



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:14 am GMT

PDB ID : 3ZDX  
Title : Integrin alphaIIB beta3 headpiece and RGD peptide complex  
Authors : Zhu, J.H.; Zhu, J.Q.; Springer, T.A.  
Deposited on : 2012-12-03  
Resolution : 2.45 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 : trunk28620  
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

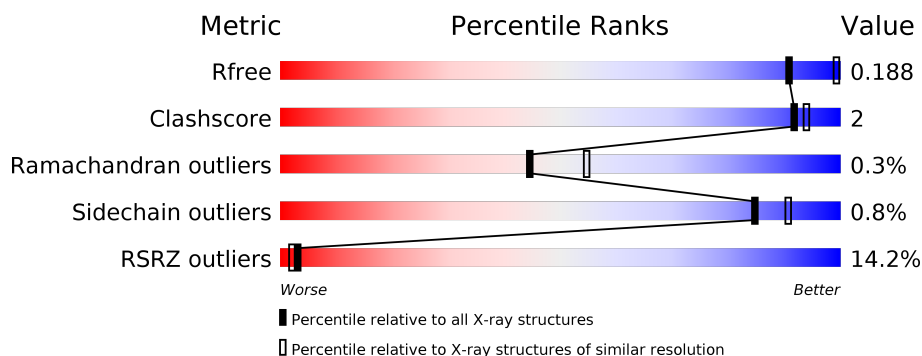
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1119 (2.48-2.44)
Clashscore	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)
RSRZ outliers	101464	1126 (2.48-2.44)

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	
1	C	457	
2	B	472	
2	D	472	
3	E	221	
3	H	221	

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Mol	Chain	Length	Quality of chain
4	F	214	<div> <div>45%</div> <div>96%</div> <div>.</div> </div>
4	L	214	<div> <div>9%</div> <div>100%</div> </div>

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
12	NAG	D	3371	-	-	-	X
5	GOL	A	1459	-	-	-	X
6	SO4	A	1461	-	-	-	X
6	SO4	A	1462	-	-	-	X
6	SO4	C	1456	-	-	-	X
6	SO4	C	1457	-	-	-	X
6	SO4	C	1458	-	-	-	X
6	SO4	C	1459	-	-	-	X
6	SO4	C	1460	-	-	-	X
6	SO4	D	1472	-	-	-	X
8	CL	B	1468	-	-	X	-

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 42688 atoms, of which 20255 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	457	Total	C	H	N	O	S	0	9	0
			6904	2248	3369	606	673	8			
1	C	453	Total	C	H	N	O	S	0	3	0
			6807	2218	3317	601	663	8			

- Molecule 2 is a protein called INTEGRIN BETA-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	464	Total	C	H	N	O	S	6	5	0
			7132	2248	3525	615	710	34			
2	D	469	Total	C	H	N	O	S	10	1	0
			7154	2258	3531	618	713	34			

- Molecule 3 is a protein called 10E5 FAB, HEAVY CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	216	Total	C	H	N	O	S	0	0	0
			3239	1041	1597	266	329	6			
3	H	216	Total	C	H	N	O	S	0	0	0
			3239	1041	1597	266	329	6			

- Molecule 4 is a protein called 10E5 FAB, LIGHT CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	214	Total	C	H	N	O	S	0	0	0
			3187	1019	1550	268	341	9			
4	L	214	Total	C	H	N	O	S	0	0	0
			3187	1019	1550	268	341	9			

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Ca	0	0
			4	4		
7	C	4	Total	Ca	0	0
			4	4		

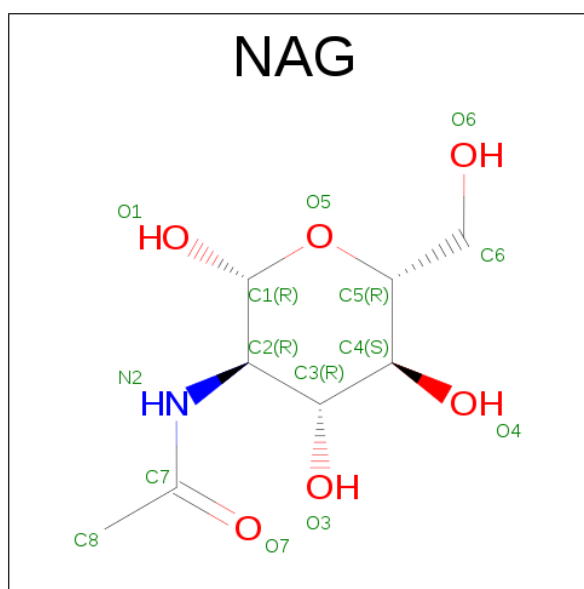
- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		

- Molecule 9 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	3	Total	Mn	0	0
			3	3		
9	D	3	Total	Mn	0	0
			3	3		

- Molecule 10 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
10	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 11 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	5	Total	C	H	N	O	0	0
			113	34	52	2	25		

- Molecule 12 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
12	D	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 13 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	D	4	Total	C	H	N	O	0	0
			93	28	43	2	20		

- Molecule 14 is water.

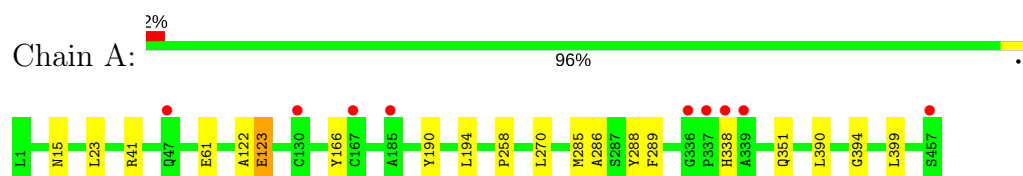
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	527	Total	O	0	0
			527	527		
14	B	221	Total	O	0	0
			221	221		
14	C	307	Total	O	0	0
			307	307		
14	D	177	Total	O	0	0
			177	177		
14	E	11	Total	O	0	0
			11	11		
14	F	8	Total	O	0	0
			8	8		
14	H	39	Total	O	0	0
			39	39		
14	L	34	Total	O	0	0
			34	34		



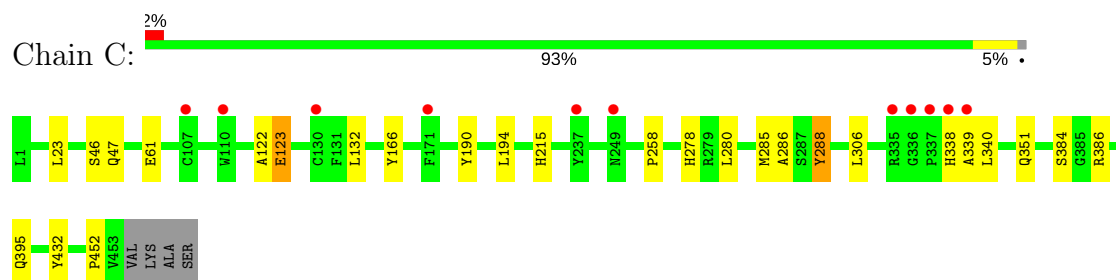
### 3 Residue-property plots [i](#)

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.

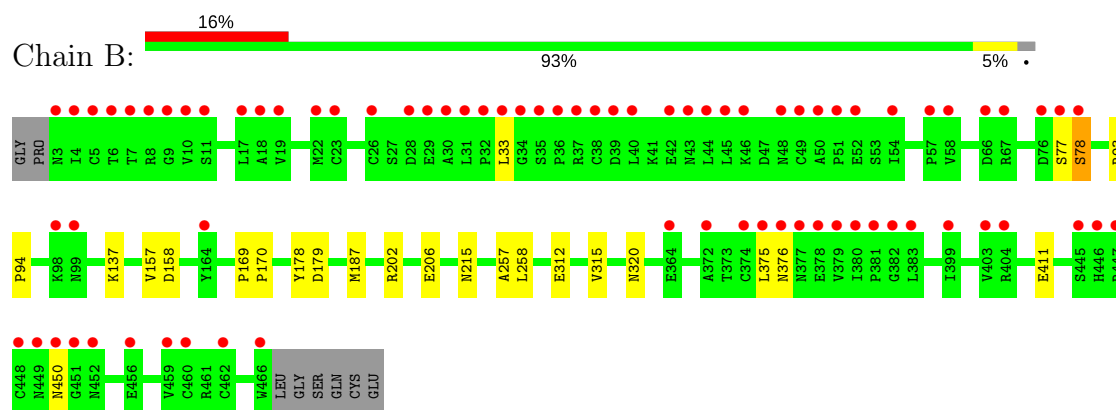
#### • Molecule 1: INTEGRIN ALPHA-IIB



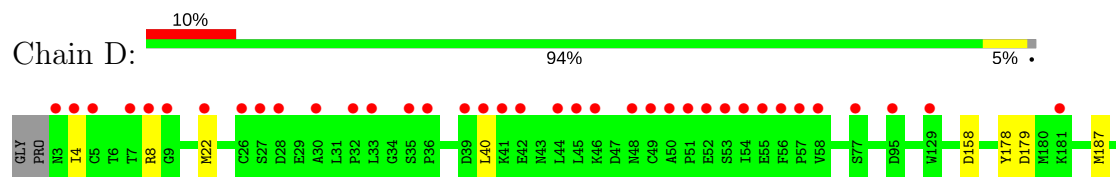
#### • Molecule 1: INTEGRIN ALPHA-IIB

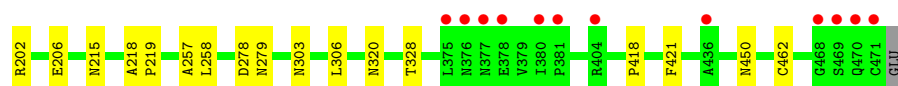


#### • Molecule 2: INTEGRIN BETA-3

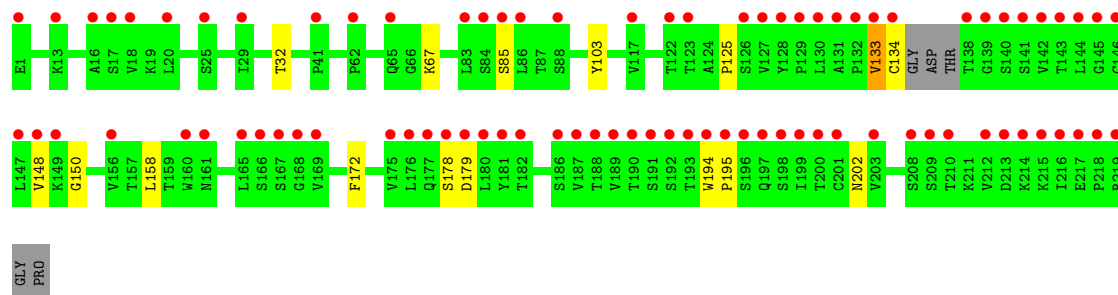
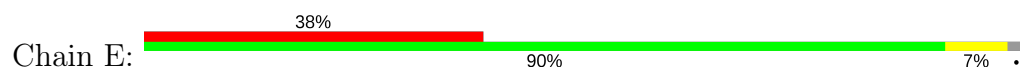


#### • Molecule 2: INTEGRIN BETA-3

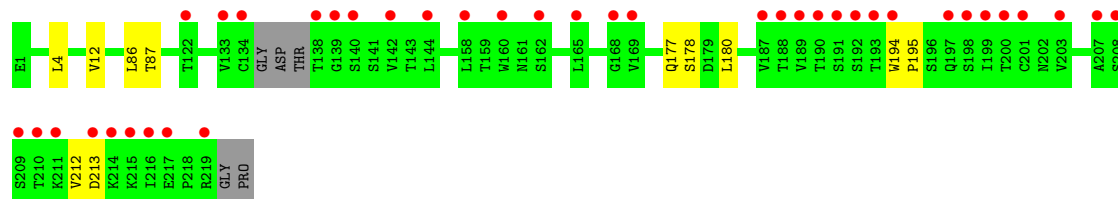




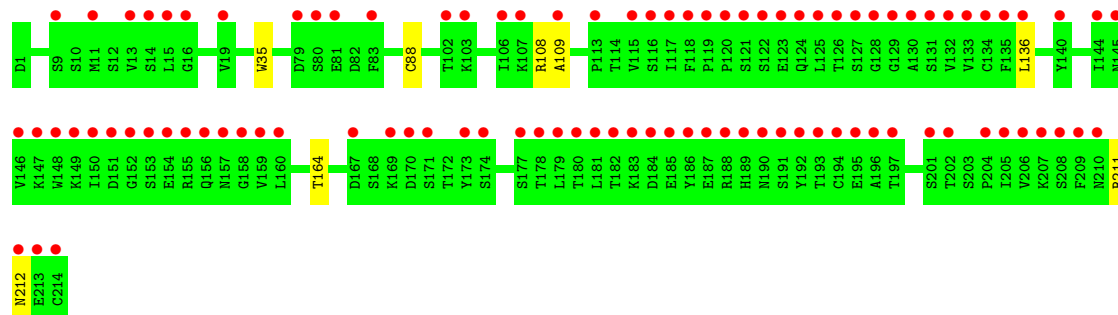
• Molecule 3: 10E5 FAB, HEAVY CHAIN



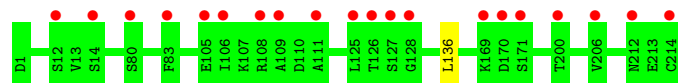
• Molecule 3: 10E5 FAB, HEAVY CHAIN



• Molecule 4: 10E5 FAB, LIGHT CHAIN



• Molecule 4: 10E5 FAB, LIGHT CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	259.71 Å   144.96 Å   104.77 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	48.36 – 2.45 48.36 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.36-2.45) 99.9 (48.36-2.45)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.45 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.163   ,   0.197 0.150   ,   0.188	Depositor DCC
$R_{free}$ test set	1003 reflections (0.69%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 61.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	42688	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, CL, CA, MN, 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	0.25	0/3659	0.43	0/4987
1	C	0.23	0/3596	0.41	0/4900
2	B	0.22	0/3685	0.40	0/4996
2	D	0.22	0/3694	0.39	0/5009
3	E	0.21	0/1684	0.39	0/2305
3	H	0.22	0/1684	0.40	0/2305
4	F	0.21	0/1673	0.38	0/2269
4	L	0.22	0/1673	0.39	0/2269
All	All	0.23	0/21348	0.40	0/29040

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3535	3369	3386	13	0
1	C	3490	3317	3328	18	1
2	B	3607	3525	3534	15	0
2	D	3623	3531	3537	12	0
3	E	1642	1597	1600	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	1597	1600	6	0
4	F	1637	1550	1553	5	0
4	L	1637	1550	1553	1	0
5	A	18	24	24	0	0
5	B	6	8	8	0	0
5	C	12	16	16	1	0
6	A	10	0	0	0	0
6	C	25	0	0	0	0
6	D	10	0	0	0	0
6	L	5	0	0	0	0
7	A	4	0	0	0	0
7	C	4	0	0	0	0
8	B	1	0	0	3	0
9	B	3	0	0	0	0
9	D	3	0	0	0	0
10	B	14	13	13	0	0
10	D	14	13	13	0	0
11	B	61	52	52	0	0
12	B	28	25	25	0	0
12	D	28	25	25	0	0
13	D	50	43	43	0	0
14	A	527	0	0	5	4
14	B	221	0	0	4	0
14	C	307	0	0	4	3
14	D	177	0	0	0	0
14	E	11	0	0	0	0
14	F	8	0	0	0	0
14	H	39	0	0	0	0
14	L	34	0	0	0	0
All	All	22433	20255	20310	78	4

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 (78) 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)
8:B:1468:CL:CL	14:B:4039:HOH:O	2.25	0.92
8:B:1468:CL:CL	14:B:4040:HOH:O	2.29	0.86
8:B:1468:CL:CL	14:B:4124:HOH:O	2.32	0.83
1:A:41:ARG:NH2	14:A:4043:HOH:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:GLN:OE1	14:C:4265:HOH:O	2.11	0.69
1:C:338:HIS:O	14:C:4178:HOH:O	2.13	0.67
1:A:15[A]:ASN:ND2	14:A:4033:HOH:O	2.29	0.66
1:A:338:HIS:O	14:A:4402:HOH:O	2.12	0.66
2:D:202:ARG:NH2	2:D:206:GLU:OE2	2.30	0.64
1:C:384:SER:OG	14:C:4254:HOH:O	2.17	0.58
3:H:177:GLN:N	3:H:180:LEU:O	2.38	0.57
1:A:122:ALA:O	1:A:123:GLU:HB2	2.05	0.56
2:B:77:SER:O	2:B:78:SER:HB3	2.04	0.56
1:C:122:ALA:O	1:C:123:GLU:HB2	2.05	0.56
3:H:213:ASP:OD1	3:H:213:ASP:N	2.38	0.56
2:D:257:ALA:O	2:D:258:LEU:HB2	2.07	0.55
2:B:137:LYS:NZ	14:B:4060:HOH:O	2.40	0.54
3:H:194:TRP:CG	3:H:195:PRO:HA	2.43	0.54
1:A:351:GLN:OE1	14:A:4418:HOH:O	2.19	0.53
3:E:67:LYS:NZ	3:E:85:SER:O	2.42	0.53
2:B:169:PRO:HD2	2:B:178:TYR:CZ	2.46	0.50
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.46	0.48
1:C:122:ALA:O	1:C:123:GLU:CB	2.61	0.48
5:C:1454:GOL:O3	5:C:1454:GOL:O1	2.30	0.48
2:D:158:ASP:HB3	2:D:187:MET:CE	2.43	0.48
2:B:312:GLU:HA	2:B:315:VAL:HG23	1.95	0.48
2:B:257:ALA:O	2:B:258:LEU:HB2	2.14	0.47
2:D:450:ASN:ND2	2:D:450:ASN:O	2.47	0.47
1:A:122:ALA:O	1:A:123:GLU:CB	2.63	0.47
2:B:450:ASN:ND2	2:B:450:ASN:O	2.47	0.47
1:C:46:SER:O	1:C:47:GLN:HB2	2.15	0.47
4:F:136:LEU:N	4:F:136:LEU:HD12	2.30	0.46
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.97	0.46
3:E:133:VAL:O	3:E:134:CYS:SG	2.73	0.46
2:B:158:ASP:HB3	2:B:187[A]:MET:CE	2.45	0.46
1:C:285:MET:SD	2:D:320:ASN:HB3	2.56	0.46
2:B:169:PRO:HB2	2:B:170:PRO:HD2	1.98	0.45
1:C:215:HIS:CE1	3:E:103:TYR:CE1	3.04	0.45
2:D:178:TYR:CG	2:D:179:ASP:N	2.84	0.45
2:D:218:ALA:HB3	2:D:219:PRO:HD3	1.98	0.45
3:H:12:VAL:HG21	3:H:86:LEU:CD1	2.47	0.45
4:L:136:LEU:N	4:L:136:LEU:HD12	2.32	0.45
1:C:258:PRO:HB2	1:C:288:TYR:CD2	2.52	0.45
1:C:194:LEU:HD12	1:C:194:LEU:C	2.38	0.44
1:A:194:LEU:C	1:A:194:LEU:HD12	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:172:PHE:CD2	4:F:164:THR:HG23	2.52	0.44
3:E:194:TRP:CG	3:E:195:PRO:HA	2.52	0.44
2:B:376:ASN:O	2:B:376:ASN:ND2	2.51	0.44
1:C:432:TYR:CZ	1:C:452:PRO:HA	2.52	0.44
1:C:278[A]:HIS:CE1	1:C:340:LEU:O	2.71	0.43
3:H:212:VAL:HG12	3:H:213:ASP:N	2.34	0.43
2:B:77:SER:O	2:B:78:SER:CB	2.65	0.42
2:D:418:PRO:HB2	2:D:421:PHE:CD1	2.53	0.42
3:E:178:SER:O	3:E:179:ASP:HB2	2.20	0.42
1:C:351:GLN:OE1	14:C:4228:HOH:O	2.22	0.42
2:D:4:ILE:O	2:D:8:ARG:HG2	2.19	0.42
2:D:306:LEU:HB3	2:D:328:THR:HG22	2.01	0.42
4:F:211:ARG:O	4:F:212:ASN:HB2	2.20	0.42
1:C:278[A]:HIS:CD2	1:C:339:ALA:HB1	2.55	0.42
2:B:178:TYR:CG	2:B:179:ASP:N	2.87	0.42
1:A:285:MET:O	1:A:286:ALA:HB3	2.20	0.41
1:A:258:PRO:HA	1:A:289:PHE:O	2.20	0.41
1:C:280:LEU:CD1	1:C:306:LEU:HD23	2.51	0.41
1:C:132:LEU:HD12	1:C:132:LEU:N	2.36	0.41
4:F:35:TRP:CZ3	4:F:88:CYS:HB3	2.56	0.41
1:C:215:HIS:CE1	3:E:32:THR:HG22	2.55	0.41
1:C:285:MET:O	1:C:286:ALA:HB3	2.20	0.41
1:A:394:GLY:HA2	1:A:399:LEU:HD23	2.03	0.41
1:A:285:MET:SD	2:B:320:ASN:HB3	2.61	0.41
2:D:22:MET:HG2	2:D:40:LEU:CD2	2.51	0.41
1:A:390:LEU:HD12	1:A:390:LEU:N	2.35	0.41
2:B:157:VAL:HG11	2:B:187[B]:MET:SD	2.60	0.41
3:E:125:PRO:HB2	3:E:148:VAL:HG13	2.03	0.41
4:F:108:ARG:HG2	4:F:109:ALA:N	2.36	0.40
3:E:158:LEU:C	3:E:158:LEU:HD23	2.42	0.40
3:H:4:LEU:N	3:H:4:LEU:HD12	2.37	0.40
1:A:41:ARG:NH1	14:A:4070:HOH:O	2.54	0.40
2:D:278:ASP:O	2:D:279:ASN:HB2	2.21	0.40

All (4) 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)
14:A:4459:HOH:O	14:C:4260:HOH:O[1_554]	1.92	0.28
14:A:4459:HOH:O	14:C:4282:HOH:O[1_554]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:4480:HOH:O	14:C:4279:HOH:O[1_554]	2.09	0.11
1:C:386:ARG:NH1	14:A:4485:HOH:O[1_556]	2.16	0.04

## 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	A	464/457 (102%)	446 (96%)	17 (4%)	1 (0%)	51	62
1	C	454/457 (99%)	441 (97%)	12 (3%)	1 (0%)	51	62
2	B	467/472 (99%)	444 (95%)	20 (4%)	3 (1%)	28	34
2	D	468/472 (99%)	451 (96%)	17 (4%)	0	100	100
3	E	212/221 (96%)	200 (94%)	10 (5%)	2 (1%)	20	23
3	H	212/221 (96%)	200 (94%)	11 (5%)	1 (0%)	32	39
4	F	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
4	L	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
All	All	2701/2728 (99%)	2589 (96%)	104 (4%)	8 (0%)	44	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	33	LEU
2	B	78	SER
2	B	375	LEU
3	E	133	VAL
1	C	123	GLU
3	H	178	SER
3	E	150	GLY



### 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	372/364 (102%)	366 (98%)	6 (2%)	68	79
1	C	364/364 (100%)	359 (99%)	5 (1%)	71	82
2	B	416/417 (100%)	414 (100%)	2 (0%)	91	94
2	D	416/417 (100%)	413 (99%)	3 (1%)	87	92
3	E	187/190 (98%)	186 (100%)	1 (0%)	91	94
3	H	187/190 (98%)	186 (100%)	1 (0%)	91	94
4	F	188/188 (100%)	188 (100%)	0	100	100
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2318/2318 (100%)	2300 (99%)	18 (1%)	85	90

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	61	GLU
1	A	166	TYR
1	A	190	TYR
1	A	270	LEU
1	A	288	TYR
2	B	215	ASN
2	B	411	GLU
1	C	23	LEU
1	C	61	GLU
1	C	166	TYR
1	C	190	TYR
1	C	288	TYR
2	D	215	ASN
2	D	303	ASN
2	D	462	CYS
3	E	202	ASN
3	H	87	THR

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

Mol	Chain	Res	Type
2	B	3	ASN
1	C	158	ASN
3	E	202	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 ⓘ

13 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	$\# Z  > 2$
11	NAG	B	3320	11,2	14,14,15	0.55	0	15,19,21	0.63	0
11	NAG	B	3321	11	14,14,15	0.58	0	15,19,21	0.69	0
11	BMA	B	3322	11	11,11,12	0.62	0	13,15,17	0.82	0
11	MAN	B	3323	11	11,11,12	0.58	0	13,15,17	0.87	0
11	MAN	B	3324	11	11,11,12	0.59	0	13,15,17	0.52	0
12	NAG	B	3371	12,2	14,14,15	0.56	0	15,19,21	0.66	0
12	NAG	B	3372	12	14,14,15	0.53	0	15,19,21	0.53	0
13	NAG	D	3320	13,2	14,14,15	0.51	0	15,19,21	0.62	0
13	NAG	D	3321	13	14,14,15	0.59	0	15,19,21	0.71	0
13	BMA	D	3322	13	11,11,12	0.65	0	13,15,17	0.83	1 (7%)
13	MAN	D	3323	13	11,11,12	0.63	0	13,15,17	0.74	0
12	NAG	D	3371	12,2	14,14,15	0.61	0	15,19,21	0.79	0
12	NAG	D	3372	12	14,14,15	0.53	0	15,19,21	0.51	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
11	NAG	B	3320	11,2	-	0/6/23/26	0/1/1/1
11	NAG	B	3321	11	-	0/6/23/26	0/1/1/1
11	BMA	B	3322	11	-	0/2/19/22	0/1/1/1
11	MAN	B	3323	11	-	0/2/19/22	0/1/1/1
11	MAN	B	3324	11	-	0/2/19/22	0/1/1/1
12	NAG	B	3371	12,2	-	0/6/23/26	0/1/1/1
12	NAG	B	3372	12	-	0/6/23/26	0/1/1/1
13	NAG	D	3320	13,2	-	0/6/23/26	0/1/1/1
13	NAG	D	3321	13	-	0/6/23/26	0/1/1/1
13	BMA	D	3322	13	-	0/2/19/22	0/1/1/1
13	MAN	D	3323	13	-	0/2/19/22	0/1/1/1
12	NAG	D	3371	12,2	-	0/6/23/26	0/1/1/1
12	NAG	D	3372	12	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	3322	BMA	C1-C2-C3	2.54	112.86	109.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

Of 33 ligands modelled in this entry, 15 are monoatomic - leaving 18 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
5	GOL	A	1458	-	5,5,5	0.36	0	5,5,5	0.24	0
5	GOL	A	1459	-	5,5,5	0.35	0	5,5,5	0.22	0
5	GOL	A	1460	-	5,5,5	0.35	0	5,5,5	0.15	0
6	SO4	A	1461	-	4,4,4	0.15	0	6,6,6	0.07	0
6	SO4	A	1462	-	4,4,4	0.14	0	6,6,6	0.06	0
5	GOL	B	1467	-	5,5,5	0.35	0	5,5,5	0.22	0
10	NAG	B	3099	2	14,14,15	0.50	0	15,19,21	0.66	0
5	GOL	C	1454	-	5,5,5	0.33	0	5,5,5	0.28	0
5	GOL	C	1455	-	5,5,5	0.34	0	5,5,5	0.23	0
6	SO4	C	1456	-	4,4,4	0.16	0	6,6,6	0.06	0
6	SO4	C	1457	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	C	1458	-	4,4,4	0.15	0	6,6,6	0.06	0
6	SO4	C	1459	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	C	1460	-	4,4,4	0.15	0	6,6,6	0.05	0
6	SO4	D	1472	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	D	1473	9	4,4,4	0.16	0	6,6,6	0.08	0
10	NAG	D	3099	2	14,14,15	0.50	0	15,19,21	0.50	0
6	SO4	L	1215	-	4,4,4	0.15	0	6,6,6	0.05	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
5	GOL	A	1458	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1459	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1460	-	-	0/4/4/4	0/0/0/0
6	SO4	A	1461	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1462	-	-	0/0/0/0	0/0/0/0
5	GOL	B	1467	-	-	0/4/4/4	0/0/0/0
10	NAG	B	3099	2	-	0/6/23/26	0/1/1/1
5	GOL	C	1454	-	-	0/4/4/4	0/0/0/0
5	GOL	C	1455	-	-	0/4/4/4	0/0/0/0
6	SO4	C	1456	-	-	0/0/0/0	0/0/0/0
6	SO4	C	1457	-	-	0/0/0/0	0/0/0/0
6	SO4	C	1458	-	-	0/0/0/0	0/0/0/0
6	SO4	C	1459	-	-	0/0/0/0	0/0/0/0
6	SO4	C	1460	-	-	0/0/0/0	0/0/0/0
6	SO4	D	1472	-	-	0/0/0/0	0/0/0/0
6	SO4	D	1473	9	-	0/0/0/0	0/0/0/0
10	NAG	D	3099	2	-	0/6/23/26	0/1/1/1
6	SO4	L	1215	-	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1454	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	457/457 (100%)	0.37	9 (1%) 65 62	9, 20, 53, 124	1 (0%)
1	C	453/457 (99%)	0.23	11 (2%) 59 55	16, 34, 68, 112	0
2	B	464/472 (98%)	0.97	77 (16%) 2 1	10, 46, 124, 181	2 (0%)
2	D	469/472 (99%)	0.50	49 (10%) 7 6	17, 45, 107, 163	2 (0%)
3	E	216/221 (97%)	2.14	84 (38%) 0 0	40, 103, 180, 201	0
3	H	216/221 (97%)	0.67	39 (18%) 1 1	24, 70, 124, 143	0
4	F	214/214 (100%)	2.20	96 (44%) 0 0	40, 92, 166, 237	0
4	L	214/214 (100%)	0.44	20 (9%) 9 7	28, 56, 89, 173	0
All	All	2703/2728 (99%)	0.79	385 (14%) 3 2	9, 46, 132, 237	5 (0%)

All (385) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	216	ILE	12.9
4	F	214	CYS	12.8
2	B	77	SER	11.7
2	D	469	SER	11.6
3	E	199	ILE	11.6
3	E	133	VAL	11.4
4	F	181	LEU	11.2
3	E	134	CYS	9.6
2	B	36	PRO	9.6
3	E	138	THR	9.2
4	F	125	LEU	8.9
3	E	194	TRP	8.8
3	E	201	CYS	8.7
3	E	144	LEU	8.7
4	F	126	THR	8.7
4	F	193	THR	8.3

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Mol	Chain	Res	Type	RSRZ
2	B	33	LEU	8.2
4	F	212	ASN	8.0
4	L	214	CYS	7.7
3	E	217	GLU	7.6
3	E	130	LEU	7.6
3	E	219	ARG	7.4
3	E	200	THR	7.2
4	F	150	ILE	6.9
3	E	212	VAL	6.9
3	E	131	ALA	6.9
2	B	44	LEU	6.9
4	F	182	THR	6.7
3	E	195	PRO	6.7
3	E	210	THR	6.7
3	E	128	TYR	6.7
2	B	4	ILE	6.7
3	E	132	PRO	6.5
4	F	158	GLY	6.5
4	F	130	ALA	6.4
3	E	142	VAL	6.4
4	F	122	SER	6.4
4	F	129	GLY	6.3
3	H	189	VAL	6.3
3	E	196	SER	6.3
4	F	192	TYR	6.3
4	F	120	PRO	6.2
2	B	10	VAL	6.2
2	B	8	ARG	6.2
3	E	160	TRP	6.2
4	F	194	CYS	6.2
4	F	213	GLU	6.1
2	B	32	PRO	6.1
4	F	209	PHE	6.1
4	F	180	THR	6.0
4	F	210	ASN	6.0
3	E	215	LYS	6.0
4	F	208	SER	5.8
4	F	186	TYR	5.7
1	A	337	PRO	5.7
2	B	34	GLY	5.7
2	B	375	LEU	5.7
2	D	51	PRO	5.7

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Mol	Chain	Res	Type	RSRZ
3	H	134	CYS	5.5
4	F	132	VAL	5.4
2	D	48	ASN	5.4
4	F	127	SER	5.4
2	D	4	ILE	5.4
2	B	39	ASP	5.4
2	B	5	CYS	5.4
2	D	471	CYS	5.3
3	E	187	VAL	5.3
2	D	33	LEU	5.2
2	B	67	ARG	5.2
2	B	51	PRO	5.1
4	F	179	LEU	5.1
4	F	119	PRO	5.1
2	D	9	GLY	5.1
4	F	131	SER	5.1
3	H	133	VAL	5.1
2	D	44	LEU	5.0
2	B	28	ASP	4.9
4	F	115	VAL	4.9
3	E	143	THR	4.9
3	E	165	LEU	4.8
4	F	206	VAL	4.8
2	B	35	SER	4.8
3	E	129	PRO	4.8
4	F	124	GLN	4.7
3	E	218	PRO	4.7
3	E	189	VAL	4.7
4	F	118	PHE	4.7
2	B	446	HIS	4.7
4	F	205	ILE	4.7
2	B	7	THR	4.7
2	B	46	LYS	4.7
2	B	45	LEU	4.6
1	A	339	ALA	4.6
3	E	203	VAL	4.6
3	E	147	LEU	4.6
4	F	117	ILE	4.6
4	F	148	TRP	4.5
4	L	212	ASN	4.5
2	D	35	SER	4.5
2	D	46	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
4	F	128	GLY	4.4
2	B	450	ASN	4.4
4	F	191	SER	4.4
3	E	16	ALA	4.3
2	B	6	THR	4.3
2	B	30	ALA	4.3
4	F	184	ASP	4.3
4	F	133	VAL	4.3
3	E	193	THR	4.3
3	E	123	THR	4.3
3	E	148	VAL	4.2
2	B	31	LEU	4.2
2	B	22	MET	4.2
3	H	138	THR	4.2
2	D	375	LEU	4.2
4	F	190	ASN	4.1
3	E	176	LEU	4.1
2	B	3	ASN	4.0
4	F	14	SER	4.0
4	F	156	GLN	4.0
2	D	54	ILE	4.0
4	F	154	GLU	4.0
3	E	167	SER	4.0
2	B	38	CYS	4.0
2	D	5	CYS	4.0
2	D	8	ARG	3.9
3	E	214	LYS	3.9
2	D	22	MET	3.9
4	F	121	SER	3.9
2	B	50	ALA	3.9
3	E	156	VAL	3.9
1	A	338	HIS	3.9
4	F	134	CYS	3.9
4	F	106	ILE	3.8
3	E	208	SER	3.8
4	F	151	ASP	3.8
2	B	383	LEU	3.8
2	B	462	CYS	3.8
3	H	191	SER	3.7
4	F	189	HIS	3.7
4	F	107	LYS	3.7
3	H	194	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	337	PRO	3.7
3	H	199	ILE	3.6
2	D	45	LEU	3.6
3	E	29	ILE	3.6
4	F	157	ASN	3.6
4	F	135	PHE	3.6
3	H	217	GLU	3.6
2	B	445	SER	3.5
4	F	169	LYS	3.5
3	E	140	SER	3.5
1	C	249	ASN	3.5
3	E	126	SER	3.5
3	E	191	SER	3.5
2	D	404	ARG	3.5
2	B	40	LEU	3.4
3	E	192	SER	3.4
3	H	215	LYS	3.4
1	C	339	ALA	3.4
3	E	65	GLN	3.4
3	H	203	VAL	3.4
2	D	40	LEU	3.4
2	D	30	ALA	3.4
4	F	155	ARG	3.4
2	D	52	GLU	3.3
3	E	85	SER	3.3
3	H	211	LYS	3.3
2	B	379	VAL	3.3
2	B	9	GLY	3.3
3	E	139	GLY	3.3
3	E	145	GLY	3.3
2	B	78	SER	3.3
4	F	136	LEU	3.3
4	F	197	THR	3.3
2	B	404	ARG	3.3
4	F	147	LYS	3.3
4	F	183	LYS	3.3
3	H	188	THR	3.3
4	F	153	SER	3.3
4	F	196	ALA	3.3
2	D	470	GLN	3.3
3	E	197	GLN	3.3
4	L	125	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
3	E	84	SER	3.3
2	B	376	ASN	3.2
4	L	111	ALA	3.2
2	B	49	CYS	3.2
2	B	460	CYS	3.2
2	B	451	GLY	3.2
4	F	149	LYS	3.2
3	H	193	THR	3.2
2	D	42	GLU	3.2
3	E	166	SER	3.2
4	F	103	LYS	3.2
2	B	48	ASN	3.2
3	E	198	SER	3.2
4	F	173	TYR	3.2
4	F	185	GLU	3.1
2	B	448	CYS	3.1
2	B	66	ASP	3.1
3	H	216	ILE	3.1
4	F	116	SER	3.1
2	B	466	TRP	3.1
3	E	190	THR	3.1
3	E	186	SER	3.1
3	E	13	LYS	3.1
2	D	39	ASP	3.1
2	B	42	GLU	3.1
1	A	336	GLY	3.1
3	H	144	LEU	3.1
3	E	86	LEU	3.0
2	D	32	PRO	3.0
2	B	11	SER	3.0
4	F	202	THR	3.0
4	F	207	LYS	3.0
3	E	141	SER	3.0
4	F	9	SER	3.0
2	D	36	PRO	3.0
4	F	170	ASP	3.0
4	L	105	GLU	3.0
2	D	3	ASN	3.0
3	H	201	CYS	2.9
3	H	192	SER	2.9
3	H	210	THR	2.9
4	L	106	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	457	SER	2.9
1	C	336	GLY	2.9
2	D	55	GLU	2.9
3	E	177	GLN	2.9
3	E	169	VAL	2.9
3	E	25	SER	2.9
4	F	144	ILE	2.9
4	F	187	GLU	2.9
2	D	57	PRO	2.9
1	C	130	CYS	2.9
3	H	160	TRP	2.9
3	H	165	LEU	2.9
3	E	181	TYR	2.9
3	E	209	SER	2.8
3	H	139	GLY	2.8
2	B	374	CYS	2.8
2	D	181	LYS	2.8
3	H	207	ALA	2.8
4	F	188	ARG	2.8
3	H	187	VAL	2.8
3	E	83	LEU	2.8
3	E	122	THR	2.8
4	L	169	LYS	2.8
3	H	169	VAL	2.8
2	D	58	VAL	2.8
4	F	13	VAL	2.8
3	E	182	THR	2.8
4	F	83	PHE	2.8
4	L	126	THR	2.7
3	E	180	LEU	2.7
3	E	117	VAL	2.7
2	B	17	LEU	2.7
4	F	174	SER	2.7
2	B	381	PRO	2.7
2	B	382	GLY	2.7
3	E	213	ASP	2.7
2	B	57	PRO	2.7
2	B	452	ASN	2.7
4	F	146	VAL	2.7
3	E	18	VAL	2.7
2	B	403	VAL	2.7
3	E	149	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
4	L	206	VAL	2.6
2	B	98	LYS	2.6
3	E	168	GLY	2.6
3	H	209	SER	2.6
2	D	56	PHE	2.6
3	H	213	ASP	2.6
2	D	436	ALA	2.6
2	D	49	CYS	2.6
1	C	338	HIS	2.6
2	D	376	ASN	2.6
3	E	127	VAL	2.6
2	B	54	ILE	2.6
2	B	52	GLU	2.6
2	D	378	GLU	2.6
2	B	26	CYS	2.5
4	L	109	ALA	2.5
2	D	129[A]	TRP	2.5
3	E	178	SER	2.5
1	A	47	GLN	2.5
4	F	201	SER	2.5
2	D	28	ASP	2.5
4	L	12	SER	2.5
3	E	188	THR	2.5
2	B	449	ASN	2.5
3	E	161	ASN	2.5
2	B	29	GLU	2.5
3	H	198	SER	2.5
2	D	53	SER	2.5
1	A	185	ALA	2.5
2	D	377	ASN	2.5
2	D	26	CYS	2.4
3	H	158	LEU	2.4
4	F	140	TYR	2.4
4	F	167	ASP	2.4
3	E	41	PRO	2.4
3	H	142	VAL	2.4
4	L	171	SER	2.4
2	B	380	ILE	2.4
4	F	11	MET	2.4
2	D	468	GLY	2.4
2	B	76	ASP	2.4
4	F	171	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	377	ASN	2.4
2	D	7	THR	2.4
4	F	15	LEU	2.4
3	H	140	SER	2.4
2	D	27	SER	2.4
4	F	80	SER	2.4
2	B	23	CYS	2.4
2	B	378	GLU	2.3
4	F	123	GLU	2.3
4	F	178	THR	2.3
2	D	380	ILE	2.3
4	F	109	ALA	2.3
2	B	99	ASN	2.3
4	F	160	LEU	2.3
3	H	219	ARG	2.3
1	C	335	ARG	2.3
3	E	20	LEU	2.3
4	F	81	GLU	2.3
2	B	58	VAL	2.3
4	L	170	ASP	2.3
2	B	447	ARG	2.3
4	F	177	SER	2.3
3	H	200	THR	2.3
3	E	146	CYS	2.3
2	B	37	ARG	2.2
2	D	381	PRO	2.2
4	F	159	VAL	2.2
4	L	83	PHE	2.2
4	F	145	ASN	2.2
4	L	127	SER	2.2
1	C	107	CYS	2.2
3	E	17	SER	2.2
2	B	399	ILE	2.2
3	E	62	PRO	2.2
4	F	195	GLU	2.2
3	E	1	GLU	2.2
4	F	16	GLY	2.2
4	L	200	THR	2.2
1	C	171	PHE	2.2
3	E	179	ASP	2.2
3	H	162	SER	2.2
3	H	197	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
3	H	190	THR	2.2
2	D	77	SER	2.2
3	E	88	SER	2.2
2	D	50	ALA	2.1
2	B	364	GLU	2.1
4	F	113	PRO	2.1
3	H	214	LYS	2.1
2	B	372	ALA	2.1
2	B	456	GLU	2.1
4	F	102	THR	2.1
1	A	130	CYS	2.1
4	L	128	GLY	2.1
3	H	122	THR	2.1
1	C	110	TRP	2.1
4	L	14	SER	2.1
4	L	108	ARG	2.1
3	H	168	GLY	2.1
2	B	19	VAL	2.1
3	E	175	VAL	2.1
4	F	19	VAL	2.1
4	F	204	PRO	2.1
2	D	95	ASP	2.1
4	L	80	SER	2.1
2	B	43	ASN	2.1
1	A	167	CYS	2.1
4	F	79	ASP	2.0
2	B	18	ALA	2.0
2	B	459	VAL	2.0
2	D	41	LYS	2.0
1	C	237	TYR	2.0
2	B	164	TYR	2.0
3	H	208	SER	2.0
4	F	152	GLY	2.0

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

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
12	NAG	D	3371	14/15	0.84	0.30	2.20	55,95,127,136	0
12	NAG	B	3371	14/15	0.82	0.34	1.17	66,98,121,123	0
13	NAG	D	3320	14/15	0.94	0.14	-0.83	21,44,61,70	0
11	NAG	B	3320	14/15	0.96	0.12	-3.15	13,28,46,53	0
13	NAG	D	3321	14/15	0.87	0.26	-	48,77,102,108	0
11	MAN	B	3323	11/12	0.76	0.28	-	54,111,133,145	0
11	NAG	B	3321	14/15	0.92	0.16	-	47,65,96,99	0
12	NAG	D	3372	14/15	0.82	0.50	-	116,148,185,192	0
11	MAN	B	3324	11/12	0.80	0.26	-	108,127,148,152	0
12	NAG	B	3372	14/15	0.86	0.39	-	93,126,151,153	0
13	MAN	D	3323	11/12	0.75	0.22	-	104,129,153,155	0
11	BMA	B	3322	11/12	0.75	0.24	-	81,124,152,153	0
13	BMA	D	3322	11/12	0.69	0.34	-	93,132,158,161	0

### 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	SO4	D	1472	5/5	0.86	0.28	9.44	62,114,118,118	0
6	SO4	C	1458	5/5	0.93	0.24	7.42	59,107,112,117	0
6	SO4	C	1460	5/5	0.82	0.25	6.91	105,113,126,134	0
6	SO4	C	1456	5/5	0.94	0.20	3.56	56,99,110,117	0
6	SO4	C	1457	5/5	0.88	0.19	2.65	88,112,116,117	0
5	GOL	A	1459	6/6	0.90	0.28	2.56	47,71,81,86	0
6	SO4	A	1461	5/5	0.95	0.19	2.41	48,71,91,109	0
6	SO4	C	1459	5/5	0.90	0.23	2.40	132,135,136,141	0
6	SO4	A	1462	5/5	0.92	0.19	2.06	94,110,116,116	0
10	NAG	D	3099	14/15	0.87	0.30	1.77	78,100,120,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CA	A	2006	1/1	0.99	0.20	1.31	14,14,14,14	0
8	CL	B	1468	1/1	0.99	0.21	0.96	26,26,26,26	0
5	GOL	B	1467	6/6	0.92	0.20	0.90	62,87,101,104	0
6	SO4	D	1473	5/5	0.98	0.17	0.61	19,55,61,81	0
5	GOL	A	1460	6/6	0.86	0.19	0.58	50,67,81,89	0
5	GOL	A	1458	6/6	0.95	0.20	0.54	42,62,82,82	0
5	GOL	C	1454	6/6	0.90	0.19	0.33	46,71,85,85	0
9	MN	B	2001	1/1	1.00	0.20	0.27	23,23,23,23	0
7	CA	C	2007	1/1	0.98	0.12	-0.14	38,38,38,38	0
7	CA	C	2006	1/1	0.99	0.14	-0.18	33,33,33,33	0
9	MN	D	2001	1/1	0.99	0.14	-0.63	31,31,31,31	0
7	CA	A	2007	1/1	0.99	0.15	-0.73	14,14,14,14	0
7	CA	A	2005	1/1	0.99	0.12	-0.98	15,15,15,15	0
7	CA	C	2005	1/1	0.99	0.06	-2.36	38,38,38,38	0
9	MN	D	2003	1/1	0.99	0.13	-2.57	34,34,34,34	0
7	CA	C	2004	1/1	0.95	0.06	-2.62	47,47,47,47	0
7	CA	A	2004	1/1	0.97	0.05	-3.10	28,28,28,28	0
9	MN	B	2003	1/1	0.99	0.16	-3.79	25,25,25,25	0
9	MN	B	2002	1/1	0.97	0.07	-3.93	41,41,41,41	0
9	MN	D	2002	1/1	0.98	0.07	-8.93	43,43,43,43	0
6	SO4	L	1215	5/5	0.88	0.24	-	100,105,109,119	0
10	NAG	B	3099	14/15	0.85	0.37	-	95,127,149,154	0
5	GOL	C	1455	6/6	0.87	0.26	-	55,86,104,124	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.