



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:26 PM GMT

PDB ID : 3ZE2
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 : 2.35 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

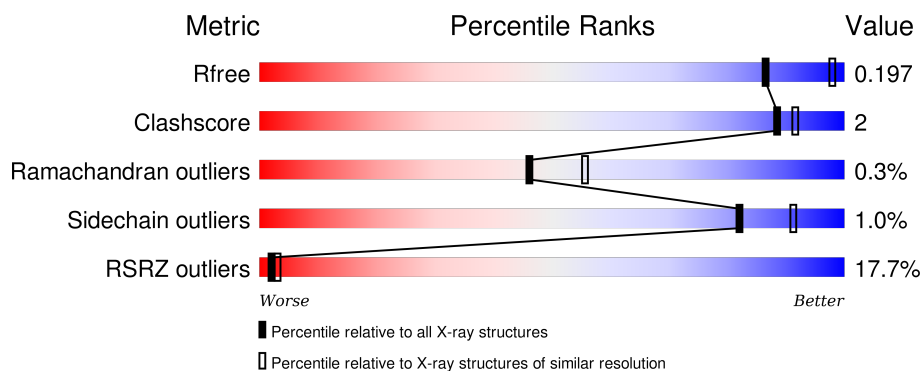
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	 93% 6%
1	C	457	 94% 5%
2	B	472	 15% 89% 10%
2	D	472	 26% 74% 22%
3	E	221	 93% 5%

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Mol	Chain	Length	Quality of chain
3	H	221	
4	F	214	
4	L	214	
5	I	6	
5	J	6	

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
6	GOL	A	1455	-	-	-	X
6	GOL	A	1456	-	-	-	X
6	GOL	C	1454	-	-	-	X
6	GOL	C	1456	-	-	-	X
6	GOL	C	1457	-	-	-	X
6	GOL	F	1215	-	-	-	X
6	GOL	F	1216	-	-	-	X
6	GOL	J	1498	-	-	-	X
7	SO4	A	1457	-	-	-	X
8	CA	A	2005	-	-	-	X
9	MN	B	2001	-	-	-	X
9	MN	D	2001	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 41569 atoms, of which 19764 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	H	N	O	S	2	5	0
			6845	2228	3341	600	668	8			
1	C	453	Total	C	H	N	O	S	1	6	0
			6840	2227	3337	602	666	8			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	469	Total	C	H	N	O	S	0	7	0
			7218	2275	3569	619	721	34			
2	D	367	Total	C	H	N	O	S	0	6	0
			5806	1834	2896	487	570	19			

- 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	2	0
			3222	1028	1569	273	343	9			
4	L	214	Total	C	H	N	O	S	0	0	0
			3187	1019	1550	268	341	9			

- Molecule 5 is a protein called RGD PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	6	Total	C	H	N	O	0	3	0
			111	32	52	15	12			
5	J	6	Total	C	H	N	O	0	0	0
			74	22	34	9	9			

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	C	1	Total	C	H	O	0	0
			14	3	8	3		
6	C	1	Total	C	H	O	0	0
			14	3	8	3		
6	C	1	Total	C	H	O	0	0
			14	3	8	3		
6	C	1	Total	C	H	O	0	0
			14	3	8	3		
6	E	1	Total	C	H	O	0	0
			14	3	8	3		
6	F	1	Total	C	H	O	0	0
			14	3	8	3		
6	F	1	Total	C	H	O	0	0
			14	3	8	3		
6	J	1	Total	C	H	O	0	0
			14	3	8	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	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- 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		

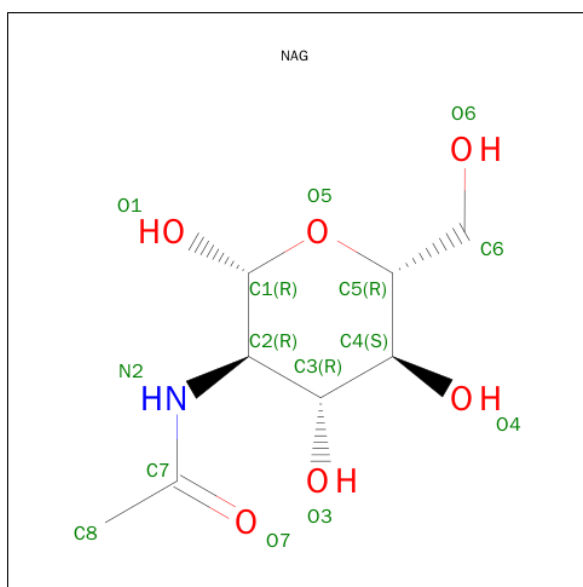
- Molecule 10 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	6	Total	C	H	N	O	0	0
			133	40	61	2	30		

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

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

- Molecule 12 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- 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	483	Total	O	0	0
			483	483		

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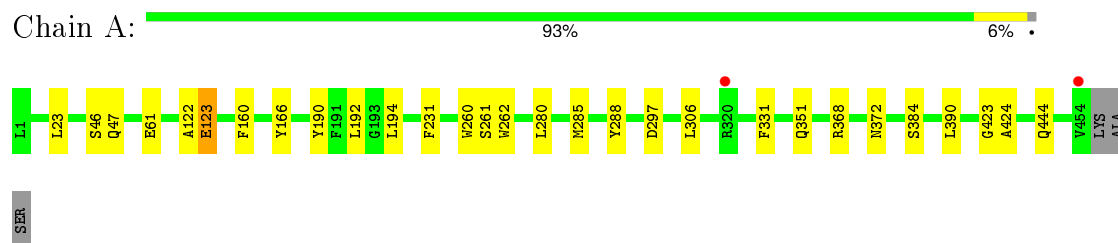
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	B	211	Total 211	O 211	0	0
14	C	283	Total 283	O 283	0	0
14	D	107	Total 107	O 107	0	0
14	E	129	Total 129	O 129	0	0
14	F	68	Total 68	O 68	0	0
14	H	18	Total 18	O 18	0	0
14	I	2	Total 2	O 2	0	0
14	J	2	Total 2	O 2	0	0
14	L	15	Total 15	O 15	0	0

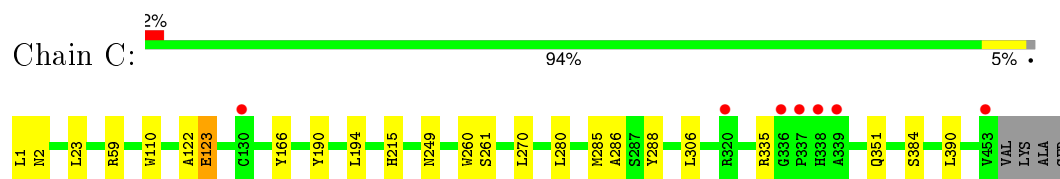
3 Residue-property plots

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

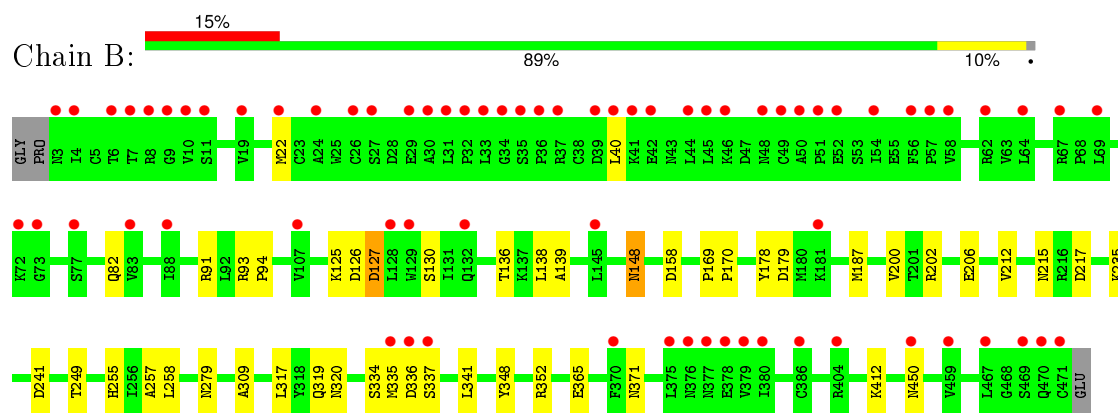
• Molecule 1: INTEGRIN ALPHA-IIB



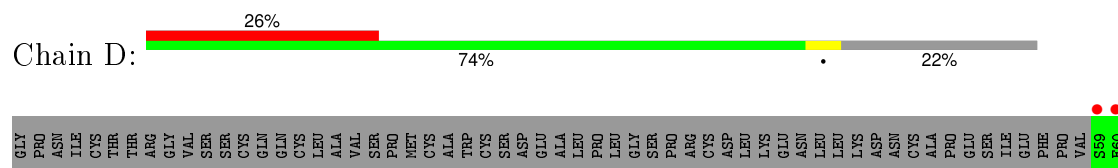
• Molecule 1: INTEGRIN ALPHA-IIB

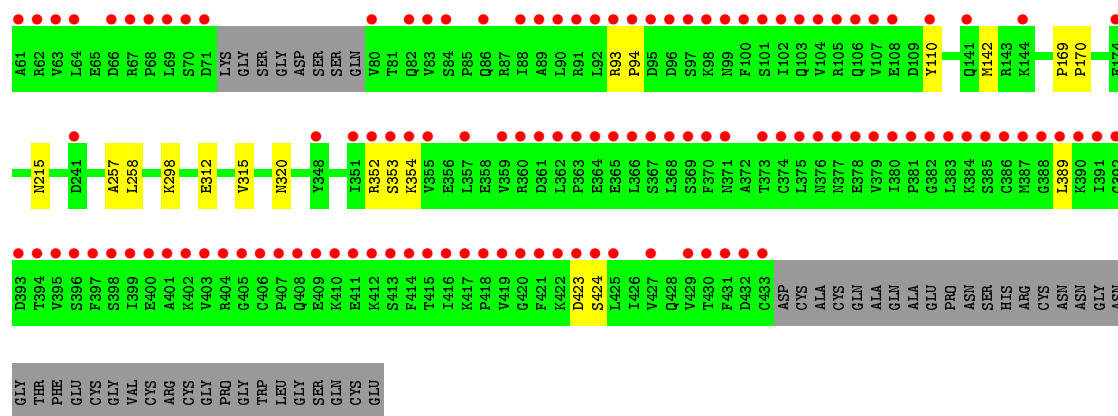


• Molecule 2: INTEGRIN BETA-3

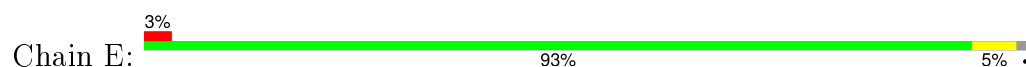


• Molecule 2: INTEGRIN BETA-3

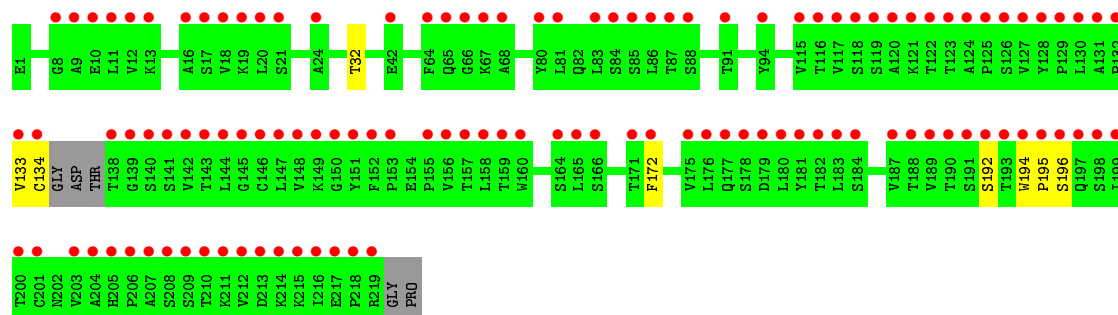




• Molecule 3: 10E5 FAB HEAVY CHAIN



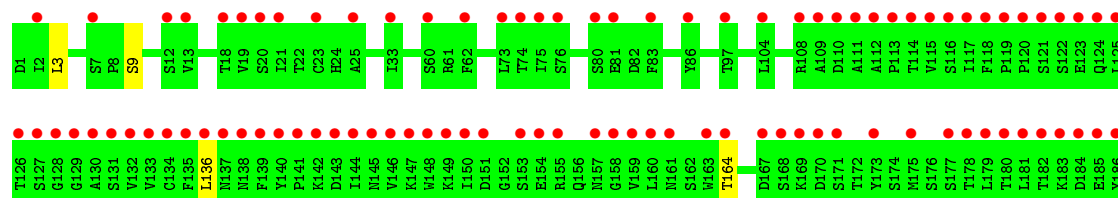
• Molecule 3: 10E5 FAB HEAVY CHAIN

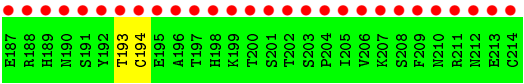


• Molecule 4: 10E5 FAB LIGHT CHAIN



• Molecule 4: 10E5 FAB LIGHT CHAIN





● Molecule 5: RGD PEPTIDE



● Molecule 5: RGD PEPTIDE



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	233.21Å 143.56Å 104.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.02 – 2.35 54.02 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.02-2.35) 100.0 (54.02-2.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.34Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.175 , 0.204 0.168 , 0.197	Depositor DCC
R_{free} test set	1011 reflections (0.69%)	DCC
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 146567 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	41569	wwPDB-VP
Average B, all atoms (Å ²)	66.0	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.*

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, BMA, NAG, 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	0.24	0/3612	0.44	0/4923
1	C	0.23	0/3615	0.41	0/4927
2	B	0.22	0/3737	0.40	0/5066
2	D	0.22	0/2976	0.39	0/4031
3	E	0.23	0/1684	0.42	0/2305
3	H	0.21	0/1684	0.38	0/2305
4	F	0.23	0/1692	0.41	0/2294
4	L	0.22	0/1673	0.37	0/2269
5	I	0.20	0/59	0.40	0/76
5	J	0.18	0/40	0.39	0/52
All	All	0.23	0/20772	0.41	0/28248

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3504	3341	3348	20	0
1	C	3503	3337	3345	18	0
2	B	3649	3569	3575	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2910	2896	2900	11	0
3	E	1642	1597	1600	5	0
3	H	1642	1597	1600	5	0
4	F	1653	1569	1571	6	0
4	L	1637	1550	1553	4	0
5	I	59	52	51	6	0
5	J	40	34	34	0	0
6	A	12	16	16	0	0
6	C	24	32	32	1	0
6	E	6	8	8	0	0
6	F	12	16	16	0	0
6	J	6	8	8	0	0
7	A	10	0	0	1	0
8	A	4	0	0	0	0
8	C	4	0	0	0	0
9	B	3	0	0	0	0
9	D	3	0	0	0	0
10	B	72	61	61	0	0
11	B	28	25	25	2	0
12	C	14	13	13	0	0
13	D	50	43	43	0	0
14	A	483	0	0	6	1
14	B	211	0	0	6	0
14	C	283	0	0	6	1
14	D	107	0	0	1	0
14	E	129	0	0	0	0
14	F	68	0	0	0	0
14	H	18	0	0	0	0
14	I	2	0	0	0	0
14	J	2	0	0	0	0
14	L	15	0	0	1	0
All	All	21805	19764	19799	99	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (99) 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)
14:A:3238:HOH:O	5:I:492[B]:GLY:N	2.03	0.90
14:A:3222:HOH:O	5:I:493[A]:ARG:NH2	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:SER:OG	14:C:3243:HOH:O	2.05	0.74
1:A:384:SER:OG	14:A:3430:HOH:O	2.06	0.73
7:A:1457:SO4:O3	14:A:3482:HOH:O	2.09	0.70
2:B:148:ASN:OD1	14:B:3048:HOH:O	2.10	0.70
2:B:335:MET:O	14:B:3040:HOH:O	2.10	0.68
1:C:249:ASN:ND2	14:C:3170:HOH:O	2.27	0.68
1:C:2[B]:ASN:OD1	14:C:3001:HOH:O	2.12	0.67
2:B:126:ASP:OD1	14:B:3039:HOH:O	2.13	0.67
1:C:351:GLN:OE1	14:C:3221:HOH:O	2.13	0.66
2:B:130[B]:SER:OG	2:B:336:ASP:OD2	2.14	0.65
2:B:319[B]:GLN:OE1	14:B:3169:HOH:O	2.13	0.65
1:C:1:LEU:N	1:C:2[B]:ASN:HA	2.11	0.65
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.32	0.62
11:B:3371:NAG:O3	11:B:3372:NAG:O5	2.13	0.62
1:C:1:LEU:N	1:C:2[A]:ASN:HA	2.12	0.60
2:B:82:GLN:NE2	14:B:3017:HOH:O	2.36	0.56
1:A:122:ALA:O	1:A:123:GLU:HB2	2.06	0.56
1:C:122:ALA:O	1:C:123:GLU:HB2	2.06	0.55
2:B:235:LYS:NZ	14:B:3109:HOH:O	2.36	0.55
2:B:178[B]:TYR:CD1	2:B:179:ASP:N	2.74	0.55
1:C:335:ARG:NH2	14:C:3212:HOH:O	2.40	0.55
1:A:192:LEU:HD13	5:I:493[A]:ARG:NH1	2.22	0.55
1:C:59:ARG:NH1	14:C:3050:HOH:O	2.39	0.55
2:B:130[A]:SER:OG	2:B:337[A]:SER:OG	2.25	0.55
2:D:423:ASP:OD1	2:D:424:SER:N	2.40	0.55
1:A:280[B]:LEU:HD23	1:A:331:PHE:CZ	2.44	0.53
2:B:127:ASP:N	2:B:127:ASP:OD1	2.41	0.52
4:L:9:SER:OG	14:L:3004:HOH:O	2.19	0.52
1:A:351:GLN:OE1	14:A:3394:HOH:O	2.19	0.51
2:B:450:ASN:ND2	2:B:450:ASN:O	2.44	0.51
1:A:280[B]:LEU:HD23	1:A:331:PHE:CE1	2.45	0.51
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.93	0.51
3:H:192:SER:O	3:H:196:SER:OG	2.29	0.50
2:B:365:GLU:OE2	2:B:412:LYS:NZ	2.42	0.50
3:E:133:VAL:O	3:E:134:CYS:SG	2.70	0.50
2:D:257:ALA:O	2:D:258:LEU:HB2	2.12	0.50
2:D:298:LYS:NZ	14:D:3079:HOH:O	2.43	0.48
2:B:257:ALA:O	2:B:258:LEU:HB2	2.14	0.48
1:A:122:ALA:O	1:A:123:GLU:CB	2.62	0.48
2:B:371:ASN:ND2	11:B:3371:NAG:C7	2.77	0.48
2:B:158:ASP:HB3	2:B:187:MET:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280[A]:LEU:CD1	1:A:306:LEU:HD23	2.44	0.48
2:B:249[B]:THR:HG22	2:B:309:ALA:HB3	1.95	0.47
1:C:122:ALA:O	1:C:123:GLU:CB	2.63	0.47
3:E:194:TRP:CG	3:E:195:PRO:HA	2.49	0.47
1:A:160:PHE:HB2	5:I:493[B]:ARG:HD3	1.97	0.46
1:A:280[B]:LEU:HD12	1:A:280[B]:LEU:N	2.30	0.46
3:H:194:TRP:CG	3:H:195:PRO:HA	2.50	0.46
2:D:110:TYR:OH	2:D:354:LYS:O	2.25	0.46
2:B:22:MET:HG2	2:B:40:LEU:CD2	2.46	0.45
3:H:172:PHE:CD2	4:L:164:THR:HG23	2.51	0.45
1:A:46:SER:O	1:A:47:GLN:HB2	2.17	0.45
2:D:352:ARG:CG	2:D:352:ARG:O	2.64	0.45
2:D:169:PRO:HB2	2:D:170:PRO:HD2	1.98	0.45
1:A:285:MET:SD	2:B:320:ASN:HB3	2.57	0.45
5:I:492[B]:GLY:O	5:I:494[B]:GLY:N	2.50	0.45
1:C:194:LEU:C	1:C:194:LEU:HD12	2.38	0.44
1:C:280:LEU:CD1	1:C:306:LEU:HD23	2.46	0.44
1:C:390:LEU:HD12	1:C:390:LEU:N	2.32	0.44
3:E:67:LYS:NZ	3:E:84:SER:O	2.50	0.44
4:L:136:LEU:N	4:L:136:LEU:HD12	2.33	0.43
2:D:312:GLU:HA	2:D:315:VAL:HG23	2.00	0.43
1:A:390:LEU:N	1:A:390:LEU:HD12	2.34	0.43
2:B:235:LYS:CE	2:B:279:ASN:OD1	2.67	0.43
2:B:139:ALA:HB2	2:B:200:VAL:HG11	1.99	0.43
2:B:348:TYR:CZ	2:B:352:ARG:HD2	2.53	0.43
2:B:125:LYS:HA	2:B:212:VAL:HG11	2.01	0.43
4:F:91:TYR:HB2	4:F:96:TYR:CZ	2.53	0.43
3:H:133:VAL:O	3:H:134:CYS:SG	2.77	0.43
1:C:215:HIS:CE1	3:H:32:THR:HG22	2.53	0.43
3:E:12:VAL:HG21	3:E:86:LEU:CD1	2.49	0.43
5:I:492[B]:GLY:C	5:I:494[B]:GLY:N	2.72	0.43
1:A:192:LEU:HD11	1:A:231:PHE:CD1	2.53	0.43
1:C:285:MET:SD	2:D:320:ASN:HB3	2.59	0.42
1:C:260:TRP:CE3	1:C:261:SER:HB2	2.54	0.42
2:B:169:PRO:HB2	2:B:170:PRO:HD2	1.99	0.42
1:A:194:LEU:C	1:A:194:LEU:HD12	2.39	0.42
2:B:138:LEU:HA	2:B:341:LEU:HD13	2.00	0.42
2:D:354:LYS:HG3	2:D:354:LYS:O	2.19	0.42
4:L:193:THR:HG22	4:L:194:CYS:N	2.34	0.42
1:A:260:TRP:CE3	1:A:261:SER:HB2	2.55	0.42
3:E:125:PRO:HB2	3:E:148:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:211:ARG:NH1	4:F:212:ASN:OD1	2.53	0.42
4:F:43:SER:OG	4:F:44:PHE:N	2.50	0.41
1:A:423:GLY:O	1:A:424:ALA:HB3	2.20	0.41
1:C:285:MET:O	1:C:286:ALA:HB3	2.20	0.41
2:D:353:SER:HB2	2:D:389:LEU:N	2.35	0.41
1:A:444:GLN:NE2	14:A:3478:HOH:O	2.53	0.41
4:F:136:LEU:N	4:F:136:LEU:HD12	2.36	0.41
1:A:262:TRP:HB3	2:B:317:LEU:HD13	2.03	0.41
4:F:140:TYR:CG	4:F:141:PRO:HA	2.56	0.41
2:B:217:ASP:OD2	2:B:255:HIS:NE2	2.55	0.40
2:D:93:ARG:HB2	2:D:94:PRO:HD2	2.03	0.40
2:B:169:PRO:HD2	2:B:178[B]:TYR:CE1	2.56	0.40
4:F:211:ARG:O	4:F:212:ASN:HB2	2.22	0.40
1:A:297:ASP:O	1:A:372:ASN:HB2	2.21	0.40
1:C:110:TRP:HB3	6:C:1457:GOL:H31	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:3480:HOH:O	14:C:3252:HOH:O[1_554]	2.18	0.02

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%)	445 (97%)	11 (2%)	1 (0%)	52 63
1	C	457/457 (100%)	440 (96%)	16 (4%)	1 (0%)	52 63
2	B	474/472 (100%)	460 (97%)	13 (3%)	1 (0%)	52 63
2	D	369/472 (78%)	355 (96%)	13 (4%)	1 (0%)	46 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	212/221 (96%)	202 (95%)	9 (4%)	1 (0%)	34	39
3	H	212/221 (96%)	200 (94%)	12 (6%)	0	100	100
4	F	214/214 (100%)	206 (96%)	8 (4%)	0	100	100
4	L	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
5	I	6/6 (100%)	2 (33%)	0	4 (67%)	0	0
5	J	4/6 (67%)	4 (100%)	0	0	100	100
All	All	2617/2740 (96%)	2514 (96%)	94 (4%)	9 (0%)	46	55

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	D	142	MET
1	C	123	GLU
5	I	493[A]	ARG
5	I	493[B]	ARG
2	B	334	SER
5	I	494[A]	GLY
5	I	494[B]	GLY
3	E	133	VAL

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%)	361 (98%)	6 (2%)	70	83
1	C	367/364 (101%)	362 (99%)	5 (1%)	74	86
2	B	422/417 (101%)	416 (99%)	6 (1%)	74	86
2	D	336/417 (81%)	335 (100%)	1 (0%)	94	98
3	E	187/190 (98%)	186 (100%)	1 (0%)	92	97
3	H	187/190 (98%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	190/188 (101%)	188 (99%)	2 (1%)	80	90
4	L	188/188 (100%)	187 (100%)	1 (0%)	92	97
5	I	5/4 (125%)	3 (60%)	2 (40%)	0	0
5	J	4/4 (100%)	4 (100%)	0	100	100
All	All	2253/2326 (97%)	2229 (99%)	24 (1%)	82	90

All (24) 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	288	TYR
1	A	368	ARG
2	B	91	ARG
2	B	127	ASP
2	B	136	THR
2	B	148	ASN
2	B	215	ASN
2	B	241	ASP
1	C	23	LEU
1	C	166	TYR
1	C	190	TYR
1	C	270	LEU
1	C	288	TYR
2	D	215	ASN
3	E	202	ASN
4	F	108[A]	ARG
4	F	108[B]	ARG
5	I	493[A]	ARG
5	I	493[B]	ARG
4	L	3	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
2	B	450	ASN
1	C	338	HIS

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Mol	Chain	Res	Type
2	D	316	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 ⓘ

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	0.59	0	15,19,21	0.66	0
10	NAG	B	3321	10	14,14,15	0.53	0	15,19,21	0.81	0
10	BMA	B	3322	10	11,11,12	0.60	0	14,15,17	0.75	1 (7%)
10	MAN	B	3323	10	11,11,12	0.62	0	14,15,17	0.66	0
10	MAN	B	3324	10	11,11,12	0.62	0	14,15,17	0.73	0
10	MAN	B	3325	10	11,11,12	0.62	0	14,15,17	0.62	0
11	NAG	B	3371	11,2	14,14,15	0.49	0	15,19,21	0.74	0
11	NAG	B	3372	11	14,14,15	0.52	0	15,19,21	0.58	0
13	NAG	D	3320	13,2	14,14,15	0.45	0	15,19,21	0.82	1 (6%)
13	NAG	D	3321	13	14,14,15	0.59	0	15,19,21	0.82	0
13	BMA	D	3322	13	11,11,12	0.61	0	14,15,17	0.70	0
13	MAN	D	3323	13	11,11,12	0.58	0	14,15,17	0.69	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	BMA	B	3322	10	-	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
10	MAN	B	3325	10	-	0/2/19/22	0/1/1/1
11	NAG	B	3371	11,2	-	0/6/23/26	0/1/1/1
11	NAG	B	3372	11	-	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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	3322	BMA	C1-C2-C3	2.04	111.95	109.54
13	D	3320	NAG	C1-O5-C5	2.20	115.05	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	3371	NAG	2	0
11	B	3372	NAG	1	0

5.6 Ligand geometry

Of 27 ligands modelled in this entry, 14 are monoatomic - leaving 13 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	1455	-	5,5,5	0.36	0	5,5,5	0.11	0
6	GOL	A	1456	-	5,5,5	0.35	0	5,5,5	0.18	0
7	SO4	A	1457	-	4,4,4	0.22	0	6,6,6	0.11	0
7	SO4	A	1458	-	4,4,4	0.22	0	6,6,6	0.06	0
6	GOL	C	1454	-	5,5,5	0.35	0	5,5,5	0.27	0
6	GOL	C	1455	-	5,5,5	0.35	0	5,5,5	0.22	0
6	GOL	C	1456	-	5,5,5	0.35	0	5,5,5	0.28	0
6	GOL	C	1457	-	5,5,5	0.35	0	5,5,5	0.17	0
12	NAG	C	2015	1	14,14,15	0.52	0	15,19,21	0.75	0
6	GOL	E	1220	-	5,5,5	0.36	0	5,5,5	0.23	0
6	GOL	F	1215	-	5,5,5	0.37	0	5,5,5	0.20	0
6	GOL	F	1216	-	5,5,5	0.33	0	5,5,5	0.23	0
6	GOL	J	1498	-	5,5,5	0.34	0	5,5,5	0.25	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	1455	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1456	-	-	0/4/4/4	0/0/0/0
7	SO4	A	1457	-	-	0/0/0/0	0/0/0/0
7	SO4	A	1458	-	-	0/0/0/0	0/0/0/0
6	GOL	C	1454	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1455	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1456	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1457	-	-	0/4/4/4	0/0/0/0
12	NAG	C	2015	1	-	0/6/23/26	0/1/1/1
6	GOL	E	1220	-	-	0/4/4/4	0/0/0/0
6	GOL	F	1215	-	-	0/4/4/4	0/0/0/0
6	GOL	F	1216	-	-	0/4/4/4	0/0/0/0
6	GOL	J	1498	-	-	0/4/4/4	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1457	SO4	1	0
6	C	1457	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, 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%)	0.43	2 (0%) 93 97	15, 26, 52, 116	4 (0%)
1	C	453/457 (99%)	0.34	7 (1%) 76 85	22, 38, 72, 130	1 (0%)
2	B	469/472 (99%)	0.97	71 (15%) 3 5	16, 48, 118, 193	127 (27%)
2	D	367/472 (77%)	2.22	122 (33%) 0 0	23, 53, 179, 217	76 (20%)
3	E	216/221 (97%)	0.10	6 (2%) 56 69	26, 42, 70, 107	0
3	H	216/221 (97%)	2.85	118 (54%) 0 0	49, 107, 160, 211	0
4	F	214/214 (100%)	0.50	14 (6%) 22 33	30, 48, 86, 192	2 (0%)
4	L	214/214 (100%)	3.25	122 (57%) 0 0	59, 114, 205, 233	1 (0%)
5	I	6/6 (100%)	1.68	2 (33%) 0 0	27, 33, 51, 56	0
5	J	6/6 (100%)	0.76	0 100 100	31, 38, 70, 72	0
All	All	2615/2740 (95%)	1.18	464 (17%) 2 3	15, 45, 157, 233	211 (8%)

All (464) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	409	GLU	24.1
4	L	181	LEU	21.8
4	L	214	CYS	16.5
4	L	130	ALA	15.9
2	D	395	VAL	14.8
2	B	7	THR	13.3
2	D	375	LEU	13.3
2	D	391	ILE	13.3
2	D	401	ALA	13.1
2	D	433	CYS	13.1
4	F	214	CYS	12.9
3	H	133	VAL	12.6
4	L	193	THR	12.5

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Mol	Chain	Res	Type	RSRZ
4	L	148	TRP	12.3
2	D	412	LYS	11.6
2	D	419	VAL	11.4
3	H	147	LEU	11.3
2	D	431	PHE	11.2
2	D	389	LEU	11.1
4	L	136	LEU	11.0
2	D	103	GLN	10.9
2	D	93	ARG	10.3
2	D	399	ILE	10.2
4	L	209	PHE	10.2
2	D	407	PRO	10.1
2	D	397	PHE	9.9
2	D	363	PRO	9.8
2	D	92	LEU	9.4
4	F	212	ASN	9.2
2	D	381	PRO	9.2
3	H	217	GLU	9.1
2	B	469	SER	9.1
2	D	405	GLY	9.0
3	H	128	TYR	9.0
3	H	130	LEU	9.0
2	D	408	GLN	8.9
3	H	131	ALA	8.8
4	L	129	GLY	8.7
2	D	420	GLY	8.5
2	D	376	ASN	8.5
3	H	134	CYS	8.5
3	H	11	LEU	8.4
2	D	106	GLN	8.4
2	D	429	VAL	8.4
2	D	425	LEU	8.4
4	L	213	GLU	8.3
3	H	132	PRO	8.3
3	H	209	SER	8.3
2	D	100	PHE	8.1
3	H	156	VAL	8.1
4	L	150	ILE	8.0
4	L	186	TYR	8.0
2	D	102	ILE	8.0
2	D	380	ILE	8.0
3	H	219	ARG	7.9

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Mol	Chain	Res	Type	RSRZ
2	B	471	CYS	7.9
3	H	216	ILE	7.9
4	L	117	ILE	7.8
4	L	192	TYR	7.7
2	D	62	ARG	7.7
3	H	218	PRO	7.7
2	D	410	LYS	7.6
2	D	400	GLU	7.6
2	D	88	ILE	7.6
2	D	99	ASN	7.5
3	H	138	THR	7.4
3	H	140	SER	7.4
2	D	104	VAL	7.4
4	L	125	LEU	7.3
4	L	206	VAL	7.3
4	L	203	SER	7.3
2	D	390	LYS	7.2
3	H	199	ILE	7.2
4	L	155	ARG	7.2
2	D	406	CYS	7.2
4	L	128	GLY	7.1
2	D	71	ASP	7.1
4	L	119	PRO	7.0
4	L	160	LEU	7.0
2	D	403	VAL	7.0
4	L	145	ASN	6.9
4	L	183	LYS	6.9
2	D	90	LEU	6.9
2	D	94	PRO	6.9
2	D	352	ARG	6.9
2	D	392	GLY	6.9
3	H	152	PHE	6.8
4	L	115	VAL	6.8
4	L	208	SER	6.8
3	H	18	VAL	6.8
2	D	64	LEU	6.8
2	B	33	LEU	6.7
1	C	337	PRO	6.7
4	L	114	THR	6.7
3	H	144	LEU	6.7
4	L	158	GLY	6.7
2	D	61	ALA	6.7

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Mol	Chain	Res	Type	RSRZ
2	D	105	ARG	6.7
4	L	190	ASN	6.6
4	L	132	VAL	6.6
4	L	212	ASN	6.6
4	L	205	ILE	6.6
3	H	200	THR	6.6
2	D	364	GLU	6.6
2	D	404	ARG	6.5
3	H	148	VAL	6.5
2	D	377	ASN	6.5
2	B	335	MET	6.5
3	H	127	VAL	6.5
2	B	32	PRO	6.5
3	H	151	TYR	6.5
2	B	9	GLY	6.5
4	L	197	THR	6.5
2	B	470	GLN	6.5
3	H	17	SER	6.5
2	D	386	CYS	6.5
4	L	196	ALA	6.4
2	D	379	VAL	6.4
2	D	83	VAL	6.4
4	L	194	CYS	6.4
2	B	8	ARG	6.3
2	B	10	VAL	6.3
3	H	146	CYS	6.3
4	L	126	THR	6.3
2	D	427	VAL	6.3
2	B	129	TRP	6.3
4	L	180	THR	6.2
2	D	402	LYS	6.2
2	D	432	ASP	6.1
2	D	107	VAL	6.1
3	H	176	LEU	6.1
2	D	371	ASN	6.1
4	L	182	THR	6.1
3	H	121	LYS	6.1
2	D	370	PHE	6.0
2	D	394	THR	6.0
3	H	117	VAL	5.9
4	L	113	PRO	5.9
4	L	146	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
3	H	159	THR	5.9
2	D	416	ILE	5.9
4	L	144	ILE	5.9
3	H	158	LEU	5.9
4	L	159	VAL	5.9
2	D	101	SER	5.9
2	D	97	SER	5.8
4	L	120	PRO	5.8
2	D	393	ASP	5.8
2	B	54	ILE	5.7
3	H	189	VAL	5.7
2	D	84	SER	5.7
2	D	366	LEU	5.7
4	L	179	LEU	5.7
2	D	430	THR	5.7
2	D	423	ASP	5.7
2	D	383	LEU	5.6
4	L	195	GLU	5.6
3	H	194	TRP	5.6
4	L	131	SER	5.6
2	B	50	ALA	5.6
2	B	51	PRO	5.6
4	L	188	ARG	5.4
4	L	175	MET	5.4
2	D	108	GLU	5.4
3	H	177	GLN	5.4
2	D	368	LEU	5.4
2	D	374	CYS	5.4
4	L	121	SER	5.3
4	L	154	GLU	5.3
2	D	355	VAL	5.3
3	H	205	HIS	5.3
2	D	369	SER	5.3
2	D	387	MET	5.3
3	H	210	THR	5.2
4	L	211	ARG	5.2
4	L	135	PHE	5.2
2	D	396	SER	5.2
4	L	210	ASN	5.2
4	L	118	PHE	5.2
3	H	157	THR	5.2
2	B	128	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
2	D	96	ASP	5.1
3	H	122	THR	5.1
4	L	122	SER	5.1
3	H	126	SER	5.1
3	H	208	SER	5.1
3	H	203	VAL	5.1
2	D	59	SER	5.1
2	D	63	VAL	5.1
2	B	375	LEU	5.0
2	D	378	GLU	5.0
1	C	453	VAL	5.0
2	B	44	LEU	5.0
2	D	357	LEU	5.0
2	D	362	LEU	5.0
2	D	98	LYS	4.9
1	A	454	VAL	4.9
2	D	95	ASP	4.9
3	H	215	LYS	4.9
3	H	198	SER	4.9
4	L	111	ALA	4.9
2	D	373	THR	4.9
2	B	31	LEU	4.9
4	L	123	GLU	4.9
3	H	118	SER	4.8
3	H	149	LYS	4.8
3	H	201	CYS	4.8
1	C	336	GLY	4.8
2	B	3	ASN	4.8
2	D	110	TYR	4.8
3	H	125	PRO	4.8
4	L	149	LYS	4.8
3	H	86	LEU	4.8
2	B	4	ILE	4.8
2	B	48	ASN	4.7
3	H	212	VAL	4.7
5	I	492[A]	GLY	4.7
2	B	49	CYS	4.7
2	B	36	PRO	4.6
3	H	142	VAL	4.6
4	L	127	SER	4.6
4	L	201	SER	4.6
4	L	147	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
3	H	191	SER	4.6
3	H	24	ALA	4.6
4	L	199	LYS	4.6
4	L	207	LYS	4.6
2	B	6	THR	4.6
4	L	178	THR	4.6
2	B	35	SER	4.6
3	H	195	PRO	4.6
3	H	180	LEU	4.6
4	L	204	PRO	4.5
3	H	211	LYS	4.5
3	H	141	SER	4.5
2	D	382	GLY	4.5
2	D	398	SER	4.4
3	H	12	VAL	4.4
2	D	354	LYS	4.4
4	L	177	SER	4.4
2	D	82	GLN	4.3
2	B	39	ASP	4.3
3	H	8	GLY	4.3
3	H	145	GLY	4.3
2	D	68	PRO	4.3
4	L	164	THR	4.3
2	D	60	GLU	4.2
2	B	22	MET	4.2
1	C	320	ARG	4.2
2	B	450	ASN	4.2
3	H	182	THR	4.1
2	B	404	ARG	4.1
2	D	421	PHE	4.1
4	L	124	GLN	4.1
4	L	133	VAL	4.1
2	D	415	THR	4.1
2	D	86	GLN	4.0
4	L	184	ASP	4.0
3	H	119	SER	4.0
4	L	168	SER	4.0
4	L	142	LYS	4.0
3	H	123	THR	4.0
4	L	141	PRO	4.0
3	H	115	VAL	4.0
3	H	83	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	336	ASP	3.9
3	H	184	SER	3.9
4	L	139	PHE	3.9
4	L	134	CYS	3.9
4	L	163	TRP	3.9
5	I	493[A]	ARG	3.8
2	D	353	SER	3.8
4	L	189	HIS	3.8
2	B	30	ALA	3.8
2	B	379	VAL	3.8
2	B	337[A]	SER	3.8
2	B	459	VAL	3.8
3	H	150	GLY	3.7
3	E	133	VAL	3.7
4	L	200	THR	3.7
2	D	70	SER	3.7
2	B	37	ARG	3.7
2	D	367	SER	3.7
2	D	385	SER	3.7
4	L	187	GLU	3.7
3	H	13	LYS	3.6
3	H	21	SER	3.6
3	H	183	LEU	3.6
3	H	129	PRO	3.6
4	L	191	SER	3.6
3	H	64	PHE	3.6
4	F	129	GLY	3.6
4	L	202	THR	3.6
2	D	89	ALA	3.6
3	H	139	GLY	3.6
4	L	169	LYS	3.5
3	H	94	TYR	3.5
3	H	206	PRO	3.5
3	H	81	LEU	3.5
4	L	151	ASP	3.5
3	H	153	PRO	3.5
4	F	122	SER	3.5
4	L	25	ALA	3.5
3	H	175	VAL	3.5
2	B	41	LYS	3.5
2	B	45	LEU	3.5
2	B	376	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
4	F	213	GLU	3.4
4	L	83	PHE	3.4
2	B	26	CYS	3.4
2	B	40	LEU	3.3
4	L	20	SER	3.3
4	L	109	ALA	3.3
3	H	143	THR	3.3
2	D	91	ARG	3.3
3	H	160	TRP	3.3
4	L	198	HIS	3.3
2	D	414	PHE	3.3
3	E	134	CYS	3.3
3	H	193	THR	3.3
3	H	192	SER	3.3
4	F	191	SER	3.3
4	L	137	ASN	3.3
3	H	214	LYS	3.3
4	L	21	ILE	3.3
2	D	413	SER	3.3
2	B	19	VAL	3.3
3	E	131	ALA	3.3
4	L	185	GLU	3.2
4	L	157	ASN	3.2
3	H	207	ALA	3.2
3	H	84	SER	3.2
2	B	42	GLU	3.2
3	H	172	PHE	3.2
3	H	42	GLU	3.2
4	L	19	VAL	3.2
4	L	171	SER	3.2
3	H	20	LEU	3.2
3	H	116	THR	3.2
2	B	46	LYS	3.1
2	D	69	LEU	3.1
4	L	86	TYR	3.1
3	H	187	VAL	3.1
3	H	120	ALA	3.0
4	L	12	SER	3.0
3	H	155	PRO	3.0
4	L	140	TYR	3.0
4	F	186	TYR	3.0
2	B	29	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	422	LYS	3.0
3	H	91	THR	3.0
2	B	52	GLU	2.9
3	E	130	LEU	2.9
4	L	143	ASP	2.9
2	B	77	SER	2.9
2	D	241	ASP	2.9
4	F	190	ASN	2.9
2	B	24	ALA	2.8
2	B	380	ILE	2.8
4	F	184	ASP	2.8
4	L	112	ALA	2.8
2	B	11	SER	2.8
2	D	411	GLU	2.8
2	D	424	SER	2.8
2	B	72	LYS	2.8
3	H	68	ALA	2.8
2	B	107	VAL	2.8
4	L	73	LEU	2.8
2	D	365	GLU	2.8
4	L	110	ASP	2.8
3	H	188	THR	2.8
2	D	417	LYS	2.7
2	B	73	GLY	2.7
3	H	197	GLN	2.7
4	L	116	SER	2.7
3	H	181	TYR	2.7
4	L	76	SER	2.7
4	L	153	SER	2.7
3	H	66	GLY	2.7
2	B	378	GLU	2.7
2	B	64	LEU	2.7
3	H	165	LEU	2.7
4	F	150	ILE	2.7
4	L	2	ILE	2.7
3	H	204	ALA	2.7
4	F	192	TYR	2.7
4	L	161	ASN	2.6
3	H	9	ALA	2.6
2	B	132	GLN	2.6
2	D	67	ARG	2.6
3	H	10	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
3	H	67	LYS	2.6
3	E	219	ARG	2.6
3	H	164	SER	2.6
4	L	18	THR	2.6
3	H	190	THR	2.6
4	L	75	ILE	2.6
2	D	388	GLY	2.5
4	L	167	ASP	2.5
3	H	171	THR	2.5
4	L	62	PHE	2.5
2	D	384	LYS	2.5
4	L	170	ASP	2.5
2	B	58	VAL	2.5
2	B	67	ARG	2.4
2	D	360	ARG	2.4
3	H	80	TYR	2.4
2	B	88	ILE	2.4
3	H	85	SER	2.4
2	B	145	LEU	2.4
4	L	80	SER	2.4
2	D	144	LYS	2.4
4	F	179	LEU	2.4
4	L	108	ARG	2.4
2	D	361	ASP	2.4
2	D	348	TYR	2.4
4	L	138	ASN	2.3
3	H	124	ALA	2.3
4	L	33	ILE	2.3
2	B	386	CYS	2.3
4	F	125	LEU	2.3
4	L	74	THR	2.3
2	B	69	LEU	2.3
2	D	66	ASP	2.3
4	L	173	TYR	2.3
2	D	141	GLN	2.3
1	C	338	HIS	2.3
3	H	196	SER	2.3
3	H	179	ASP	2.3
4	L	23	CYS	2.2
2	B	27	SER	2.2
1	C	130	CYS	2.2
2	B	370	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	467	LEU	2.2
3	H	178	SER	2.2
3	H	65	GLN	2.2
2	B	377	ASN	2.2
2	D	359	VAL	2.2
2	B	56	PHE	2.2
1	A	320	ARG	2.2
3	H	19	LYS	2.2
2	B	57	PRO	2.2
4	L	104	LEU	2.2
3	H	87	THR	2.2
3	H	16	ALA	2.2
2	D	80	VAL	2.1
4	L	60	SER	2.1
1	C	339	ALA	2.1
2	D	418	PRO	2.1
4	F	127	SER	2.1
3	H	213	ASP	2.1
4	L	97	THR	2.1
2	B	34	GLY	2.1
2	D	351	ILE	2.1
2	B	83	VAL	2.1
4	L	13	VAL	2.1
2	B	181	LYS	2.1
3	E	129	PRO	2.1
2	B	62	ARG	2.1
3	H	88	SER	2.1
3	H	166	SER	2.1
2	D	174[A]	GLU	2.0
4	L	7	SER	2.0
4	L	81	GLU	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, 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	B	3371	14/15	0.85	0.24	0.86	77,95,114,119	0
13	NAG	D	3320	14/15	0.92	0.12	-0.03	41,55,74,79	0
10	BMA	B	3322	11/12	0.81	0.16	-	58,74,92,95	0
10	MAN	B	3325	11/12	0.89	0.15	-	73,78,93,95	0
10	MAN	B	3324	11/12	0.84	0.14	-	65,72,87,89	0
10	NAG	B	3320	14/15	0.97	0.16	-	16,30,47,55	0
13	MAN	D	3323	11/12	0.69	0.44	-	106,115,138,138	0
13	BMA	D	3322	11/12	0.73	0.30	-	103,113,135,136	0
10	NAG	B	3321	14/15	0.96	0.14	-	34,48,64,68	0
11	NAG	B	3372	14/15	0.60	0.38	-	112,122,145,150	0
10	MAN	B	3323	11/12	0.85	0.15	-	71,78,92,95	0
13	NAG	D	3321	14/15	0.85	0.23	-	66,86,99,105	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
6	GOL	C	1454	6/6	0.64	0.40	9.07	86,104,110,114	0
6	GOL	C	1456	6/6	0.92	0.23	8.96	62,79,89,95	0
6	GOL	C	1457	6/6	0.72	0.35	7.33	65,78,87,92	0
6	GOL	F	1215	6/6	0.88	0.19	5.88	70,84,86,86	0
6	GOL	A	1456	6/6	0.68	0.29	5.68	64,84,100,103	0
7	SO4	A	1457	5/5	0.88	0.22	5.49	72,79,82,82	0
6	GOL	A	1455	6/6	0.89	0.26	5.12	56,67,77,79	0
6	GOL	J	1498	6/6	0.84	0.30	4.27	68,82,86,88	0
9	MN	D	2001	1/1	1.00	0.20	2.97	25,25,25,25	0
6	GOL	F	1216	6/6	0.85	0.19	2.59	58,70,80,83	0
8	CA	A	2005	1/1	1.00	0.16	2.22	23,23,23,23	0
9	MN	B	2001	1/1	1.00	0.20	2.17	23,23,23,23	0
8	CA	C	2005	1/1	0.98	0.15	1.95	46,46,46,46	0
7	SO4	A	1458	5/5	0.87	0.23	1.73	95,97,98,102	0
9	MN	D	2002	1/1	1.00	0.18	1.47	30,30,30,30	0
8	CA	A	2006	1/1	0.99	0.17	1.29	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	CA	A	2007	1/1	1.00	0.17	1.25	23,23,23,23	0
6	GOL	E	1220	6/6	0.83	0.19	0.97	67,81,85,85	0
9	MN	B	2002	1/1	0.97	0.18	0.74	52,52,52,52	0
8	CA	C	2007	1/1	0.98	0.14	0.68	41,41,41,41	0
8	CA	A	2004	1/1	0.99	0.14	0.19	27,27,27,27	0
6	GOL	C	1455	6/6	0.81	0.20	-0.13	85,102,105,107	0
8	CA	C	2006	1/1	0.99	0.12	-0.43	42,42,42,42	0
8	CA	C	2004	1/1	0.98	0.11	-0.56	53,53,53,53	0
9	MN	D	2003	1/1	0.99	0.12	-2.59	33,33,33,33	0
9	MN	B	2003	1/1	1.00	0.13	-2.76	28,28,28,28	0
12	NAG	C	2015	14/15	0.65	0.35	-	86,102,119,129	0

6.5 Other polymers [i](#)

There are no such residues in this entry.