASN	3.5
3	E	168	GLY	3.5
2	D	30	ALA	3.5
3	E	16	ALA	3.5
2	D	35	SER	3.5

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Mol	Chain	Res	Type	RSRZ
3	H	216	ILE	3.5
3	H	158	LEU	3.4
4	F	206	VAL	3.4
2	B	9	GLY	3.4
2	D	22	MET	3.4
4	F	177	SER	3.4
3	E	187	VAL	3.4
3	E	177	GLN	3.3
3	H	144	LEU	3.3
1	A	336	GLY	3.3
3	E	149	LYS	3.3
1	C	336	GLY	3.3
3	E	191	SER	3.3
2	D	52	GLU	3.3
4	F	153	SER	3.3
4	F	209	PHE	3.3
2	D	3	ASN	3.3
4	F	159	VAL	3.3
2	B	26	CYS	3.2
2	D	375	LEU	3.2
4	F	121	SER	3.2
2	D	78	SER	3.2
3	E	85	SER	3.2
3	E	176	LEU	3.2
4	F	107	LYS	3.2
3	E	66	GLY	3.2
1	A	338	HIS	3.2
2	B	11	SER	3.2
4	F	145	ASN	3.2
4	F	192	TYR	3.2
2	B	445	SER	3.2
2	D	378	GLU	3.2
3	E	25	SER	3.1
3	E	189	VAL	3.1
4	F	133	VAL	3.1
3	H	215	LYS	3.1
4	L	202	THR	3.1
3	E	92	ALA	3.1
4	F	144	ILE	3.1
4	F	178	THR	3.0
2	D	468	GLY	3.0
4	F	106	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	48	ASN	3.0
4	F	185	GLU	3.0
4	F	117	ILE	3.0
3	E	175	VAL	3.0
3	H	169	VAL	3.0
2	D	42	GLU	3.0
4	F	151	ASP	3.0
4	F	204	PRO	3.0
1	C	338	HIS	3.0
3	E	122	THR	3.0
1	C	339	ALA	2.9
4	F	201	SER	2.9
4	F	128	GLY	2.9
4	L	205	ILE	2.9
2	B	381	PRO	2.9
2	D	32	PRO	2.9
3	E	214	LYS	2.9
4	F	146	VAL	2.9
2	B	6	THR	2.9
4	F	205	ILE	2.9
3	H	160	TRP	2.9
4	F	169	LYS	2.9
2	D	380	ILE	2.9
2	B	382	GLY	2.8
3	E	82	GLN	2.8
4	F	156	GLN	2.8
2	B	38	CYS	2.8
4	F	14	SER	2.8
4	L	212	ASN	2.8
4	L	206	VAL	2.8
2	B	458	GLY	2.8
2	B	5	CYS	2.8
2	B	455	PHE	2.7
3	H	203	VAL	2.7
4	F	123	GLU	2.7
3	E	84	SER	2.7
3	H	201	CYS	2.7
4	F	194	CYS	2.7
2	B	380	ILE	2.7
3	E	124	ALA	2.7
3	H	131	ALA	2.7
3	E	11	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	H	130	LEU	2.7
2	D	77	SER	2.7
3	H	117	VAL	2.7
4	F	109	ALA	2.6
3	E	121	LYS	2.6
4	F	80	SER	2.6
3	H	129	PRO	2.6
2	B	49	CYS	2.6
2	D	49	CYS	2.6
4	F	197	THR	2.6
3	E	209	SER	2.6
3	H	209	SER	2.6
3	E	89	GLU	2.6
2	B	397	PHE	2.6
4	F	173	TYR	2.6
3	E	205	HIS	2.6
2	B	54	ILE	2.6
3	H	143	THR	2.5
4	F	211	ARG	2.5
3	E	156	VAL	2.5
2	D	40	LEU	2.5
4	L	213	GLU	2.5
4	F	190	ASN	2.5
2	D	129[A]	TRP	2.5
2	D	53	SER	2.5
3	H	166	SER	2.5
4	F	191	SER	2.5
1	C	130	CYS	2.5
2	B	462	CYS	2.5
1	C	337	PRO	2.5
2	B	378	GLU	2.5
2	D	28	ASP	2.5
3	E	151	TYR	2.5
2	B	437	CYS	2.5
1	C	340	LEU	2.4
4	F	103	LYS	2.4
3	H	17	SER	2.4
2	B	373	THR	2.4
3	E	17	SER	2.4
4	F	124	GLN	2.4
4	F	149	LYS	2.4
4	F	11	MET	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	48	ASN	2.4
3	E	20	LEU	2.3
4	F	83	PHE	2.3
2	D	26	CYS	2.3
2	D	143	ARG	2.3
3	H	208	SER	2.3
3	H	213	ASP	2.3
2	D	34	GLY	2.3
3	E	182	THR	2.3
4	F	168	SER	2.3
3	E	65	GLN	2.3
2	B	50	ALA	2.3
3	H	122	THR	2.3
2	D	5	CYS	2.3
3	H	139	GLY	2.3
4	F	12	SER	2.3
1	C	246	GLY	2.2
3	H	162	SER	2.2
4	F	203	SER	2.2
1	C	169	ALA	2.2
3	E	188	THR	2.2
2	B	57	PRO	2.2
1	C	302	GLY	2.2
3	H	138	THR	2.2
4	F	199	LYS	2.2
2	B	27	SER	2.2
4	F	171	SER	2.2
4	F	8	PRO	2.2
2	B	438	GLN	2.2
4	F	189	HIS	2.2
2	B	451	GLY	2.2
2	B	461	ARG	2.1
3	H	142	VAL	2.1
4	F	202	THR	2.1
3	H	212	VAL	2.1
4	L	83	PHE	2.1
1	C	249	ASN	2.1
4	F	161	ASN	2.1
2	D	404	ARG	2.1
3	E	1	GLU	2.1
3	E	88	SER	2.1
4	L	80	SER	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	143	ASP	2.1
2	B	24	ALA	2.1
3	E	140	SER	2.1
3	H	194	TRP	2.1
2	D	27	SER	2.1
2	D	56	PHE	2.1
3	H	140	SER	2.1
3	H	198	SER	2.1
3	H	211	LYS	2.1
1	A	45	PRO	2.1
4	L	117	ILE	2.1
2	B	66	ASP	2.1
2	B	377	ASN	2.1
4	L	105	GLU	2.0
3	H	210	THR	2.0
1	A	96	SER	2.0
2	B	98	LYS	2.0
3	E	193	THR	2.0
2	D	450	ASN	2.0
4	L	201	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](#)

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
11	NAG	D	3371	14/15	0.86	0.26	1.98	55,84,97,112	0
11	NAG	B	3371	14/15	0.86	0.25	0.46	58,87,99,110	0
12	NAG	D	3320	14/15	0.94	0.13	-	25,41,53,57	0
10	NAG	B	3320	14/15	0.97	0.11	-	17,28,41,46	0
10	MAN	B	3324	11/12	0.67	0.24	-	106,113,118,118	0
12	NAG	D	3321	14/15	0.88	0.26	-	57,71,87,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
10	NAG	B	3321	14/15	0.90	0.12	-	40,53,63,76	0
10	MAN	B	3322	11/12	0.79	0.26	-	52,93,109,113	0
12	MAN	D	3322	11/12	0.51	0.31	-	100,108,110,110	0
11	NAG	B	3372	14/15	0.84	0.31	-	108,117,121,123	0
11	NAG	D	3372	14/15	0.73	0.45	-	118,126,130,131	0
10	MAN	B	3323	11/12	0.69	0.23	-	64,77,88,90	0

## 6.4 Ligands

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
8	MG	D	2001	1/1	0.87	0.72	21.72	41,41,41,41	1
7	SO4	L	215	5/5	0.81	0.44	11.63	101,106,112,115	0
7	SO4	D	473	5/5	0.72	0.39	9.70	131,133,136,137	0
6	GOL	C	458	6/6	0.83	0.30	8.64	45,61,71,79	0
6	GOL	A	463	6/6	0.73	0.30	7.75	77,79,83,84	0
6	GOL	A	460	6/6	0.81	0.27	6.14	68,70,78,84	0
7	SO4	H	222	5/5	0.83	0.36	5.69	112,116,118,123	0
7	SO4	C	461	5/5	0.88	0.26	5.64	55,75,85,87	0
7	SO4	B	473	5/5	0.76	0.30	4.50	90,98,103,108	0
7	SO4	C	460	5/5	0.90	0.19	3.61	39,53,83,84	0
7	SO4	A	464	5/5	0.86	0.17	3.09	97,98,107,112	0
7	SO4	D	472	5/5	0.79	0.25	2.66	73,92,98,108	0
6	GOL	A	461	6/6	0.92	0.18	1.49	28,50,57,71	0
6	GOL	B	472	6/6	0.83	0.17	1.43	65,70,72,77	0
5	CA	A	2006	1/1	0.99	0.15	0.56	16,16,16,16	0
8	MG	B	2001	1/1	0.97	0.16	0.22	26,26,26,26	1
5	CA	C	2007	1/1	0.97	0.14	0.17	36,36,36,36	0
5	CA	A	2005	1/1	0.99	0.12	-0.41	19,19,19,19	0
5	CA	C	2006	1/1	0.97	0.11	-0.51	34,34,34,34	0
5	CA	B	2003	1/1	0.99	0.17	-0.65	13,13,13,13	0
5	CA	A	2007	1/1	1.00	0.13	-0.70	16,16,16,16	0
5	CA	D	2003	1/1	0.99	0.16	-0.89	22,22,22,22	0
7	SO4	C	463	5/5	0.93	0.12	-1.14	84,91,98,98	0
5	CA	A	2004	1/1	0.99	0.06	-1.84	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CA	D	2002	1/1	0.95	0.12	-2.05	31,31,31,31	0
5	CA	C	2004	1/1	0.97	0.04	-2.22	45,45,45,45	0
5	CA	C	2005	1/1	0.99	0.05	-3.76	38,38,38,38	0
5	CA	B	2002	1/1	0.96	0.05	-4.01	35,35,35,35	0
6	GOL	A	458	6/6	0.86	0.20	-	28,51,56,58	0
6	GOL	A	459	6/6	0.93	0.16	-	42,45,58,58	0
6	GOL	C	459	6/6	0.79	0.27	-	52,67,73,74	0
6	GOL	A	462	6/6	0.84	0.21	-	47,61,65,70	0
9	NAG	B	3099	14/15	0.88	0.38	-	85,98,104,106	0
9	NAG	D	3099	14/15	0.79	0.29	-	76,90,95,96	0
7	SO4	C	462	5/5	0.85	0.18	-	110,113,117,118	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.