



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:16 am 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 : 1.7.2 (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

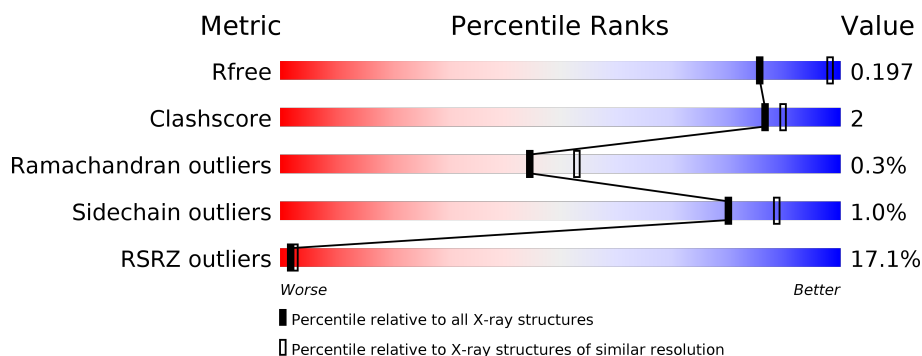
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (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	<div> <div></div> <div>93% 6% .</div> </div>
1	C	457	<div> <div>2%</div> <div>94% 5% .</div> </div>
2	B	472	<div> <div>14%</div> <div>89% 10% .</div> </div>
2	D	472	<div> <div>25%</div> <div>74% . 22%</div> </div>
3	E	221	<div> <div>2%</div> <div>93% 5% .</div> </div>
3	H	221	<div> <div>52%</div> <div>94% . .</div> </div>

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Mol	Chain	Length	Quality of chain
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
8	CA	C	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.

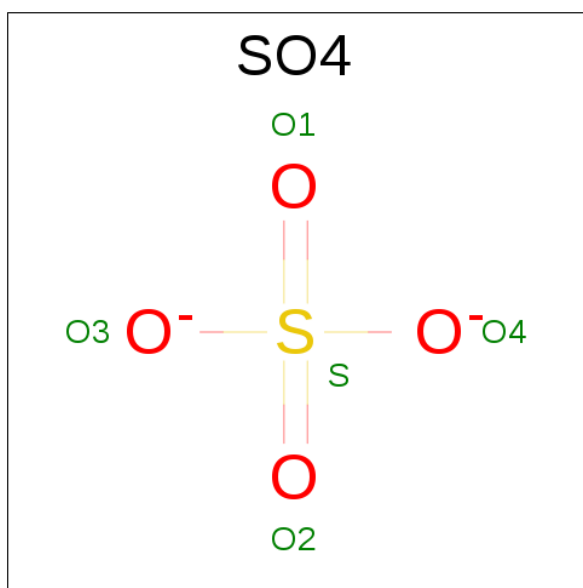
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	6	Total	C	H	N	O	0	3	0
			111	32	52	15	12			
5	J	6	Total	C	H	N	O	0	0	0
			74	22	34	9	9			

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



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		

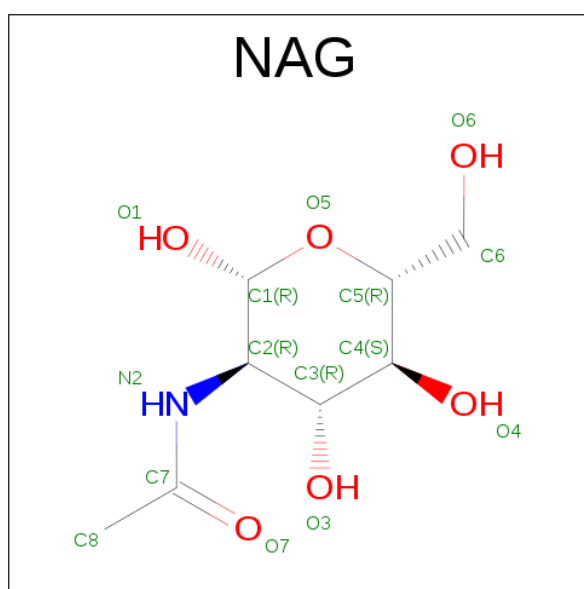
- Molecule 10 is a polymer of unknown type called SUGAR (6-MER).

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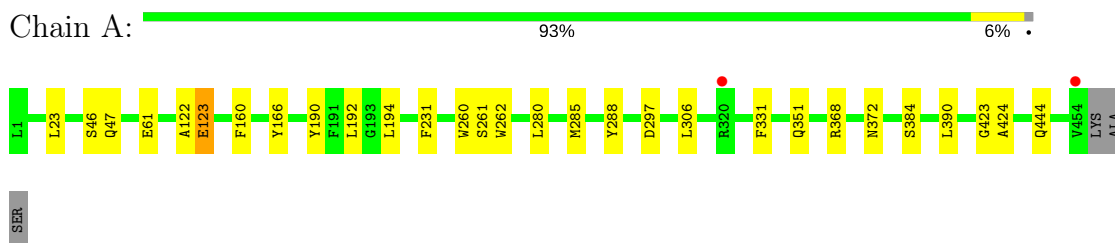
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	B	211	Total 211	O 211	0	0
14	C	283	Total 283	O 283	0	0
14	D	107	Total 107	O 107	0	0
14	E	129	Total 129	O 129	0	0
14	F	68	Total 68	O 68	0	0
14	H	18	Total 18	O 18	0	0
14	I	2	Total 2	O 2	0	0
14	J	2	Total 2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

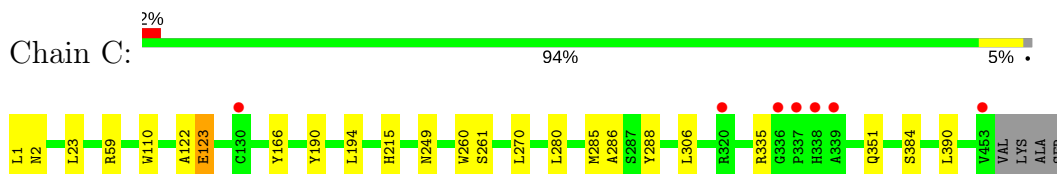
3 Residue-property plots

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

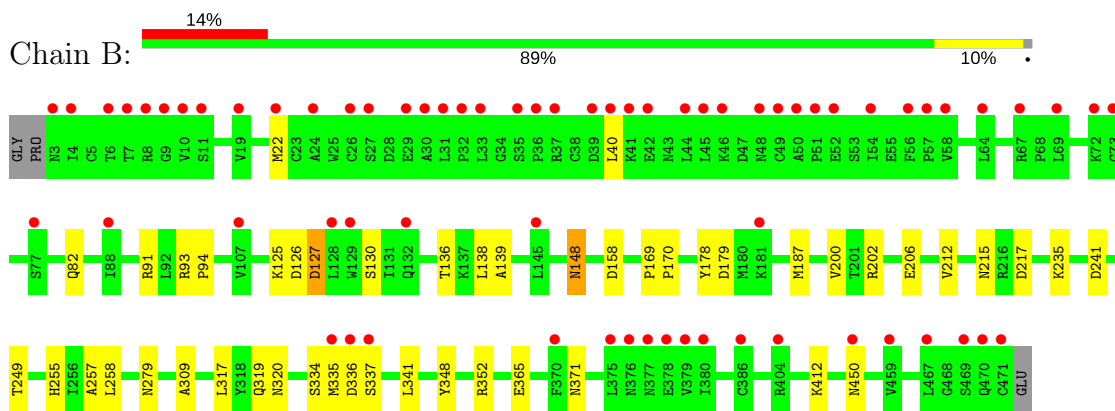
• Molecule 1: INTEGRIN ALPHA-IIB



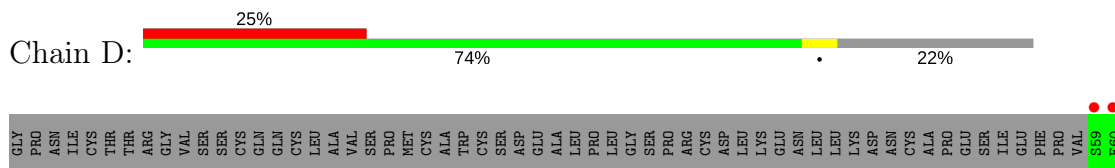
• Molecule 1: INTEGRIN ALPHA-IIB

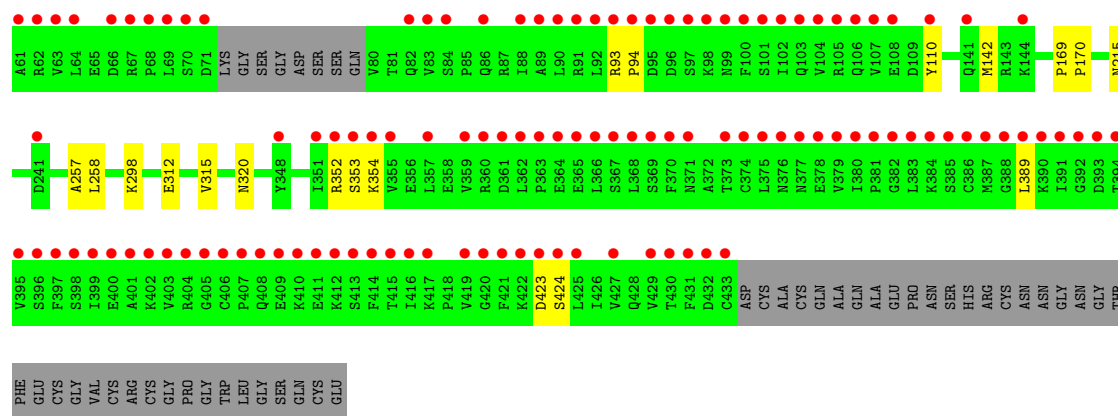


• Molecule 2: INTEGRIN BETA-3

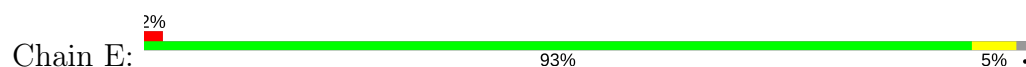


• Molecule 2: INTEGRIN BETA-3

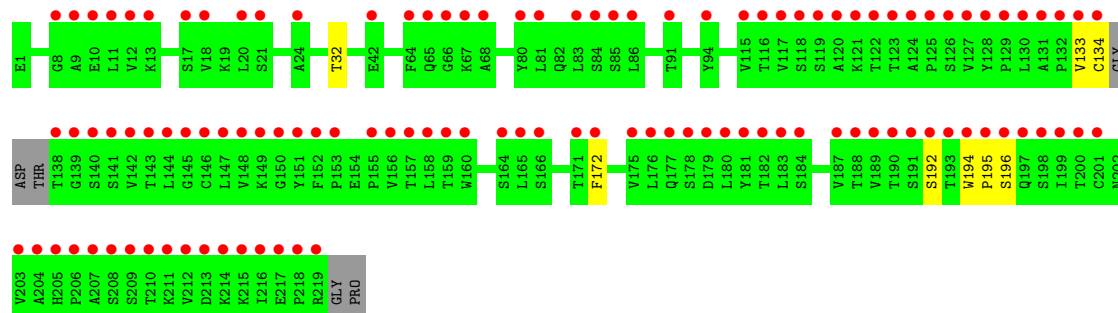




• Molecule 3: 10E5 FAB HEAVY CHAIN



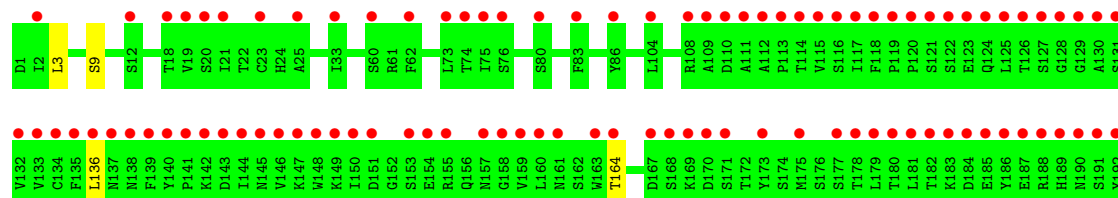
• Molecule 3: 10E5 FAB HEAVY CHAIN

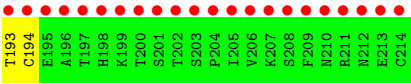


• Molecule 4: 10E5 FAB LIGHT CHAIN



• Molecule 4: 10E5 FAB LIGHT CHAIN





● 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 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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:178[B]:TYR:CD1	2:B:179:ASP:N	2.74	0.55
2:B:235:LYS:NZ	14:B:3109:HOH:O	2.36	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
2:D:257:ALA:O	2:D:258:LEU:HB2	2.12	0.50
3:E:133:VAL:O	3:E:134:CYS:SG	2.70	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:158:ASP:HB3	2:B:187:MET:CE	2.44	0.48
2:B:371:ASN:ND2	11:B:3371:NAG:C7	2.77	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
1:A:46:SER:O	1:A:47:GLN:HB2	2.17	0.45
3:H:172:PHE:CD2	4:L:164:THR:HG23	2.51	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:139:ALA:HB2	2:B:200:VAL:HG11	1.99	0.43
2:B:235:LYS:CE	2:B:279:ASN:OD1	2.67	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
1:C:215:HIS:CE1	3:H:32:THR:HG22	2.53	0.43
3:H:133:VAL:O	3:H:134:CYS:SG	2.77	0.43
3:E:12:VAL:HG21	3:E:86:LEU:CD1	2.49	0.43
1:A:192:LEU:HD11	1:A:231:PHE:CD1	2.53	0.43
5:I:492[B]:GLY:C	5:I:494[B]:GLY:N	2.72	0.43
1:C:260:TRP:CE3	1:C:261:SER:HB2	2.54	0.42
1:C:285:MET:SD	2:D:320:ASN:HB3	2.59	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%)	51 61
1	C	457/457 (100%)	440 (96%)	16 (4%)	1 (0%)	51 61
2	B	474/472 (100%)	460 (97%)	13 (3%)	1 (0%)	51 61
2	D	369/472 (78%)	355 (96%)	13 (4%)	1 (0%)	44 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	212/221 (96%)	202 (95%)	9 (4%)	1 (0%)	32	37
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%)	44	53

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%)	68	79
1	C	367/364 (101%)	362 (99%)	5 (1%)	71	82
2	B	422/417 (101%)	416 (99%)	6 (1%)	71	82
2	D	336/417 (81%)	335 (100%)	1 (0%)	94	97
3	E	187/190 (98%)	186 (100%)	1 (0%)	91	95
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%)	78	87
4	L	188/188 (100%)	187 (100%)	1 (0%)	91	95
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%)	80	87

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	0.60	0	15,19,21	0.62	0
10	NAG	B	3321	10	14,14,15	0.55	0	15,19,21	0.78	0
10	BMA	B	3322	10	11,11,12	0.62	0	13,15,17	0.68	0
10	MAN	B	3323	10	11,11,12	0.64	0	13,15,17	0.62	0
10	MAN	B	3324	10	11,11,12	0.64	0	13,15,17	0.71	0
10	MAN	B	3325	10	11,11,12	0.63	0	13,15,17	0.59	0
11	NAG	B	3371	11,2	14,14,15	0.51	0	15,19,21	0.66	0
11	NAG	B	3372	11	14,14,15	0.53	0	15,19,21	0.54	0
13	NAG	D	3320	13,2	14,14,15	0.46	0	15,19,21	0.85	1 (6%)
13	NAG	D	3321	13	14,14,15	0.60	0	15,19,21	0.74	0
13	BMA	D	3322	13	11,11,12	0.63	0	13,15,17	0.57	0
13	MAN	D	3323	13	11,11,12	0.60	0	13,15,17	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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	3320	NAG	C1-O5-C5	2.09	115.05	112.17

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	0.10	0
6	GOL	A	1456	-	5,5,5	0.35	0	5,5,5	0.18	0
7	SO4	A	1457	-	4,4,4	0.14	0	6,6,6	0.11	0
7	SO4	A	1458	-	4,4,4	0.15	0	6,6,6	0.07	0
6	GOL	C	1454	-	5,5,5	0.35	0	5,5,5	0.28	0
6	GOL	C	1455	-	5,5,5	0.35	0	5,5,5	0.23	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	0.54	0	15,19,21	0.81	0
6	GOL	E	1220	-	5,5,5	0.36	0	5,5,5	0.23	0
6	GOL	F	1215	-	5,5,5	0.38	0	5,5,5	0.21	0
6	GOL	F	1216	-	5,5,5	0.33	0	5,5,5	0.24	0
6	GOL	J	1498	-	5,5,5	0.34	0	5,5,5	0.26	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%)	0.34	2 (0%) 92 96	15, 26, 52, 116	4 (0%)
1	C	453/457 (99%)	0.26	7 (1%) 74 83	22, 38, 72, 130	1 (0%)
2	B	469/472 (99%)	0.87	68 (14%) 3 5	16, 48, 118, 193	127 (27%)
2	D	367/472 (77%)	2.08	119 (32%) 0 0	23, 53, 179, 217	76 (20%)
3	E	216/221 (97%)	0.02	5 (2%) 61 71	26, 42, 70, 107	0
3	H	216/221 (97%)	2.69	114 (52%) 0 0	49, 107, 160, 211	0
4	F	214/214 (100%)	0.42	13 (6%) 22 31	30, 48, 86, 192	2 (0%)
4	L	214/214 (100%)	3.08	118 (55%) 0 0	59, 114, 205, 233	1 (0%)
5	I	6/6 (100%)	1.55	2 (33%) 0 0	27, 33, 51, 56	0
5	J	6/6 (100%)	0.68	0 100 100	31, 38, 70, 72	0
All	All	2615/2740 (95%)	1.06	448 (17%) 2 2	15, 45, 157, 233	211 (8%)

All (448) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	409	GLU	24.2
4	L	181	LEU	21.4
4	L	214	CYS	15.6
4	L	130	ALA	15.1
2	D	395	VAL	13.8
2	B	7	THR	12.8
2	D	401	ALA	12.8
2	D	375	LEU	12.7
2	D	391	ILE	12.6
2	D	433	CYS	12.5
4	F	214	CYS	12.5
4	L	193	THR	12.2
3	H	133	VAL	12.0

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Mol	Chain	Res	Type	RSRZ
4	L	148	TRP	11.9
2	D	412	LYS	11.3
3	H	147	LEU	10.8
2	D	419	VAL	10.7
2	D	103	GLN	10.5
2	D	431	PHE	10.5
2	D	389	LEU	10.5
4	L	136	LEU	10.5
2	D	93	ARG	10.4
2	D	399	ILE	10.0
4	L	209	PHE	9.9
2	D	407	PRO	9.5
2	D	363	PRO	9.4
2	D	397	PHE	9.2
2	D	381	PRO	9.0
4	F	212	ASN	8.8
2	D	92	LEU	8.8
2	B	469	SER	8.8
3	H	128	TYR	8.7
3	H	217	GLU	8.7
3	H	130	LEU	8.7
3	H	131	ALA	8.7
2	D	408	GLN	8.6
2	D	425	LEU	8.3
4	L	129	GLY	8.3
3	H	134	CYS	8.2
2	D	420	GLY	8.1
2	D	429	VAL	8.1
2	D	376	ASN	8.1
2	D	106	GLN	8.1
4	L	213	GLU	8.0
3	H	132	PRO	8.0
2	D	405	GLY	8.0
3	H	11	LEU	8.0
3	H	209	SER	7.9
3	H	219	ARG	7.9
4	L	186	TYR	7.8
4	L	150	ILE	7.7
2	D	380	ILE	7.7
2	D	100	PHE	7.7
3	H	156	VAL	7.6
4	L	117	ILE	7.6

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Mol	Chain	Res	Type	RSRZ
3	H	216	ILE	7.6
2	B	471	CYS	7.5
2	D	102	ILE	7.5
2	D	62	ARG	7.5
2	D	410	LYS	7.5
4	L	192	TYR	7.4
3	H	218	PRO	7.3
2	D	99	ASN	7.3
2	D	400	GLU	7.3
2	D	88	ILE	7.3
3	H	138	THR	7.0
4	L	125	LEU	7.0
3	H	140	SER	7.0
2	D	104	VAL	7.0
2	D	390	LYS	7.0
3	H	199	ILE	7.0
2	D	71	ASP	6.9
4	L	155	ARG	6.9
4	L	183	LYS	6.9
4	L	203	SER	6.9
2	D	352	ARG	6.9
4	L	128	GLY	6.8
2	D	90	LEU	6.8
2	D	94	PRO	6.8
4	L	160	LEU	6.8
4	L	206	VAL	6.8
2	D	64	LEU	6.7
4	L	119	PRO	6.7
4	L	145	ASN	6.7
2	D	406	CYS	6.6
4	L	158	GLY	6.6
4	L	208	SER	6.6
3	H	18	VAL	6.6
2	D	403	VAL	6.6
3	H	144	LEU	6.5
2	D	105	ARG	6.5
2	D	392	GLY	6.5
2	D	61	ALA	6.5
2	D	364	GLU	6.4
4	L	115	VAL	6.4
2	B	33	LEU	6.4
3	H	152	PHE	6.4

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Mol	Chain	Res	Type	RSRZ
4	L	190	ASN	6.4
2	B	8	ARG	6.3
4	L	197	THR	6.3
4	L	205	ILE	6.3
1	C	337	PRO	6.3
2	D	404	ARG	6.3
3	H	151	TYR	6.3
4	L	114	THR	6.3
2	B	9	GLY	6.3
2	B	32	PRO	6.2
2	D	377	ASN	6.2
4	L	212	ASN	6.2
3	H	127	VAL	6.2
4	L	132	VAL	6.2
3	H	148	VAL	6.2
3	H	200	THR	6.2
2	B	470	GLN	6.2
4	L	196	ALA	6.2
3	H	17	SER	6.1
4	L	182	THR	6.1
2	D	379	VAL	6.1
4	L	180	THR	6.0
2	D	83	VAL	6.0
2	B	335	MET	6.0
4	L	194	CYS	6.0
2	D	427	VAL	6.0
2	D	386	CYS	6.0
2	D	402	LYS	6.0
2	B	10	VAL	6.0
4	L	126	THR	5.9
2	D	371	ASN	5.9
3	H	176	LEU	5.9
3	H	146	CYS	5.9
3	H	121	LYS	5.8
2	B	129	TRP	5.8
2	D	370	PHE	5.8
2	D	432	ASP	5.8
2	D	416	ILE	5.7
4	L	159	VAL	5.7
2	D	107	VAL	5.7
4	L	144	ILE	5.7
3	H	117	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
2	D	394	THR	5.6
2	D	383	LEU	5.6
3	H	158	LEU	5.5
4	L	113	PRO	5.5
4	L	179	LEU	5.5
2	D	393	ASP	5.5
3	H	189	VAL	5.5
2	D	97	SER	5.5
2	D	101	SER	5.5
4	L	146	VAL	5.5
3	H	159	THR	5.5
2	D	84	SER	5.4
4	L	120	PRO	5.4
2	D	423	ASP	5.4
2	B	54	ILE	5.4
4	L	195	GLU	5.4
2	D	366	LEU	5.4
3	H	194	TRP	5.3
4	L	131	SER	5.3
2	D	108	GLU	5.3
2	D	430	THR	5.3
2	B	50	ALA	5.3
2	B	51	PRO	5.2
2	D	368	LEU	5.2
4	L	175	MET	5.2
4	L	154	GLU	5.2
4	L	188	ARG	5.1
3	H	177	GLN	5.1
2	D	369	SER	5.1
2	D	387	MET	5.1
4	L	211	ARG	5.1
4	L	121	SER	5.1
2	D	355	VAL	5.0
3	H	205	HIS	5.0
4	L	135	PHE	5.0
4	L	210	ASN	5.0
3	H	210	THR	5.0
4	L	118	PHE	5.0
2	B	128	LEU	4.9
3	H	157	THR	4.9
2	D	59	SER	4.9
2	D	374	CYS	4.8

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Mol	Chain	Res	Type	RSRZ
2	D	96	ASP	4.8
2	B	44	LEU	4.8
3	H	122	THR	4.8
3	H	208	SER	4.8
4	L	123	GLU	4.8
2	D	378	GLU	4.8
2	D	357	LEU	4.8
3	H	126	SER	4.8
4	L	149	LYS	4.8
2	D	396	SER	4.8
1	C	453	VAL	4.8
2	B	375	LEU	4.8
2	D	98	LYS	4.8
3	H	118	SER	4.7
4	L	122	SER	4.7
2	D	362	LEU	4.7
2	D	63	VAL	4.7
3	H	203	VAL	4.7
2	B	31	LEU	4.7
3	H	215	LYS	4.7
2	D	373	THR	4.7
3	H	149	LYS	4.6
2	B	3	ASN	4.6
3	H	198	SER	4.6
4	L	147	LYS	4.6
3	H	212	VAL	4.6
4	L	127	SER	4.6
1	C	336	GLY	4.6
1	A	454	VAL	4.6
2	D	110	TYR	4.6
3	H	201	CYS	4.5
3	H	86	LEU	4.5
2	B	4	ILE	4.5
3	H	125	PRO	4.5
3	H	211	LYS	4.5
2	D	95	ASP	4.5
3	H	191	SER	4.4
4	L	111	ALA	4.4
4	L	199	LYS	4.4
4	L	204	PRO	4.4
4	L	207	LYS	4.4
2	B	48	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
3	H	142	VAL	4.4
2	B	36	PRO	4.4
5	I	492[A]	GLY	4.4
2	B	49	CYS	4.4
2	B	6	THR	4.4
4	L	178	THR	4.4
2	B	35	SER	4.4
2	D	382	GLY	4.3
3	H	141	SER	4.3
3	H	180	LEU	4.3
2	D	82	GLN	4.3
4	L	177	SER	4.3
2	D	354	LYS	4.2
3	H	195	PRO	4.2
3	H	24	ALA	4.2
4	L	201	SER	4.2
2	D	398	SER	4.2
2	D	68	PRO	4.2
3	H	12	VAL	4.2
2	D	421	PHE	4.1
2	B	22	MET	4.1
2	D	60	GLU	4.1
3	H	145	GLY	4.1
3	H	8	GLY	4.1
2	B	39	ASP	4.0
1	C	320	ARG	4.0
4	L	164	THR	4.0
2	B	450	ASN	4.0
4	L	142	LYS	4.0
2	B	404	ARG	4.0
2	D	415	THR	4.0
3	H	119	SER	4.0
4	L	124	GLN	3.9
4	L	133	VAL	3.9
3	H	182	THR	3.9
2	D	86	GLN	3.8
4	L	141	PRO	3.8
4	L	184	ASP	3.8
3	H	123	THR	3.8
3	H	184	SER	3.7
3	H	115	VAL	3.7
2	B	336	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	70	SER	3.7
4	L	168	SER	3.7
5	I	493[A]	ARG	3.7
2	D	353	SER	3.7
4	L	134	CYS	3.6
3	H	83	LEU	3.6
2	B	337[A]	SER	3.6
4	L	189	HIS	3.6
4	L	163	TRP	3.6
2	B	30	ALA	3.6
4	L	139	PHE	3.6
2	B	459	VAL	3.5
3	H	13	LYS	3.5
3	H	150	GLY	3.5
3	E	133	VAL	3.5
2	B	37	ARG	3.5
2	D	385	SER	3.5
3	H	183	LEU	3.5
2	B	379	VAL	3.5
3	H	21	SER	3.5
4	L	200	THR	3.4
4	L	20	SER	3.4
3	H	81	LEU	3.4
3	H	139	GLY	3.4
4	L	187	GLU	3.4
3	H	64	PHE	3.4
2	D	367	SER	3.4
3	H	206	PRO	3.4
2	D	89	ALA	3.4
4	L	191	SER	3.4
4	L	169	LYS	3.4
4	L	151	ASP	3.3
3	H	94	TYR	3.3
2	B	41	LYS	3.3
4	F	122	SER	3.3
4	F	129	GLY	3.3
3	H	129	PRO	3.3
3	H	175	VAL	3.3
4	L	25	ALA	3.3
2	B	45	LEU	3.3
4	L	202	THR	3.3
4	L	109	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	376	ASN	3.2
3	H	153	PRO	3.2
4	F	213	GLU	3.2
4	L	185	GLU	3.2
2	D	91	ARG	3.2
4	L	83	PHE	3.2
3	H	214	LYS	3.2
3	H	160	TRP	3.1
3	H	172	PHE	3.1
3	H	42	GLU	3.1
2	B	40	LEU	3.1
4	L	198	HIS	3.1
4	L	19	VAL	3.1
3	E	134	CYS	3.1
4	L	137	ASN	3.1
2	B	26	CYS	3.1
4	L	21	ILE	3.1
2	B	46	LYS	3.1
2	D	414	PHE	3.1
2	D	422	LYS	3.1
4	F	191	SER	3.1
2	B	42	GLU	3.1
3	H	143	THR	3.0
3	E	131	ALA	3.0
4	L	157	ASN	3.0
2	D	69	LEU	3.0
3	H	207	ALA	3.0
3	H	192	SER	3.0
3	H	116	THR	3.0
3	H	193	THR	3.0
3	H	20	LEU	2.9
2	D	413	SER	2.9
3	H	84	SER	2.9
2	D	411	GLU	2.9
2	B	19	VAL	2.9
4	L	171	SER	2.9
3	H	155	PRO	2.9
3	H	187	VAL	2.9
4	L	86	TYR	2.9
4	L	140	TYR	2.9
4	F	186	TYR	2.9
2	B	29	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
3	H	120	ALA	2.9
4	L	143	ASP	2.9
2	B	52	GLU	2.8
2	B	72	LYS	2.8
3	E	130	LEU	2.8
4	L	12	SER	2.8
2	D	365	GLU	2.8
2	B	380	ILE	2.8
4	F	184	ASP	2.7
4	F	190	ASN	2.7
2	D	241	ASP	2.7
2	B	77	SER	2.7
3	H	91	THR	2.7
3	H	68	ALA	2.7
2	B	24	ALA	2.6
4	L	112	ALA	2.6
2	D	417	LYS	2.6
4	F	192	TYR	2.6
4	L	18	THR	2.6
2	B	11	SER	2.6
2	D	424	SER	2.6
4	L	116	SER	2.6
3	H	188	THR	2.6
4	L	161	ASN	2.6
3	H	67	LYS	2.6
3	H	165	LEU	2.6
4	L	110	ASP	2.6
2	B	73	GLY	2.6
2	B	64	LEU	2.5
3	H	197	GLN	2.5
3	H	181	TYR	2.5
4	L	76	SER	2.5
2	B	107	VAL	2.5
2	D	384	LYS	2.5
4	L	73	LEU	2.5
2	B	132	GLN	2.5
3	H	9	ALA	2.5
4	L	2	ILE	2.5
3	H	66	GLY	2.4
2	D	67	ARG	2.4
4	L	153	SER	2.4
2	B	378	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	150	ILE	2.4
4	L	75	ILE	2.4
2	D	360	ARG	2.4
3	E	219	ARG	2.4
3	H	164	SER	2.4
3	H	10	GLU	2.4
2	D	388	GLY	2.4
3	H	190	THR	2.4
3	H	80	TYR	2.3
2	B	58	VAL	2.3
2	B	67	ARG	2.3
4	L	170	ASP	2.3
2	B	145	LEU	2.3
3	H	204	ALA	2.3
2	D	144	LYS	2.3
4	L	62	PHE	2.3
2	B	88	ILE	2.3
3	H	171	THR	2.3
4	L	108	ARG	2.3
4	L	138	ASN	2.3
4	L	167	ASP	2.3
4	F	179	LEU	2.3
2	D	348	TYR	2.3
3	H	85	SER	2.3
2	B	69	LEU	2.2
4	L	33	ILE	2.2
2	D	361	ASP	2.2
3	H	179	ASP	2.2
2	D	141	GLN	2.2
2	B	386	CYS	2.2
4	L	80	SER	2.2
2	D	66	ASP	2.1
4	F	125	LEU	2.1
3	H	124	ALA	2.1
4	L	74	THR	2.1
2	B	377	ASN	2.1
3	H	196	SER	2.1
4	L	173	TYR	2.1
3	H	178	SER	2.1
4	L	23	CYS	2.1
3	H	65	GLN	2.1
2	B	27	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	57	PRO	2.1
2	D	359	VAL	2.1
2	B	467	LEU	2.1
2	B	56	PHE	2.1
2	B	370	PHE	2.1
1	C	130	CYS	2.0
1	C	338	HIS	2.0
2	B	181	LYS	2.0
2	D	351	ILE	2.0
1	C	339	ALA	2.0
3	H	166	SER	2.0
4	L	60	SER	2.0
3	H	213	ASP	2.0
4	L	104	LEU	2.0
1	A	320	ARG	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	0.88	77,95,114,119	0
13	NAG	D	3320	14/15	0.92	0.12	0.08	41,55,74,79	0
10	BMA	B	3322	11/12	0.82	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	0.85	0.13	-	65,72,87,89	0
10	NAG	B	3320	14/15	0.97	0.15	-	16,30,47,55	0
13	MAN	D	3323	11/12	0.70	0.43	-	106,115,138,138	0
13	BMA	D	3322	11/12	0.74	0.29	-	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	0.61	0.38	-	112,122,145,150	0
10	MAN	B	3323	11/12	0.85	0.15	-	71,78,92,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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(\AA^2)	Q<0.9
6	GOL	C	1454	6/6	0.65	0.39	8.82	86,104,110,114	0
6	GOL	C	1456	6/6	0.92	0.23	8.39	62,79,89,95	0
6	GOL	C	1457	6/6	0.73	0.35	7.37	65,78,87,92	0
6	GOL	F	1215	6/6	0.88	0.18	5.77	70,84,86,86	0
6	GOL	A	1456	6/6	0.69	0.29	5.62	64,84,100,103	0
7	SO4	A	1457	5/5	0.88	0.22	5.55	72,79,82,82	0
6	GOL	A	1455	6/6	0.89	0.26	5.18	56,67,77,79	0
6	GOL	J	1498	6/6	0.84	0.30	4.18	68,82,86,88	0
9	MN	D	2001	1/1	1.00	0.20	3.08	25,25,25,25	0
6	GOL	F	1216	6/6	0.86	0.18	2.48	58,70,80,83	0
8	CA	A	2005	1/1	1.00	0.16	2.30	23,23,23,23	0
8	CA	C	2005	1/1	0.98	0.15	2.18	46,46,46,46	0
9	MN	B	2001	1/1	1.00	0.20	2.18	23,23,23,23	0
7	SO4	A	1458	5/5	0.87	0.23	1.86	95,97,98,102	0
9	MN	D	2002	1/1	1.00	0.18	1.38	30,30,30,30	0
8	CA	A	2007	1/1	1.00	0.17	1.38	23,23,23,23	0
8	CA	A	2006	1/1	0.99	0.17	1.30	19,19,19,19	0
6	GOL	E	1220	6/6	0.83	0.19	0.99	67,81,85,85	0
8	CA	C	2007	1/1	0.98	0.14	0.83	41,41,41,41	0
9	MN	B	2002	1/1	0.97	0.17	0.68	52,52,52,52	0
8	CA	A	2004	1/1	1.00	0.14	0.33	27,27,27,27	0
6	GOL	C	1455	6/6	0.81	0.19	-0.14	85,102,105,107	0
8	CA	C	2006	1/1	0.99	0.12	-0.36	42,42,42,42	0
8	CA	C	2004	1/1	0.98	0.11	-0.51	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	-2.70	28,28,28,28	0
12	NAG	C	2015	14/15	0.66	0.35	-	86,102,119,129	0

6.5 Other polymers [i](#)

There are no such residues in this entry.