



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:56 AM GMT

PDB ID : 3NID
Title : The Closed Headpiece of Integrin α IIb β 3 and its Complex with an α IIb β 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

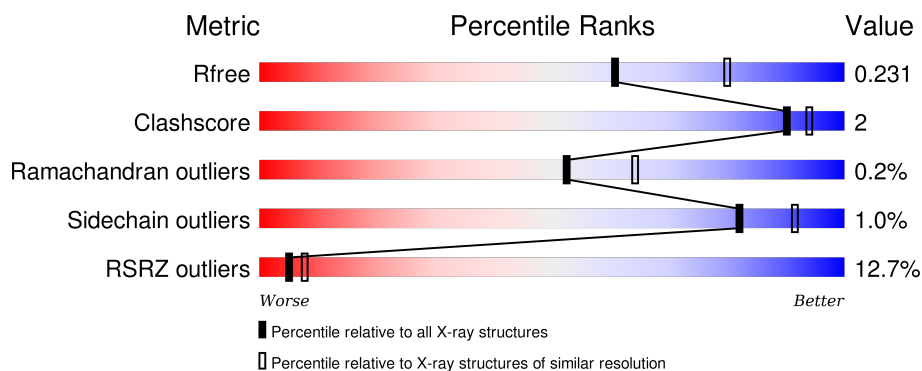
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 ≥ 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>94%</div> <div>5%</div> </div>
1	C	457	<div> <div>3%</div> <div>94%</div> <div>5%</div> </div>
2	B	471	<div> <div>14%</div> <div>91%</div> <div>7%</div> </div>
2	D	471	<div> <div>10%</div> <div>95%</div> <div>5%</div> </div>
3	E	221	<div> <div>35%</div> <div>87%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	221	
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: O₄S).

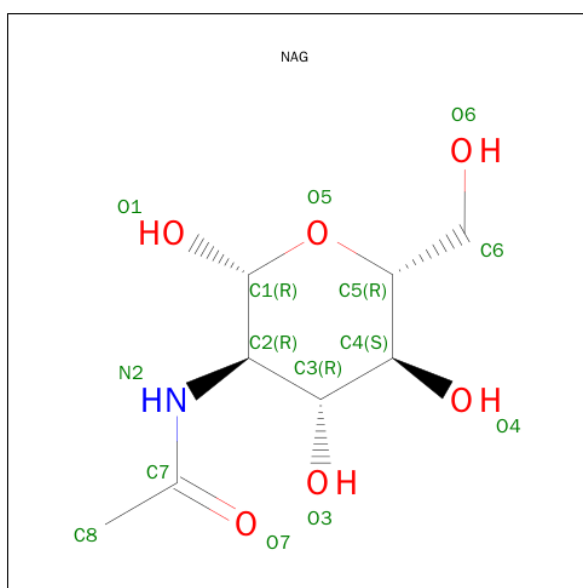


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	L	1	Total	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: C₈H₁₅NO₆).



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		

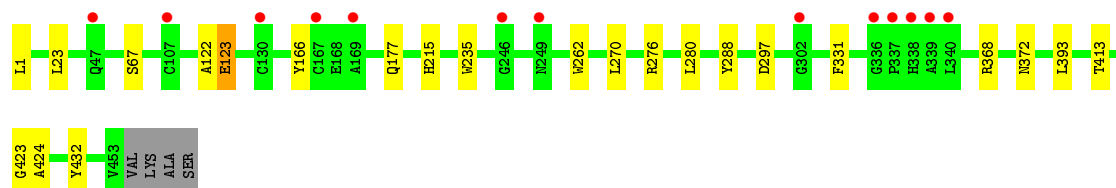
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

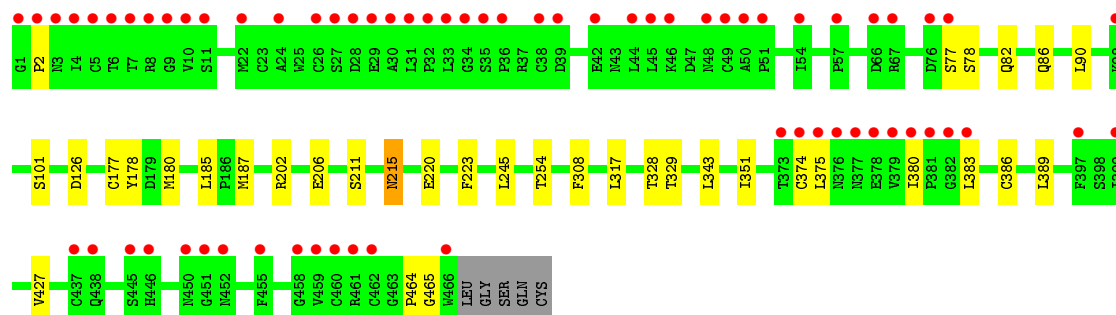
- Molecule 1: Integrin alpha-IIb



- Molecule 1: Integrin alpha-IIb

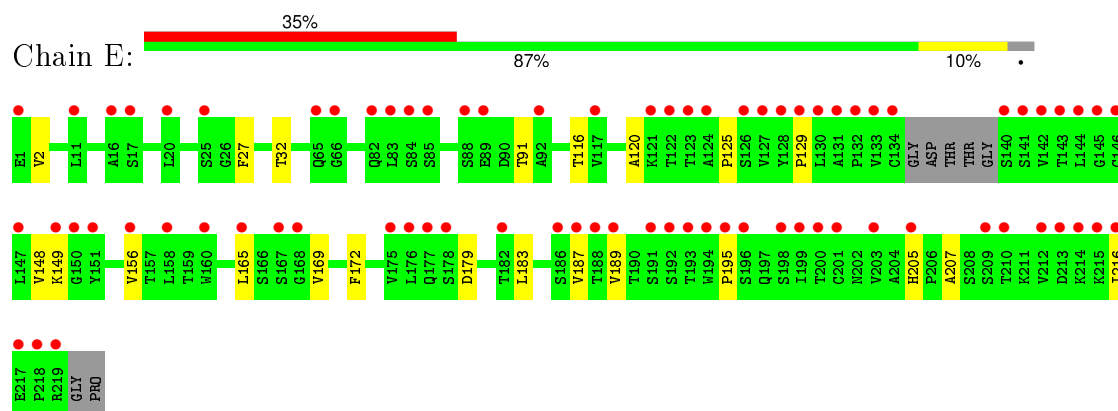


- Molecule 2: Integrin beta-3

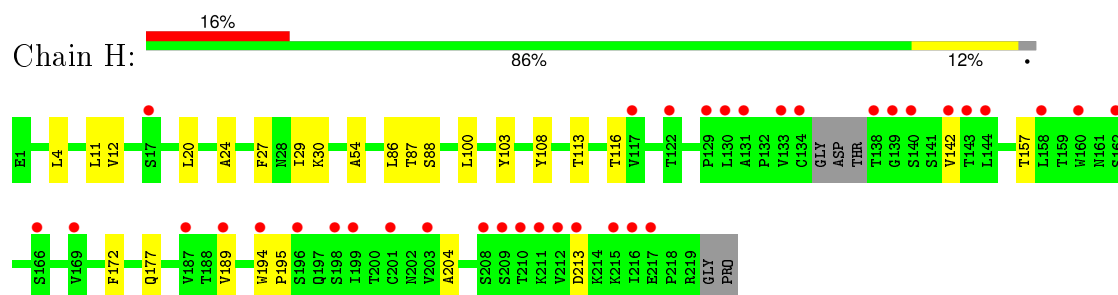




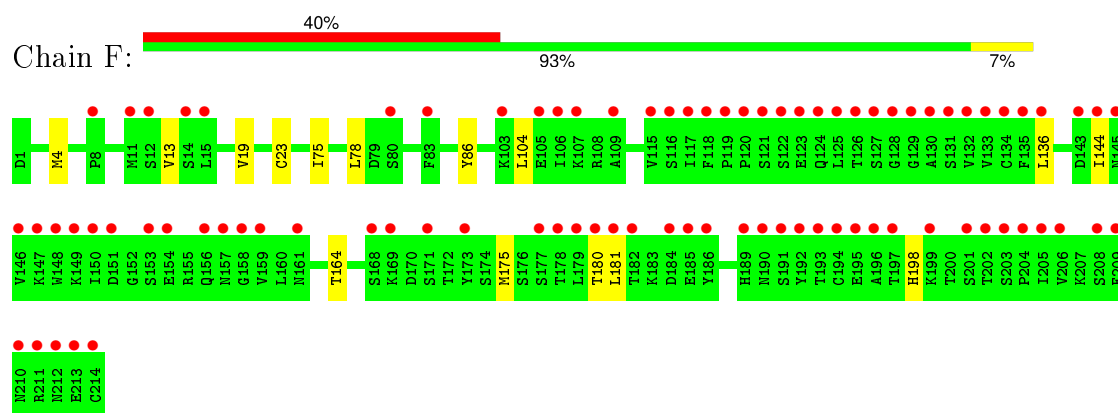
• Molecule 3: Monoclonal antibody 10E5 heavy chain



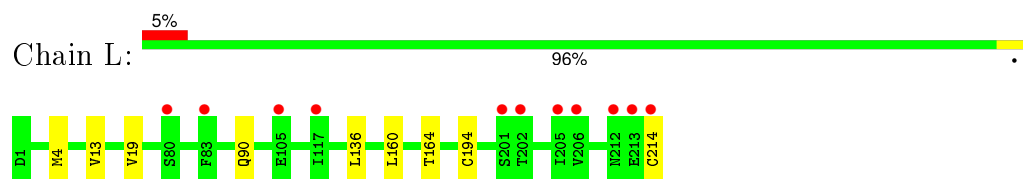
• Molecule 3: Monoclonal antibody 10E5 heavy chain



• 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 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	32.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 169848 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22131	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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:177:GLN:HB2	4:L:160:LEU:HD21	1.92	0.51
3:H:4:LEU:N	3:H:4:LEU:HD12	2.26	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:D:202:ARG:NH1	13:D:515:HOH:O	2.40	0.47
2:B:185:LEU:HG	2:B:211:SER:OG	2.15	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
4:L:4:MET:HE2	4:L:90:GLN:HB3	1.98	0.46
2:B:386:CYS:HB3	2:B:389:LEU:HD11	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
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:B:220:GLU:OE1	2:B:220:GLU:HA	2.18	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
4:F:4:MET:CE	4:F:23:CYS:SG	3.06	0.43
2:B:464:PRO:HA	2:B:465:GLY:HA2	1.73	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)
3:H:177:GLN:CB	4:L:160:LEU:HD21	2.50	0.42
3:E:125:PRO:HB2	3:E:148:VAL:HG13	2.01	0.42
2:D:115:TYR:CZ	2:D:236:ILE:HD12	2.55	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:87:THR:HG22	3:H:88:SER:N	2.35	0.41
3:H:194:TRP:CG	3:H:195:PRO:HA	2.56	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 [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	457/457 (100%)	444 (97%)	12 (3%)	1 (0%)	52	64
1	C	453/457 (99%)	440 (97%)	12 (3%)	1 (0%)	52	64
2	B	466/471 (99%)	451 (97%)	13 (3%)	2 (0%)	39	48
2	D	470/471 (100%)	457 (97%)	13 (3%)	0	100	100
3	E	210/221 (95%)	200 (95%)	9 (4%)	1 (0%)	34	41

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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%)	52	64

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%)	74	86
1	C	363/364 (100%)	358 (99%)	5 (1%)	74	86
2	B	414/416 (100%)	408 (99%)	6 (1%)	74	86
2	D	417/416 (100%)	413 (99%)	4 (1%)	82	91
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	186 (100%)	1 (0%)	92	97
4	F	188/188 (100%)	187 (100%)	1 (0%)	92	97
4	L	188/188 (100%)	186 (99%)	2 (1%)	80	90
All	All	2310/2316 (100%)	2286 (99%)	24 (1%)	82	91

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	0.48	0	15,19,21	0.88	1 (6%)
10	NAG	B	3321	10	14,14,15	0.55	0	15,19,21	1.17	2 (13%)
10	MAN	B	3322	10	11,11,12	0.55	0	14,15,17	1.51	3 (21%)
10	MAN	B	3323	10	11,11,12	0.54	0	14,15,17	0.66	0
10	MAN	B	3324	10	11,11,12	0.62	0	14,15,17	1.21	2 (14%)
11	NAG	B	3371	11,2	14,14,15	0.57	0	15,19,21	0.65	0
11	NAG	B	3372	11	14,14,15	0.47	0	15,19,21	0.88	0
12	NAG	D	3320	12,2	14,14,15	0.47	0	15,19,21	1.10	1 (6%)
12	NAG	D	3321	12	14,14,15	0.55	0	15,19,21	0.74	0
12	MAN	D	3322	12	11,11,12	0.46	0	14,15,17	1.68	1 (7%)
11	NAG	D	3371	11,2	14,14,15	0.54	0	15,19,21	0.58	0
11	NAG	D	3372	11	14,14,15	0.47	0	15,19,21	0.81	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 (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	3324	MAN	O5-C1-C2	-2.84	106.26	110.86
10	B	3322	MAN	O5-C1-C2	-2.10	107.45	110.86
10	B	3322	MAN	O5-C5-C6	2.07	111.82	107.35
10	B	3324	MAN	C1-O5-C5	2.14	114.96	112.25
10	B	3320	NAG	C1-O5-C5	2.60	115.55	112.25
10	B	3321	NAG	C4-C3-C2	2.62	115.31	111.23
10	B	3321	NAG	C3-C4-C5	2.72	114.94	110.20
10	B	3322	MAN	C3-C4-C5	3.43	116.18	110.20
12	D	3320	NAG	C1-O5-C5	3.70	116.95	112.25
12	D	3322	MAN	C1-O5-C5	5.51	119.24	112.25

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	0.32	0
6	GOL	A	459	-	5,5,5	0.38	0	5,5,5	0.22	0
6	GOL	A	460	-	5,5,5	0.32	0	5,5,5	0.45	0
6	GOL	A	461	-	5,5,5	0.22	0	5,5,5	0.39	0
6	GOL	A	462	-	5,5,5	0.34	0	5,5,5	0.17	0
6	GOL	A	463	-	5,5,5	0.33	0	5,5,5	0.23	0
7	SO4	A	464	-	4,4,4	0.16	0	6,6,6	0.06	0
9	NAG	B	3099	2	14,14,15	0.55	0	15,19,21	0.95	1 (6%)
6	GOL	B	472	-	5,5,5	0.30	0	5,5,5	0.24	0
7	SO4	B	473	-	4,4,4	0.19	0	6,6,6	0.12	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	0.20	0
7	SO4	C	460	-	4,4,4	0.16	0	6,6,6	0.18	0
7	SO4	C	461	-	4,4,4	0.15	0	6,6,6	0.27	0
7	SO4	C	462	-	4,4,4	0.21	0	6,6,6	0.08	0
7	SO4	C	463	-	4,4,4	0.19	0	6,6,6	0.14	0
9	NAG	D	3099	2	14,14,15	0.58	0	15,19,21	0.88	0
7	SO4	D	472	-	4,4,4	0.14	0	6,6,6	0.13	0
7	SO4	D	473	-	4,4,4	0.21	0	6,6,6	0.11	0
7	SO4	H	222	-	4,4,4	0.20	0	6,6,6	0.06	0
7	SO4	L	215	-	4,4,4	0.18	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	2.30	115.17	112.25

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, 95th 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 ²)	Q<0.9
1	A	454/457 (99%)	0.44	6 (1%) 79 84	9, 20, 49, 89	0
1	C	453/457 (99%)	0.29	13 (2%) 55 64	15, 32, 63, 106	0
2	B	466/471 (98%)	0.93	68 (14%) 3 5	10, 44, 127, 170	1 (0%)
2	D	471/471 (100%)	0.60	46 (9%) 10 14	16, 41, 101, 142	1 (0%)
3	E	214/221 (96%)	1.98	77 (35%) 0 0	41, 96, 147, 161	0
3	H	216/221 (97%)	0.73	36 (16%) 2 4	24, 73, 143, 176	0
4	F	214/214 (100%)	1.94	86 (40%) 0 0	41, 91, 143, 170	1 (0%)
4	L	214/214 (100%)	0.35	11 (5%) 32 41	26, 57, 104, 194	1 (0%)
All	All	2702/2726 (99%)	0.78	343 (12%) 5 8	9, 44, 128, 194	4 (0%)

All (343) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	212	VAL	13.9
4	F	214	CYS	13.1
3	E	133	VAL	12.1
2	B	33	LEU	11.6
3	E	201	CYS	11.4
4	F	181	LEU	9.4
3	E	216	ILE	9.0
3	E	131	ALA	8.9
3	E	134	CYS	8.7
2	B	77	SER	8.5
4	F	126	THR	8.3
2	D	469	SER	8.3
4	L	214	CYS	8.2
2	B	44	LEU	8.1
3	E	219	ARG	8.1
3	E	194	TRP	8.1

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Mol	Chain	Res	Type	RSRZ
2	B	30	ALA	8.0
2	D	471	CYS	7.7
1	A	337	PRO	7.7
2	B	36	PRO	7.7
4	F	212	ASN	7.6
4	F	125	LEU	7.5
4	F	122	SER	7.2
4	F	148	TRP	7.2
4	F	193	THR	7.1
4	F	130	ALA	6.9
3	H	134	CYS	6.7
3	H	133	VAL	6.7
3	E	142	VAL	6.6
4	F	179	LEU	6.6
3	E	144	LEU	6.5
3	E	129	PRO	6.4
2	B	375	LEU	6.4
2	B	10	VAL	6.3
3	E	200	THR	6.3
2	B	76	ASP	6.2
3	E	215	LYS	6.1
4	F	180	THR	5.8
3	E	147	LEU	5.8
2	B	34	GLY	5.7
3	E	192	SER	5.7
4	F	210	ASN	5.7
2	B	4	ILE	5.6
4	F	129	GLY	5.6
3	E	196	SER	5.6
2	D	470	GLN	5.5
2	B	2	PRO	5.4
3	E	210	THR	5.4
3	E	217	GLU	5.4
4	F	135	PHE	5.3
4	F	213	GLU	5.3
3	E	127	VAL	5.3
3	E	203	VAL	5.3
4	F	150	ILE	5.3
2	B	450	ASN	5.3
4	F	184	ASP	5.2
3	E	198	SER	5.2
4	F	158	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
4	F	118	PHE	5.2
3	E	218	PRO	5.1
2	D	51	PRO	5.0
2	B	374	CYS	5.0
3	E	130	LEU	5.0
3	E	165	LEU	4.9
2	B	446	HIS	4.9
2	B	46	LYS	4.9
4	F	119	PRO	4.9
2	B	28	ASP	4.9
2	D	44	LEU	4.8
3	E	117	VAL	4.8
2	B	32	PRO	4.8
4	F	147	LYS	4.8
2	B	45	LEU	4.7
3	E	132	PRO	4.7
3	E	199	ILE	4.7
2	B	7	THR	4.7
3	E	150	GLY	4.7
2	B	466	TRP	4.7
2	B	1	GLY	4.7
4	F	182	THR	4.7
4	F	136	LEU	4.6
4	F	208	SER	4.6
4	F	127	SER	4.5
3	E	126	SER	4.5
2	D	2	PRO	4.5
4	F	131	SER	4.4
3	E	195	PRO	4.4
2	D	33	LEU	4.4
2	B	31	LEU	4.4
2	B	8	ARG	4.4
2	B	39	ASP	4.4
2	D	9	GLY	4.4
1	A	339	ALA	4.3
3	H	187	VAL	4.3
4	F	120	PRO	4.3
2	D	1	GLY	4.3
3	E	128	TYR	4.3
4	F	115	VAL	4.3
4	F	196	ALA	4.3
4	F	134	CYS	4.2

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Mol	Chain	Res	Type	RSRZ
4	F	116	SER	4.2
3	E	186	SER	4.2
3	E	160	TRP	4.2
2	B	29	GLU	4.2
4	F	154	GLU	4.2
2	B	376	ASN	4.2
4	F	195	GLU	4.2
3	H	189	VAL	4.1
3	E	213	ASP	4.1
2	B	35	SER	4.1
2	B	42	GLU	4.1
3	E	83	LEU	4.1
2	B	22	MET	4.0
2	D	54	ILE	4.0
3	E	141	SER	4.0
3	E	145	GLY	4.0
3	E	143	THR	4.0
4	F	132	VAL	4.0
2	B	460	CYS	4.0
2	B	3	ASN	3.9
4	F	186	TYR	3.9
3	E	123	THR	3.9
3	E	146	CYS	3.9
2	D	376	ASN	3.9
2	D	36	PRO	3.9
2	B	379	VAL	3.9
4	F	157	ASN	3.8
2	D	45	LEU	3.8
2	D	46	LYS	3.8
2	B	383	LEU	3.8
2	D	8	ARG	3.8
2	B	51	PRO	3.8
3	E	167	SER	3.7
3	E	178	SER	3.7
3	H	217	GLU	3.7
2	D	4	ILE	3.7
3	H	196	SER	3.7
2	D	30	ALA	3.7
2	B	452	ASN	3.6
3	E	168	GLY	3.6
3	H	216	ILE	3.6
3	E	16	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	35	SER	3.6
4	F	206	VAL	3.6
3	H	158	LEU	3.6
3	E	187	VAL	3.5
4	F	177	SER	3.5
2	B	9	GLY	3.5
2	D	22	MET	3.5
3	H	144	LEU	3.5
4	F	153	SER	3.5
1	C	336	GLY	3.5
1	A	336	GLY	3.4
3	E	177	GLN	3.4
3	E	191	SER	3.4
4	F	159	VAL	3.4
3	E	149	LYS	3.4
2	B	26	CYS	3.4
4	F	209	PHE	3.4
2	D	52	GLU	3.4
2	D	375	LEU	3.4
3	E	176	LEU	3.4
2	D	3	ASN	3.4
2	D	78	SER	3.3
3	E	85	SER	3.3
4	F	121	SER	3.3
3	E	66	GLY	3.3
1	A	338	HIS	3.3
2	B	11	SER	3.3
2	B	445	SER	3.3
3	E	189	VAL	3.3
4	F	133	VAL	3.3
4	F	145	ASN	3.3
4	F	107	LYS	3.3
3	E	25	SER	3.2
2	D	378	GLU	3.2
4	F	192	TYR	3.2
4	L	202	THR	3.2
3	H	215	LYS	3.2
4	F	178	THR	3.2
4	F	144	ILE	3.2
3	E	92	ALA	3.2
2	D	468	GLY	3.2
3	H	169	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	106	ILE	3.1
4	F	117	ILE	3.1
3	E	175	VAL	3.1
4	F	151	ASP	3.1
2	D	48	ASN	3.1
4	F	204	PRO	3.1
4	F	185	GLU	3.1
2	D	42	GLU	3.1
4	L	205	ILE	3.1
1	C	338	HIS	3.1
3	E	122	THR	3.1
4	F	146	VAL	3.1
2	B	381	PRO	3.1
4	F	201	SER	3.1
4	F	205	ILE	3.1
1	C	339	ALA	3.1
2	B	6	THR	3.1
4	F	128	GLY	3.1
2	D	32	PRO	3.1
2	D	380	ILE	3.0
3	E	214	LYS	3.0
3	H	160	TRP	3.0
4	L	212	ASN	3.0
2	B	38	CYS	2.9
4	F	169	LYS	2.9
2	B	382	GLY	2.9
4	F	156	GLN	2.9
4	L	206	VAL	2.9
2	B	5	CYS	2.9
4	F	14	SER	2.9
3	E	82	GLN	2.9
2	B	458	GLY	2.9
3	H	203	VAL	2.9
2	B	380	ILE	2.8
2	B	455	PHE	2.8
3	H	201	CYS	2.8
4	F	194	CYS	2.8
3	E	124	ALA	2.8
3	E	84	SER	2.8
3	H	131	ALA	2.8
3	E	11	LEU	2.8
3	H	130	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
4	F	123	GLU	2.8
3	H	117	VAL	2.8
2	B	49	CYS	2.8
2	D	77	SER	2.8
4	F	109	ALA	2.8
2	D	49	CYS	2.8
3	H	129	PRO	2.7
3	E	121	LYS	2.7
3	E	209	SER	2.7
3	H	209	SER	2.7
4	F	80	SER	2.7
4	F	197	THR	2.7
3	E	156	VAL	2.7
2	B	54	ILE	2.7
3	E	89	GLU	2.7
2	B	397	PHE	2.7
3	E	205	HIS	2.6
3	H	143	THR	2.6
2	D	40	LEU	2.6
1	C	130	CYS	2.6
4	F	211	ARG	2.6
2	D	129[A]	TRP	2.6
4	F	173	TYR	2.6
4	F	190	ASN	2.6
2	D	53	SER	2.6
4	F	191	SER	2.6
4	L	213	GLU	2.6
1	C	337	PRO	2.6
2	D	28	ASP	2.6
2	B	378	GLU	2.6
2	B	437	CYS	2.6
2	B	462	CYS	2.6
3	H	166	SER	2.6
3	E	151	TYR	2.6
1	C	340	LEU	2.5
3	H	17	SER	2.5
4	F	103	LYS	2.5
2	B	373	THR	2.5
3	E	17	SER	2.5
2	B	48	ASN	2.5
4	F	149	LYS	2.4
3	E	20	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	11	MET	2.4
4	F	124	GLN	2.4
4	F	83	PHE	2.4
2	D	34	GLY	2.4
2	D	5	CYS	2.4
2	D	26	CYS	2.4
3	H	208	SER	2.4
3	E	182	THR	2.4
3	H	213	ASP	2.4
3	H	122	THR	2.4
2	D	143	ARG	2.4
1	C	246	GLY	2.4
3	H	139	GLY	2.4
4	F	12	SER	2.4
2	B	50	ALA	2.4
3	E	188	THR	2.4
3	E	65	GLN	2.4
4	F	168	SER	2.3
1	C	169	ALA	2.3
2	B	57	PRO	2.3
3	H	162	SER	2.3
4	F	203	SER	2.3
3	H	138	THR	2.3
1	C	302	GLY	2.3
2	B	27	SER	2.3
4	F	171	SER	2.3
3	H	142	VAL	2.3
3	H	212	VAL	2.3
4	F	8	PRO	2.3
4	F	189	HIS	2.3
4	F	199	LYS	2.3
2	B	438	GLN	2.2
2	B	451	GLY	2.2
4	L	83	PHE	2.2
4	F	161	ASN	2.2
4	F	202	THR	2.2
2	B	461	ARG	2.2
1	C	249	ASN	2.2
4	F	143	ASP	2.2
3	E	88	SER	2.2
2	B	24	ALA	2.2
2	D	56	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	404	ARG	2.2
3	E	140	SER	2.2
4	L	80	SER	2.2
3	E	1	GLU	2.2
4	L	117	ILE	2.2
3	H	194	TRP	2.2
1	A	45	PRO	2.2
3	H	198	SER	2.2
2	B	377	ASN	2.1
1	A	96	SER	2.1
2	D	27	SER	2.1
3	H	140	SER	2.1
3	E	193	THR	2.1
3	H	210	THR	2.1
2	B	66	ASP	2.1
4	L	105	GLU	2.1
2	D	450	ASN	2.1
3	H	211	LYS	2.1
2	B	399	ILE	2.1
1	C	167	CYS	2.1
4	L	201	SER	2.1
2	B	98	LYS	2.1
2	B	459	VAL	2.1
4	F	105	GLU	2.1
4	F	15	LEU	2.0
2	D	436	ALA	2.0
3	H	199	ILE	2.0
3	E	158	LEU	2.0
2	D	57	PRO	2.0
2	D	381	PRO	2.0
1	C	47	GLN	2.0
1	C	107	CYS	2.0
2	B	67	ARG	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 ⓘ

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, 95th 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 ²)	Q<0.9
11	NAG	D	3371	14/15	0.86	0.26	1.96	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
10	NAG	B	3321	14/15	0.90	0.12	-	40,53,63,76	0
10	MAN	B	3322	11/12	0.80	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, 95th 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 ²)	Q<0.9
8	MG	D	2001	1/1	0.87	0.71	21.14	41,41,41,41	1
7	SO4	L	215	5/5	0.81	0.44	11.55	101,106,112,115	0
7	SO4	D	473	5/5	0.73	0.39	9.71	131,133,136,137	0
6	GOL	C	458	6/6	0.83	0.30	8.73	45,61,71,79	0
6	GOL	A	463	6/6	0.73	0.30	7.83	77,79,83,84	0
6	GOL	A	460	6/6	0.81	0.27	6.12	68,70,78,84	0
7	SO4	H	222	5/5	0.83	0.36	5.70	112,116,118,123	0
7	SO4	C	461	5/5	0.88	0.25	5.54	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	3.45	39,53,83,84	0
7	SO4	A	464	5/5	0.86	0.17	3.26	97,98,107,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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	1.52	28,50,57,71	0
6	GOL	B	472	6/6	0.83	0.17	1.41	65,70,72,77	0
5	CA	A	2006	1/1	0.99	0.15	0.59	16,16,16,16	0
8	MG	B	2001	1/1	0.97	0.16	0.20	26,26,26,26	1
5	CA	C	2007	1/1	0.97	0.14	0.18	36,36,36,36	0
5	CA	A	2005	1/1	0.99	0.12	-0.38	19,19,19,19	0
5	CA	C	2006	1/1	0.97	0.11	-0.54	34,34,34,34	0
5	CA	B	2003	1/1	0.99	0.17	-0.70	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	0.11	-1.18	84,91,98,98	0
5	CA	A	2004	1/1	0.99	0.06	-1.84	29,29,29,29	0
5	CA	D	2002	1/1	0.95	0.12	-2.02	31,31,31,31	0
5	CA	C	2004	1/1	0.97	0.04	-2.21	45,45,45,45	0
5	CA	C	2005	1/1	0.99	0.05	-3.73	38,38,38,38	0
5	CA	B	2002	1/1	0.96	0.05	-4.05	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.