



wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary 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

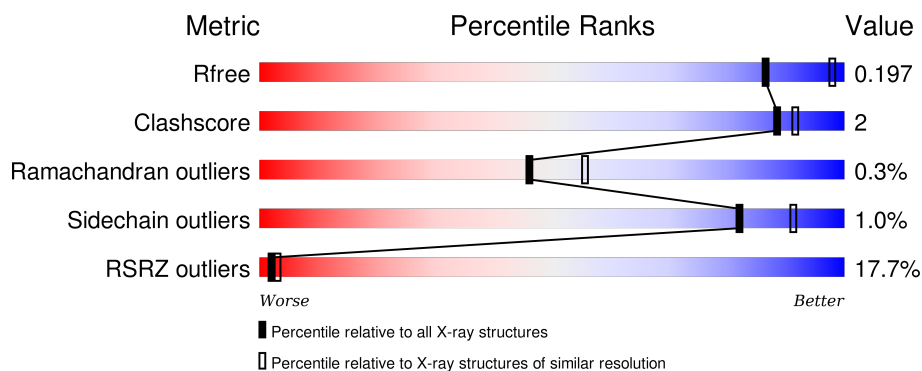
1 Overall quality at a glance

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	<div> <div style="width: 93%;"></div> <div>93%</div> <div style="width: 6%; background-color: yellow;"></div> <div>6%</div> </div>
1	C	457	<div> <div style="width: 2%; background-color: red;"></div> <div>2%</div> <div style="width: 94%;"></div> <div>94%</div> <div style="width: 5%; background-color: yellow;"></div> <div>5%</div> </div>
2	B	472	<div> <div style="width: 15%; background-color: red;"></div> <div>15%</div> <div style="width: 89%;"></div> <div>89%</div> <div style="width: 10%; background-color: yellow;"></div> <div>10%</div> </div>
2	D	472	<div> <div style="width: 26%; background-color: red;"></div> <div>26%</div> <div style="width: 74%;"></div> <div>74%</div> <div style="width: 22%; background-color: grey;"></div> <div>22%</div> </div>
3	E	221	<div> <div style="width: 3%; background-color: red;"></div> <div>3%</div> <div style="width: 93%;"></div> <div>93%</div> <div style="width: 5%; background-color: yellow;"></div> <div>5%</div> </div>

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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			

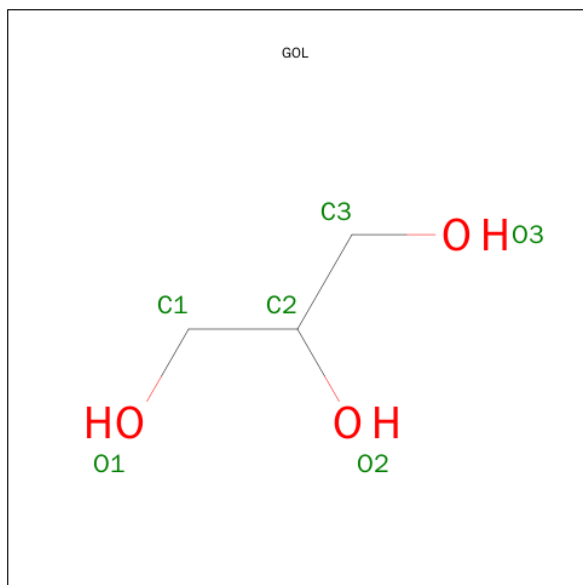
- Molecule 4 is a protein called 10E5 FAB LIGHT CHAIN.

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.

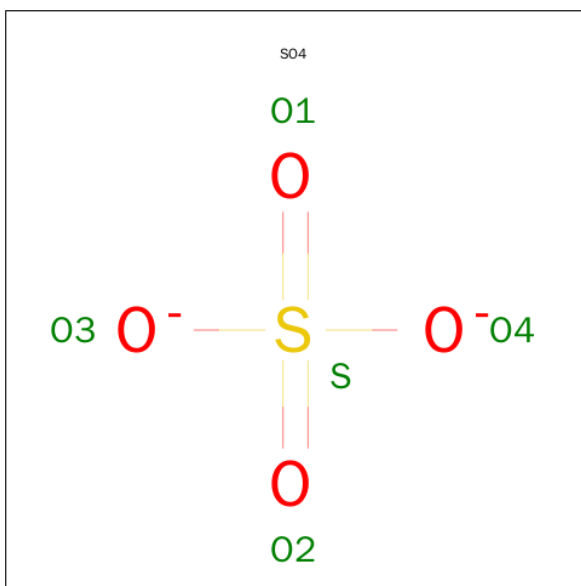
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	6	Total	C	H	N	O	0	3	0
			111	32	52	15	12			
5	J	6	Total	C	H	N	O	0	0	0
			74	22	34	9	9			

- 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		

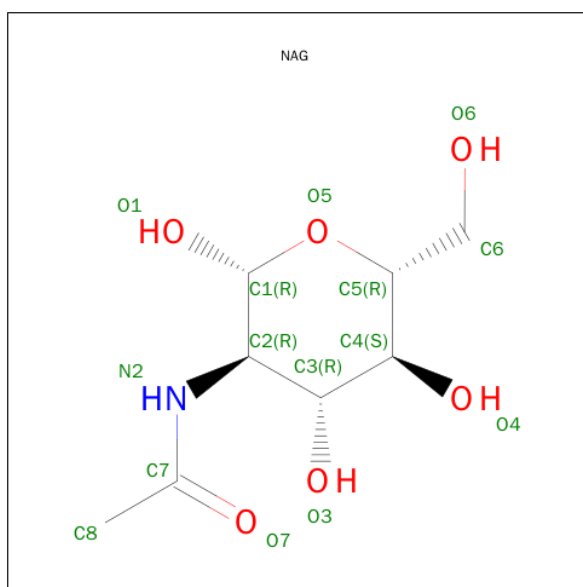
- Molecule 10 is a polymer of unknown type called SUGAR (6-MER).

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		

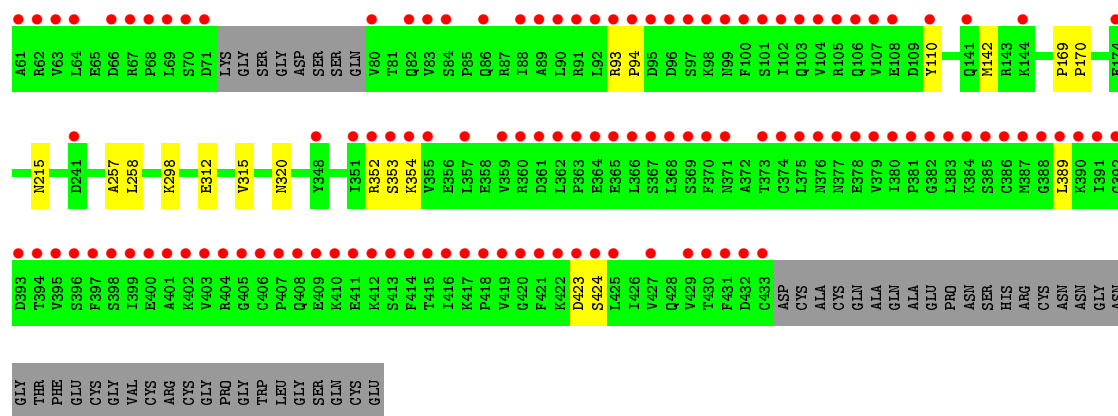
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	483	Total	O	0	0
			483	483		

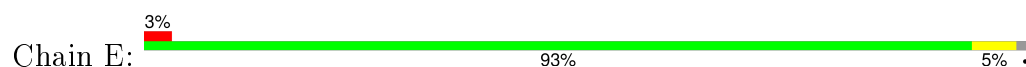
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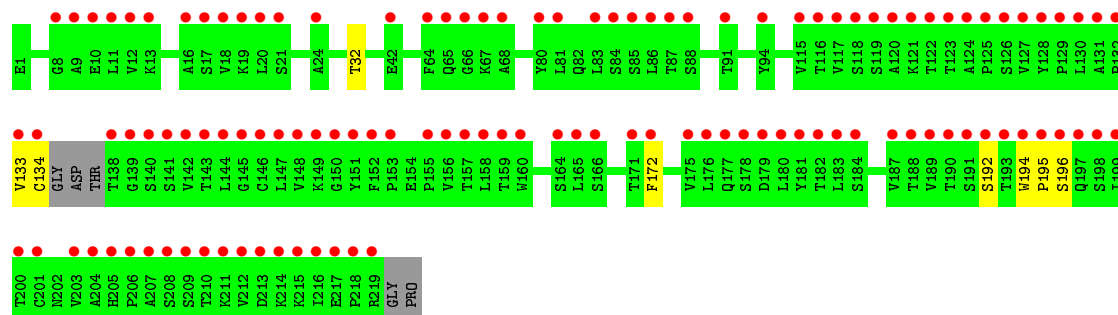
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	B	211	Total 211	O 211	0	0
14	C	283	Total 283	O 283	0	0
14	D	107	Total 107	O 107	0	0
14	E	129	Total 129	O 129	0	0
14	F	68	Total 68	O 68	0	0
14	H	18	Total 18	O 18	0	0
14	I	2	Total 2	O 2	0	0
14	J	2	Total 2	O 2	0	0
14	L	15	Total 15	O 15	0	0



• Molecule 3: 10E5 FAB HEAVY CHAIN



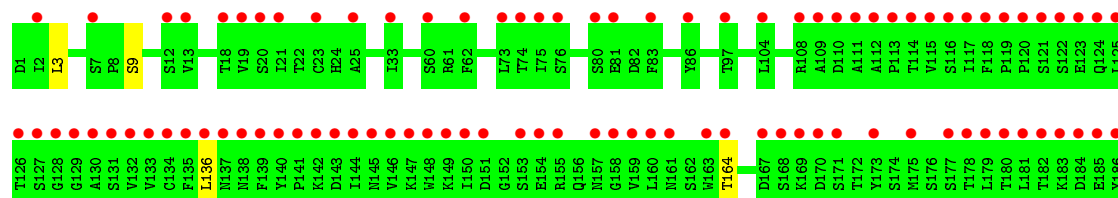
• Molecule 3: 10E5 FAB HEAVY CHAIN

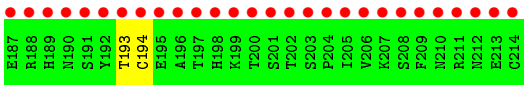


• Molecule 4: 10E5 FAB LIGHT CHAIN



• 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.

The worst 5 of 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

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
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

5 of 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

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
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

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	215	ASN
1	C	166	TYR
5	I	493[B]	ARG
2	B	241	ASP
1	C	23	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
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%)

The worst 5 of 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

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	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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 ⓘ

There are no such residues in this entry.