Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:27 PM GMT

PDB ID	:	3ZE0
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	:	2.95 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:

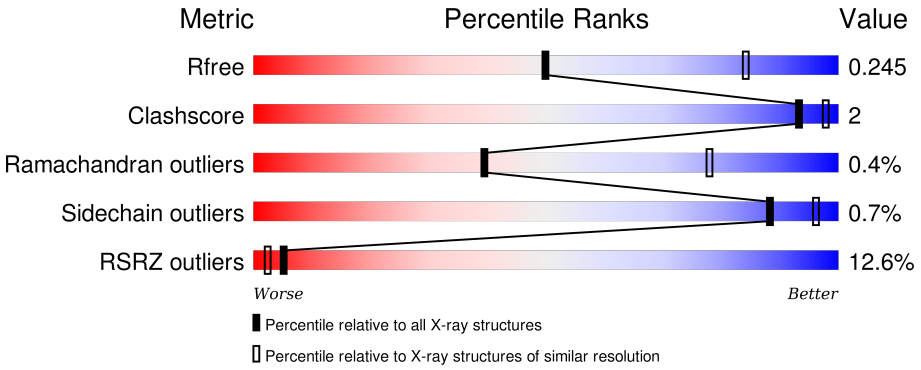
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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 <=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	95%
1	C	457	2% 96%
2	B	472	14% 92% 7%
2	D	472	19% 92% 7%
3	E	221	28% 91% 6%

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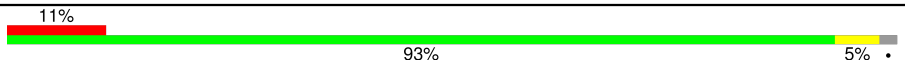
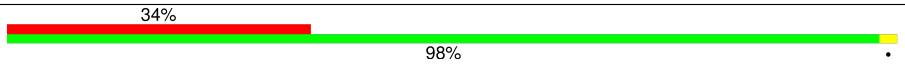
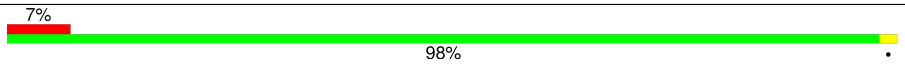
Mol	Chain	Length	Quality of chain
3	H	221	
4	F	214	
4	L	214	
5	I	6	
5	J	6	

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
12	CL	C	1455	-	-	-	X
6	SO4	A	1457	-	-	-	X
6	SO4	A	1458	-	-	-	X
9	NAG	D	3099	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 41622 atoms, of which 20222 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	455	Total	C	H	N	O	S	0	5	0
			6868	2235	3355	604	666	8			
1	C	453	Total	C	H	N	O	S	0	2	0
			6795	2214	3311	600	662	8			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	465	Total	C	H	N	O	S	6	1	0
			7098	2238	3506	613	708	33			
2	D	469	Total	C	H	N	O	S	14	1	0
			7146	2252	3526	619	715	34			

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

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

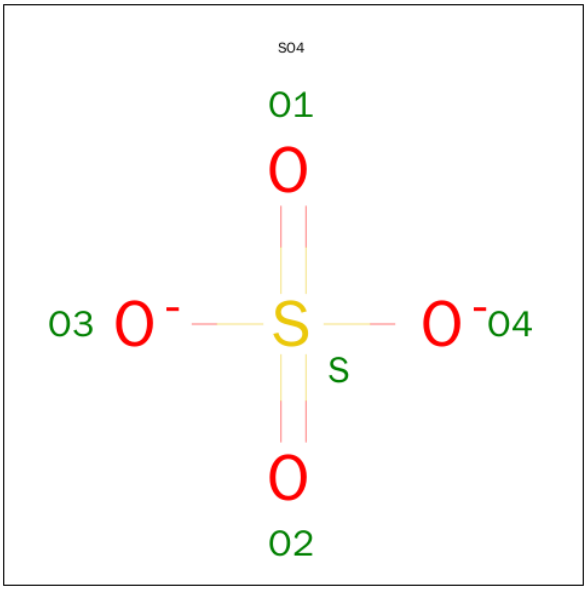
- Molecule 4 is a protein called 10E5 FAB LIGHT CHAIN.

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

- Molecule 5 is a protein called RGD PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	6	Total	C	H	N	O	0	0	0
			75	22	34	9	10			
5	J	6	Total	C	H	N	O	2	0	0
			75	22	34	9	10			

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

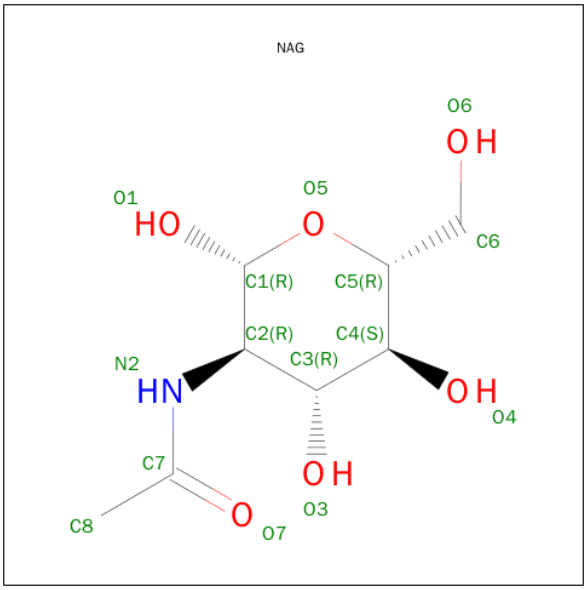
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 9 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 10 is a polymer of unknown type called SUGAR (4-MER).

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

- 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		
11	D	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	1	Total	Cl	0	0
			1	1		

- Molecule 13 is water.

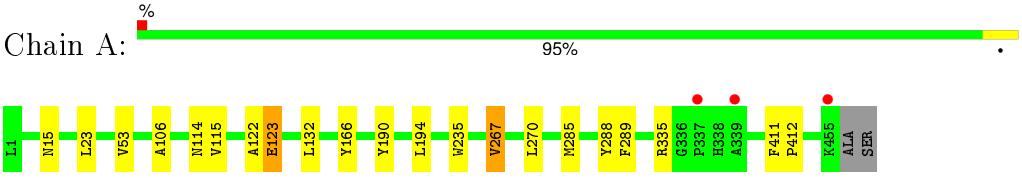
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	160	Total	O	0	0
			160	160		
13	B	71	Total	O	0	0
			71	71		
13	C	51	Total	O	0	0
			51	51		
13	D	26	Total	O	0	0
			26	26		
13	E	1	Total	O	0	0
			1	1		
13	F	1	Total	O	0	0
			1	1		
13	H	8	Total	O	0	0
			8	8		
13	I	2	Total	O	0	0
			2	2		
13	J	1	Total	O	0	0
			1	1		
13	L	6	Total	O	0	0
			6	6		

3 Residue-property plots (i)

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

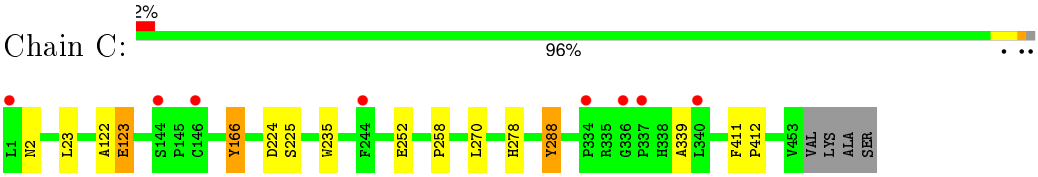
- Molecule 1: INTEGRIN ALPHA-IIB

Chain A:



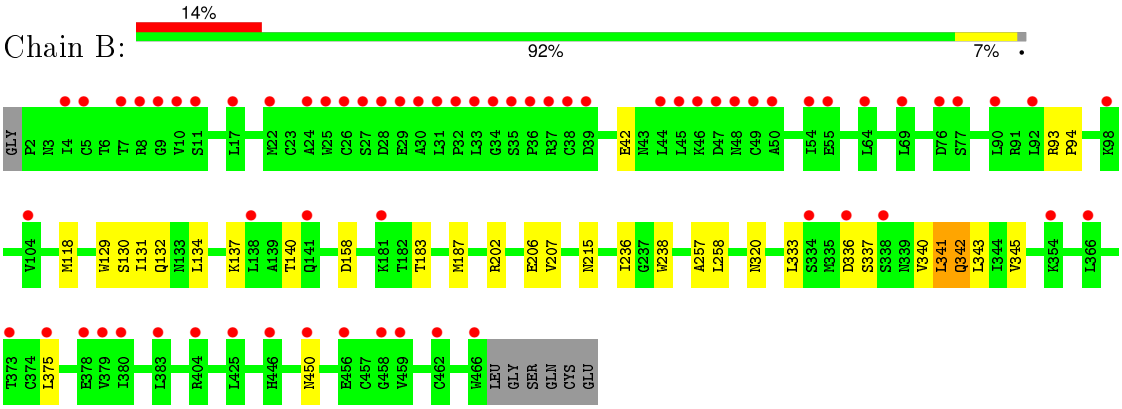
- Molecule 1: INTEGRIN ALPHA-IIB

Chain C:



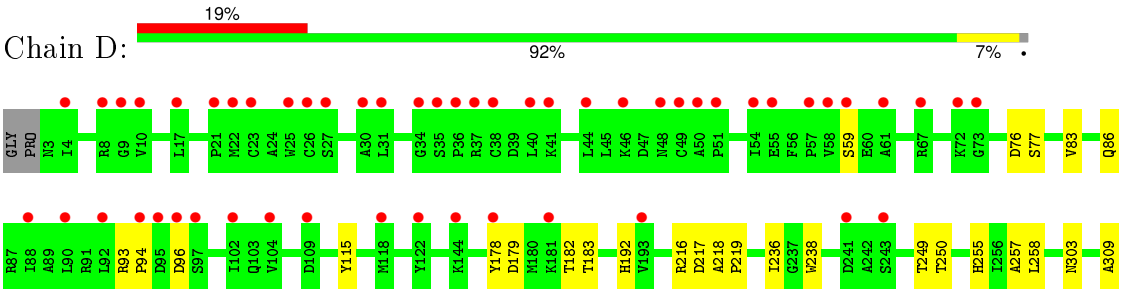
- Molecule 2: INTEGRIN BETA-3

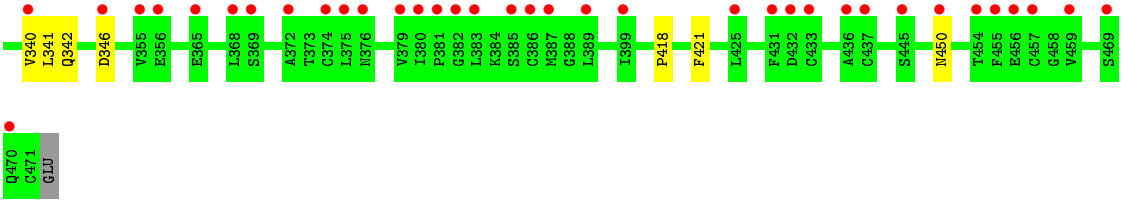
Chain B:



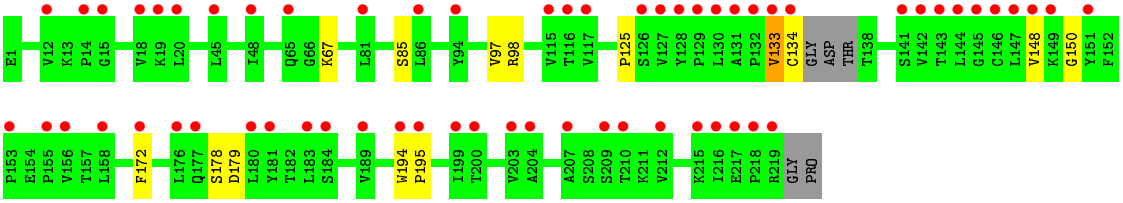
- Molecule 2: INTEGRIN BETA-3

Chain D:

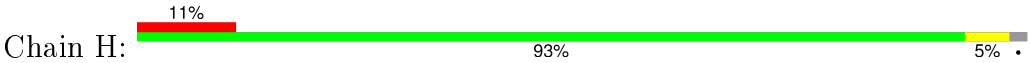


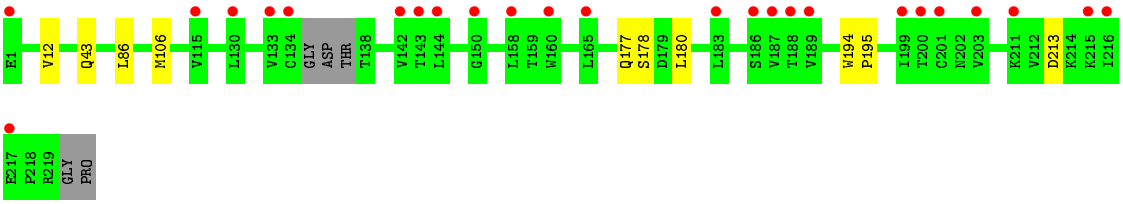


• Molecule 3: 10E5 FAB HEAVY CHAIN

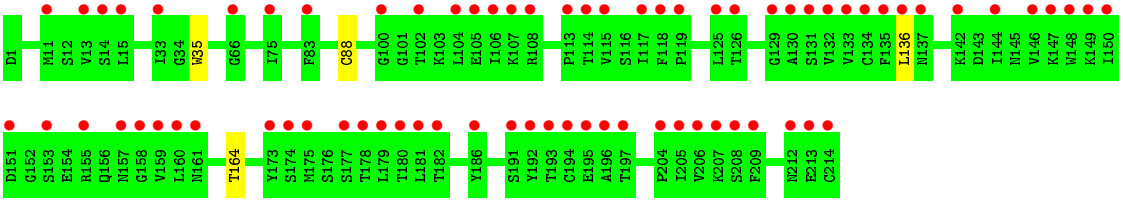


• Molecule 3: 10E5 FAB HEAVY CHAIN

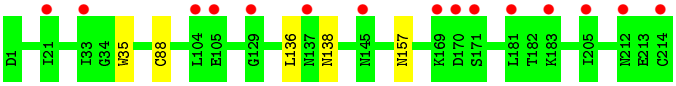




• Molecule 4: 10E5 FAB LIGHT CHAIN



• Molecule 4: 10E5 FAB LIGHT CHAIN

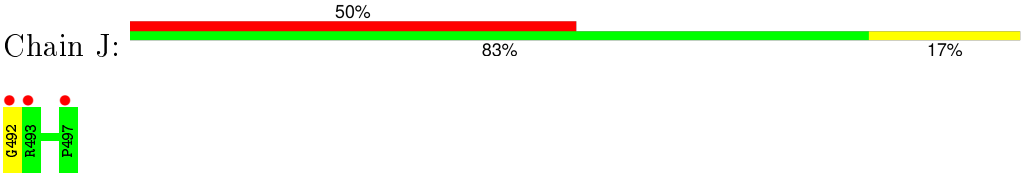


• Molecule 5: RGD PEPTIDE

There are no outlier residues recorded for this chain.

• Molecule 5: RGD PEPTIDE

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	259.64Å 144.68Å 104.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.31 – 2.95 49.03 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.31-2.95) 99.6 (49.03-2.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.96Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.185 , 0.243 0.183 , 0.245	Depositor DCC
R_{free} test set	1074 reflections (1.29%)	DCC
Wilson B-factor (Å^2)	57.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 83.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 83345 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	41622	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, NAG, CL, CA, MN, SO4, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.23	0/3625	0.40	0/4940
1	C	0.22	0/3587	0.38	0/4888
2	B	0.21	0/3662	0.39	0/4965
2	D	0.20	0/3686	0.36	0/4997
3	E	0.21	0/1684	0.38	0/2305
3	H	0.21	0/1684	0.39	0/2305
4	F	0.21	0/1673	0.37	0/2269
4	L	0.22	0/1673	0.37	0/2269
5	I	0.19	0/41	0.43	0/52
5	J	0.20	0/41	0.50	0/52
All	All	0.21	0/21356	0.38	0/29042

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	3513	3355	3364	12	0
1	C	3484	3311	3320	9	0
2	B	3592	3506	3512	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3620	3526	3531	18	0
3	E	1642	1597	1600	7	0
3	H	1642	1597	1600	5	0
4	F	1637	1550	1553	3	0
4	L	1637	1550	1553	3	0
5	I	41	34	34	0	0
5	J	41	34	34	1	0
6	A	15	0	0	1	0
6	C	5	0	0	0	0
6	L	5	0	0	0	0
7	A	4	0	0	0	0
7	C	4	0	0	0	0
8	B	3	0	0	0	0
8	D	3	0	0	0	0
9	B	14	13	13	0	0
9	D	14	13	13	1	0
10	B	50	43	43	0	0
10	D	50	43	43	0	0
11	B	28	25	25	0	0
11	D	28	25	25	1	0
12	C	1	0	0	0	0
13	A	160	0	0	3	1
13	B	71	0	0	0	0
13	C	51	0	0	0	1
13	D	26	0	0	1	0
13	E	1	0	0	0	0
13	F	1	0	0	0	0
13	H	8	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	1	0
13	L	6	0	0	1	0
All	All	21400	20222	20263	77	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 (77) 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)
2:D:115:TYR:HH	2:D:192:HIS:HD1	1.10	0.91
2:D:250:THR:OG1	13:D:4007:HOH:O	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ASP:OD1	1:C:225:SER:N	2.30	0.64
2:B:118:MET:SD	2:B:131:ILE:HD13	2.40	0.61
1:A:122:ALA:O	1:A:123:GLU:HB2	2.05	0.56
2:B:257:ALA:O	2:B:258:LEU:HB2	2.06	0.56
2:D:76:ASP:OD1	2:D:77:SER:N	2.40	0.55
2:B:130:SER:O	2:B:341:LEU:CD1	2.57	0.53
1:C:122:ALA:O	1:C:123:GLU:HB2	2.08	0.53
2:B:336:ASP:O	2:B:337:SER:OG	2.25	0.52
1:A:122:ALA:O	1:A:123:GLU:CB	2.57	0.52
9:D:3099:NAG:O6	11:D:3372:NAG:O6	2.13	0.52
3:H:194:TRP:CG	3:H:195:PRO:HA	2.44	0.52
3:H:43:GLN:N	3:H:43:GLN:OE1	2.42	0.51
2:B:131:ILE:HD12	2:B:207:VAL:HG13	1.92	0.51
2:D:342:GLN:NE2	2:D:346:ASP:OD2	2.43	0.51
6:A:1456:SO4:O3	13:A:4152:HOH:O	2.19	0.50
2:B:340:VAL:O	2:B:341:LEU:CB	2.60	0.50
2:B:342:GLN:O	2:B:345:VAL:N	2.44	0.50
1:A:267:VAL:HG12	1:A:289:PHE:CE1	2.47	0.50
3:H:177:GLN:N	3:H:180:LEU:O	2.45	0.50
2:D:217:ASP:OD2	2:D:255:HIS:NE2	2.41	0.49
2:D:450:ASN:ND2	2:D:450:ASN:O	2.47	0.48
1:C:122:ALA:O	1:C:123:GLU:CB	2.62	0.48
2:B:129:TRP:CE3	2:B:130:SER:HA	2.49	0.48
2:B:450:ASN:ND2	2:B:450:ASN:O	2.47	0.48
2:D:257:ALA:O	2:D:258:LEU:HB2	2.14	0.47
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.46	0.47
2:B:340:VAL:O	2:B:341:LEU:HB2	2.14	0.47
5:J:492:GLY:N	13:J:4001:HOH:O	2.46	0.47
2:D:182:THR:OG1	2:D:183:THR:N	2.48	0.47
1:A:15[B]:ASN:ND2	13:A:4009:HOH:O	2.48	0.46
2:D:418:PRO:HB2	2:D:421:PHE:CD1	2.51	0.46
2:D:218:ALA:HB3	2:D:219:PRO:HD3	1.97	0.46
1:A:53:VAL:HG21	1:A:106:ALA:CB	2.46	0.46
2:D:83:VAL:O	2:D:86:GLN:NE2	2.49	0.45
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.98	0.45
2:B:118:MET:SD	2:B:131:ILE:HG21	2.57	0.45
1:C:411:PHE:HB3	1:C:412:PRO:CD	2.47	0.45
3:H:213:ASP:OD1	3:H:213:ASP:N	2.49	0.45
2:D:178:TYR:CG	2:D:179:ASP:N	2.85	0.45
3:E:133:VAL:O	3:E:134:CYS:SG	2.74	0.44
1:A:15[A]:ASN:ND2	13:A:4008:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:LEU:HA	2:B:340:VAL:HG13	2.00	0.44
3:H:12:VAL:HG21	3:H:86:LEU:CD1	2.48	0.44
3:E:194:TRP:CG	3:E:195:PRO:HA	2.53	0.44
1:C:258:PRO:HB2	1:C:288:TYR:CD2	2.52	0.44
2:D:93:ARG:HB2	2:D:94:PRO:HD2	1.98	0.44
1:C:2:ASN:OD1	1:C:2:ASN:N	2.50	0.44
2:B:42:GLU:OE1	2:B:42:GLU:N	2.51	0.44
2:B:340:VAL:O	2:B:341:LEU:HG	2.18	0.43
1:A:235:TRP:CZ2	1:A:270:LEU:HD11	2.54	0.43
4:F:35:TRP:CZ3	4:F:88:CYS:HB3	2.54	0.43
1:A:132:LEU:N	1:A:132:LEU:HD12	2.33	0.43
1:A:411:PHE:HB3	1:A:412:PRO:CD	2.49	0.43
1:A:285:MET:SD	2:B:320:ASN:HB3	2.59	0.43
3:E:67:LYS:NZ	3:E:85:SER:O	2.51	0.43
1:C:235:TRP:CZ2	1:C:270:LEU:HD11	2.53	0.43
1:C:278[A]:HIS:CD2	1:C:339:ALA:HB1	2.53	0.43
3:E:172:PHE:CD2	4:F:164:THR:HG23	2.54	0.43
1:A:194:LEU:C	1:A:194:LEU:HD12	2.39	0.43
2:B:158:ASP:HB3	2:B:187:MET:CE	2.49	0.43
1:A:114:ASN:OD1	1:A:115:VAL:N	2.52	0.43
2:D:340:VAL:HG13	2:D:341:LEU:N	2.34	0.42
3:E:178:SER:O	3:E:179:ASP:HB2	2.20	0.42
2:D:59:SER:OG	2:D:96:ASP:OD2	2.26	0.42
1:C:166:TYR:CE1	2:D:216:ARG:HD3	2.54	0.42
2:D:249:THR:HG22	2:D:309:ALA:HB3	2.02	0.42
4:F:136:LEU:N	4:F:136:LEU:HD12	2.35	0.41
2:B:134:LEU:HA	2:B:137:LYS:CD	2.51	0.41
2:B:236:ILE:HG21	2:B:238:TRP:CE2	2.55	0.41
3:E:125:PRO:HB2	3:E:148:VAL:HG13	2.03	0.41
4:L:157:ASN:ND2	13:L:4006:HOH:O	2.53	0.41
2:D:236:ILE:HG21	2:D:238:TRP:CE2	2.56	0.41
4:L:136:LEU:N	4:L:136:LEU:HD12	2.36	0.40
4:L:35:TRP:CZ3	4:L:88:CYS:HB3	2.56	0.40
3:E:97:VAL:HG12	3:E:98:ARG:N	2.37	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)
13:A:4052:HOH:O	13:C:4041:HOH:O[1_554]	2.12	0.08

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	458/457 (100%)	440 (96%)	17 (4%)	1 (0%)	52	86
1	C	453/457 (99%)	428 (94%)	24 (5%)	1 (0%)	52	86
2	B	464/472 (98%)	435 (94%)	26 (6%)	3 (1%)	30	70
2	D	468/472 (99%)	436 (93%)	30 (6%)	2 (0%)	39	78
3	E	212/221 (96%)	197 (93%)	13 (6%)	2 (1%)	21	61
3	H	212/221 (96%)	196 (92%)	15 (7%)	1 (0%)	34	74
4	F	212/214 (99%)	197 (93%)	15 (7%)	0	100	100
4	L	212/214 (99%)	204 (96%)	7 (3%)	1 (0%)	34	74
5	I	4/6 (67%)	4 (100%)	0	0	100	100
5	J	4/6 (67%)	4 (100%)	0	0	100	100
All	All	2699/2740 (98%)	2541 (94%)	147 (5%)	11 (0%)	39	78

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	341	LEU
1	A	123	GLU
2	B	343	LEU
2	B	375	LEU
1	C	123	GLU
2	D	303[A]	ASN
2	D	303[B]	ASN
4	L	138	ASN
3	H	178	SER
3	E	150	GLY
3	E	133	VAL

5.3.2 Protein sidechains (i)

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	368/364 (101%)	362 (98%)	6 (2%)	70 90
1	C	363/364 (100%)	359 (99%)	4 (1%)	80 93
2	B	413/417 (99%)	408 (99%)	5 (1%)	78 93
2	D	416/417 (100%)	416 (100%)	0	100 100
3	E	187/190 (98%)	187 (100%)	0	100 100
3	H	187/190 (98%)	186 (100%)	1 (0%)	92 97
4	F	188/188 (100%)	188 (100%)	0	100 100
4	L	188/188 (100%)	188 (100%)	0	100 100
5	I	4/4 (100%)	4 (100%)	0	100 100
5	J	4/4 (100%)	4 (100%)	0	100 100
All	All	2318/2326 (100%)	2302 (99%)	16 (1%)	88 96

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	190	TYR
1	A	267	VAL
1	A	288	TYR
1	A	335	ARG
2	B	132	GLN
2	B	140	THR
2	B	183	THR
2	B	215	ASN
2	B	342	GLN
1	C	23	LEU
1	C	166	TYR
1	C	252	GLU
1	C	288	TYR
3	H	106	MET

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

Mol	Chain	Res	Type
1	A	338	HIS
2	B	450	ASN
1	C	197	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

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	0.51	0	15,19,21	0.70	0
10	NAG	B	3321	10	14,14,15	0.56	0	15,19,21	0.71	0
10	BMA	B	3322	10	11,11,12	0.59	0	14,15,17	0.86	0
10	MAN	B	3323	10	11,11,12	0.59	0	14,15,17	0.70	0
11	NAG	B	3371	11,2	14,14,15	0.57	0	15,19,21	0.81	0
11	NAG	B	3372	11	14,14,15	0.50	0	15,19,21	0.57	0
10	NAG	D	3320	10,2	14,14,15	0.49	0	15,19,21	0.64	0
10	NAG	D	3321	10	14,14,15	0.51	0	15,19,21	0.60	0
10	BMA	D	3322	10	11,11,12	0.64	0	14,15,17	0.89	1 (7%)
10	MAN	D	3323	10	11,11,12	0.63	0	14,15,17	0.71	0
11	NAG	D	3371	11,2	14,14,15	0.57	0	15,19,21	0.75	0
11	NAG	D	3372	11	14,14,15	0.51	0	15,19,21	0.61	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
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
10	NAG	D	3320	10,2	-	0/6/23/26	0/1/1/1
10	NAG	D	3321	10	-	0/6/23/26	0/1/1/1
10	BMA	D	3322	10	-	0/2/19/22	0/1/1/1
10	MAN	D	3323	10	-	0/2/19/22	0/1/1/1
11	NAG	D	3371	11,2	-	0/6/23/26	0/1/1/1
11	NAG	D	3372	11	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	3322	BMA	C1-C2-C3	2.67	112.70	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	3372	NAG	1	0

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 15 are monoatomic - leaving 7 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	SO4	A	1456	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	A	1457	-	4,4,4	0.23	0	6,6,6	0.09	0
6	SO4	A	1458	-	4,4,4	0.24	0	6,6,6	0.07	0
9	NAG	B	3099	2	14,14,15	0.50	0	15,19,21	0.68	0
6	SO4	C	1454	-	4,4,4	0.22	0	6,6,6	0.11	0
9	NAG	D	3099	2	14,14,15	0.49	0	15,19,21	0.61	0
6	SO4	L	1215	-	4,4,4	0.23	0	6,6,6	0.07	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	SO4	A	1456	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1457	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1458	-	-	0/0/0/0	0/0/0/0
9	NAG	B	3099	2	-	0/6/23/26	0/1/1/1
6	SO4	C	1454	-	-	0/0/0/0	0/0/0/0
9	NAG	D	3099	2	-	0/6/23/26	0/1/1/1
6	SO4	L	1215	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1456	SO4	1	0
9	D	3099	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	455/457 (99%)	0.34	3 (0%) 89 76	24, 43, 79, 140	0
1	C	453/457 (99%)	0.47	8 (1%) 71 51	38, 76, 118, 171	0
2	B	465/472 (98%)	0.82	65 (13%) 4 2	27, 81, 172, 213	1 (0%)
2	D	469/472 (99%)	1.08	89 (18%) 2 1	53, 113, 175, 222	2 (0%)
3	E	216/221 (97%)	1.50	61 (28%) 1 0	86, 137, 188, 213	0
3	H	216/221 (97%)	0.60	25 (11%) 6 3	51, 103, 172, 205	0
4	F	214/214 (100%)	1.63	73 (34%) 0 0	86, 140, 209, 281	1 (0%)
4	L	214/214 (100%)	0.57	15 (7%) 19 10	55, 95, 132, 234	0
5	I	6/6 (100%)	0.59	0 100 100	40, 58, 89, 90	0
5	J	6/6 (100%)	2.04	3 (50%) 0 0	43, 46, 86, 105	3 (50%)
All	All	2714/2740 (99%)	0.81	342 (12%) 5 2	24, 91, 175, 281	7 (0%)

All (342) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	193	THR	13.1
4	F	181	LEU	11.5
4	F	214	CYS	7.9
4	F	192	TYR	7.7
2	B	36	PRO	7.5
3	E	133	VAL	7.3
3	E	130	LEU	7.0
2	B	33	LEU	7.0
3	E	219	ARG	6.8
4	F	180	THR	6.7
4	F	179	LEU	6.6
3	E	142	VAL	6.4
2	B	10	VAL	6.4

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Mol	Chain	Res	Type	RSRZ
3	E	194	TRP	6.3
2	B	26	CYS	6.2
3	E	144	LEU	6.2
3	E	131	ALA	5.9
2	D	22	MET	5.8
3	E	148	VAL	5.7
2	B	48	ASN	5.7
2	D	44	LEU	5.6
3	E	132	PRO	5.5
2	D	375	LEU	5.5
4	F	130	ALA	5.4
2	B	44	LEU	5.4
3	E	200	THR	5.3
3	E	147	LEU	5.3
4	F	148	TRP	5.3
2	D	376	ASN	5.3
3	E	134	CYS	5.2
4	F	159	VAL	5.2
5	J	497	PRO	5.2
3	E	127	VAL	5.1
3	E	183	LEU	5.1
2	B	11	SER	4.9
2	D	36	PRO	4.9
4	F	125	LEU	4.9
3	H	133	VAL	4.9
4	F	115	VAL	4.9
3	E	176	LEU	4.8
4	F	186	TYR	4.8
2	D	72	LYS	4.8
4	F	133	VAL	4.8
2	D	9	GLY	4.7
4	L	214	CYS	4.7
3	E	128	TYR	4.7
3	H	142	VAL	4.7
3	E	216	ILE	4.6
4	F	135	PHE	4.6
4	F	136	LEU	4.6
4	F	212	ASN	4.5
2	D	49	CYS	4.5
4	F	147	LYS	4.5
3	E	184	SER	4.4
3	E	20	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
3	E	212	VAL	4.4
2	B	8	ARG	4.4
1	A	455	LYS	4.3
2	B	49	CYS	4.3
2	D	17	LEU	4.3
4	F	104	LEU	4.2
4	F	150	ILE	4.2
4	F	134	CYS	4.2
2	D	374	CYS	4.2
3	E	145	GLY	4.2
2	D	21	PRO	4.1
2	D	54	ILE	4.1
4	F	155	ARG	4.1
2	B	383	LEU	4.0
4	F	105	GLU	4.0
2	D	181	LYS	4.0
3	H	201	CYS	4.0
4	F	132	VAL	3.9
4	F	205	ILE	3.9
2	D	58	VAL	3.9
3	H	189	VAL	3.9
2	D	102	ILE	3.9
2	D	57	PRO	3.9
2	D	355	VAL	3.9
2	D	90	LEU	3.8
3	E	218	PRO	3.7
3	E	117	VAL	3.7
2	D	433	CYS	3.7
2	D	368	LEU	3.7
3	H	165	LEU	3.7
2	D	31	LEU	3.6
4	F	206	VAL	3.6
3	E	181	TYR	3.6
3	H	144	LEU	3.6
2	D	8	ARG	3.6
3	E	189	VAL	3.6
4	F	178	THR	3.6
3	E	129	PRO	3.6
2	D	61	ALA	3.6
2	D	35	SER	3.5
3	E	12	VAL	3.5
2	B	24	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
3	E	217	GLU	3.5
2	B	7	THR	3.5
4	F	108	ARG	3.5
4	F	149	LYS	3.5
4	F	209	PHE	3.5
3	H	216	ILE	3.5
2	D	27	SER	3.4
4	F	213	GLU	3.4
4	F	182	THR	3.4
2	D	55	GLU	3.4
2	D	454	THR	3.4
3	E	199	ILE	3.4
2	B	92	LEU	3.4
3	E	115	VAL	3.3
1	A	339	ALA	3.3
3	E	81	LEU	3.3
4	F	195	GLU	3.3
4	F	144	ILE	3.3
4	F	208	SER	3.3
4	F	113	PRO	3.3
2	B	25	TRP	3.3
2	B	28	ASP	3.3
2	B	77	SER	3.3
3	H	187	VAL	3.3
4	F	146	VAL	3.3
2	B	459	VAL	3.2
2	D	379	VAL	3.2
2	D	383	LEU	3.2
2	D	30	ALA	3.2
2	D	387	MET	3.2
2	B	34	GLY	3.2
4	F	14	SER	3.2
2	D	381	PRO	3.2
3	E	156	VAL	3.1
2	D	94	PRO	3.1
3	H	143	THR	3.1
4	F	174	SER	3.1
4	L	129	GLY	3.1
4	F	117	ILE	3.1
2	B	38	CYS	3.1
3	E	143	THR	3.1
4	F	158	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
3	E	149	LYS	3.1
4	F	191	SER	3.1
3	H	160	TRP	3.1
1	C	144	SER	3.1
3	E	126	SER	3.0
2	D	455	PHE	3.0
2	B	456	GLU	3.0
2	B	338	SER	3.0
2	B	373	THR	3.0
3	H	188	THR	3.0
3	H	1	GLU	3.0
2	B	375	LEU	3.0
4	F	107	LYS	3.0
2	D	59	SER	3.0
1	C	340	LEU	3.0
4	F	126	THR	3.0
2	B	104	VAL	3.0
2	D	46	LYS	3.0
4	L	104	LEU	3.0
4	F	13	VAL	3.0
4	F	118	PHE	3.0
2	D	386	CYS	2.9
3	E	18	VAL	2.9
2	B	27	SER	2.9
3	E	116	THR	2.9
3	E	45	LEU	2.9
2	B	54	ILE	2.9
1	C	1	LEU	2.9
2	B	141	GLN	2.9
2	D	356	GLU	2.9
2	D	10	VAL	2.9
2	D	432	ASP	2.9
2	D	459	VAL	2.9
2	B	31	LEU	2.9
4	L	205	ILE	2.9
2	D	122	TYR	2.8
3	H	130	LEU	2.8
2	D	51	PRO	2.8
4	F	197	THR	2.8
4	F	15	LEU	2.8
2	B	378	GLU	2.8
4	F	160	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	39	ASP	2.8
2	D	34	GLY	2.8
3	H	199	ILE	2.8
1	C	334	PRO	2.8
2	D	37	ARG	2.8
2	D	23	CYS	2.7
2	D	26	CYS	2.7
3	E	210	THR	2.7
2	B	181	LYS	2.7
2	D	104	VAL	2.7
2	B	380	ILE	2.7
3	E	14	PRO	2.7
2	B	17	LEU	2.7
3	H	158	LEU	2.7
3	E	86	LEU	2.7
3	E	204	ALA	2.7
4	F	100	GLY	2.7
3	H	134	CYS	2.7
2	D	92	LEU	2.7
2	D	372	ALA	2.7
2	D	369	SER	2.7
2	B	37	ARG	2.7
2	B	64	LEU	2.6
4	F	207	LYS	2.6
2	B	45	LEU	2.6
2	B	22	MET	2.6
1	C	244	PHE	2.6
2	D	50	ALA	2.6
2	D	73	GLY	2.6
4	F	175	MET	2.6
2	D	95	ASP	2.6
2	D	382	GLY	2.6
2	D	450	ASN	2.6
3	E	146	CYS	2.6
2	D	425	LEU	2.6
4	L	183	LYS	2.6
4	F	157	ASN	2.6
3	E	180	LEU	2.5
4	L	169	LYS	2.5
3	H	186	SER	2.5
4	F	106	ILE	2.5
2	D	241	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
4	L	105	GLU	2.5
4	F	75	ILE	2.5
3	E	172	PHE	2.5
2	B	90	LEU	2.5
2	D	389	LEU	2.5
2	D	97	SER	2.5
3	E	141	SER	2.5
3	E	209	SER	2.5
2	B	458	GLY	2.5
2	B	69	LEU	2.5
2	D	48	ASN	2.5
2	B	55	GLU	2.4
2	D	118	MET	2.4
2	B	32	PRO	2.4
2	B	98	LYS	2.4
2	D	178	TYR	2.4
4	F	161	ASN	2.4
3	E	177	GLN	2.4
2	D	25	TRP	2.4
2	D	470	GLN	2.4
2	B	35	SER	2.4
4	L	33	ILE	2.4
4	L	212	ASN	2.4
4	F	194	CYS	2.4
3	E	158	LEU	2.4
2	D	437	CYS	2.4
2	D	457	CYS	2.4
3	E	155	PRO	2.4
2	D	243	SER	2.4
3	E	94	TYR	2.4
2	D	340	VAL	2.4
2	B	138	LEU	2.4
2	D	40	LEU	2.4
4	F	196	ALA	2.4
2	D	399	ILE	2.4
3	E	19	LYS	2.4
2	D	346	ASP	2.4
2	B	379	VAL	2.3
2	B	450	ASN	2.3
2	B	466	TRP	2.3
4	F	83	PHE	2.3
2	B	404	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	354	LYS	2.3
2	B	446	HIS	2.3
2	B	29	GLU	2.3
2	D	96	ASP	2.3
2	D	38	CYS	2.3
4	L	170	ASP	2.3
2	D	4	ILE	2.3
4	F	119	PRO	2.3
4	F	204	PRO	2.3
1	C	146	CYS	2.3
4	F	177	SER	2.3
2	B	336	ASP	2.3
2	B	5	CYS	2.3
1	A	337	PRO	2.3
3	E	65	GLN	2.3
4	L	171	SER	2.2
4	F	66	GLY	2.2
2	B	47	ASP	2.2
2	B	4	ILE	2.2
2	B	425	LEU	2.2
4	F	33	ILE	2.2
4	F	142	LYS	2.2
2	D	445	SER	2.2
2	B	30	ALA	2.2
4	L	21	ILE	2.2
2	D	67	ARG	2.2
3	E	203	VAL	2.2
2	D	385	SER	2.2
3	H	203	VAL	2.2
3	H	217	GLU	2.2
2	B	76	ASP	2.2
4	F	151	ASP	2.2
2	B	46	LYS	2.2
4	F	11	MET	2.2
5	J	492	GLY	2.2
2	D	469	SER	2.2
3	E	207	ALA	2.2
4	F	114	THR	2.2
3	E	15	GLY	2.2
4	F	102	THR	2.2
4	F	137	ASN	2.2
4	L	137	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
3	H	211	LYS	2.1
3	H	200	THR	2.1
4	F	153	SER	2.1
2	D	431	PHE	2.1
2	B	9	GLY	2.1
2	B	50	ALA	2.1
2	D	365	GLU	2.1
2	D	41	LYS	2.1
3	E	195	PRO	2.1
5	J	493	ARG	2.1
3	H	183	LEU	2.1
2	D	436	ALA	2.1
4	F	173	TYR	2.1
1	C	336	GLY	2.1
4	F	129	GLY	2.1
2	D	380	ILE	2.1
3	E	48	ILE	2.1
4	L	145	ASN	2.1
3	H	215	LYS	2.1
4	L	181	LEU	2.1
2	B	462	CYS	2.1
3	H	150	GLY	2.1
2	D	88	ILE	2.1
3	E	151	TYR	2.1
2	D	193	VAL	2.0
4	F	131	SER	2.0
3	E	153	PRO	2.0
2	B	366	LEU	2.0
3	E	215	LYS	2.0
2	D	456	GLU	2.0
2	D	144	LYS	2.0
2	D	109	ASP	2.0
3	H	115	VAL	2.0
1	C	337	PRO	2.0
2	B	334	SER	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
11	NAG	D	3371	14/15	0.83	0.39	0.64	120,157,185,191	0
11	NAG	B	3371	14/15	0.90	0.24	-0.13	102,132,164,164	0
10	NAG	D	3320	14/15	0.95	0.18	-0.75	65,88,111,111	0
10	NAG	B	3320	14/15	0.97	0.17	-	28,45,64,85	0
11	NAG	D	3372	14/15	0.81	0.52	-	148,177,206,217	0
10	BMA	B	3322	11/12	0.81	0.15	-	98,137,174,181	0
10	NAG	B	3321	14/15	0.92	0.15	-	66,92,116,124	0
10	NAG	D	3321	14/15	0.90	0.21	-	86,119,155,164	0
11	NAG	B	3372	14/15	0.89	0.34	-	116,166,203,209	0
10	BMA	D	3322	11/12	0.77	0.24	-	151,175,210,210	0
10	MAN	D	3323	11/12	0.87	0.37	-	164,181,216,218	0
10	MAN	B	3323	11/12	0.88	0.23	-	112,141,170,172	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	SO4	A	1458	5/5	0.88	0.40	7.21	135,143,150,167	0
12	CL	C	1455	1/1	0.92	0.30	7.21	72,72,72,72	0
6	SO4	A	1457	5/5	0.94	0.26	3.64	97,98,113,136	0
9	NAG	D	3099	14/15	0.75	0.46	1.32	130,164,195,198	0
6	SO4	C	1454	5/5	0.80	0.28	1.24	137,139,143,148	0
8	MN	B	2001	1/1	1.00	0.24	0.90	42,42,42,42	0
7	CA	A	2007	1/1	1.00	0.21	0.03	39,39,39,39	0
8	MN	D	2002	1/1	0.88	0.27	-0.06	205,205,205,205	0
8	MN	D	2001	1/1	0.95	0.22	-0.13	101,101,101,101	0
8	MN	B	2002	1/1	0.99	0.21	-0.14	65,65,65,65	0
6	SO4	L	1215	5/5	0.92	0.22	-0.15	134,136,137,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	MN	B	2003	1/1	0.99	0.23	-0.16	51,51,51,51	0
7	CA	C	2007	1/1	0.99	0.15	-0.23	65,65,65,65	0
7	CA	A	2006	1/1	0.99	0.18	-0.38	38,38,38,38	0
7	CA	C	2006	1/1	0.97	0.13	-0.86	69,69,69,69	0
7	CA	A	2004	1/1	0.98	0.12	-1.02	49,49,49,49	0
7	CA	A	2005	1/1	0.99	0.15	-1.07	40,40,40,40	0
7	CA	C	2004	1/1	0.91	0.10	-1.20	111,111,111,111	0
8	MN	D	2003	1/1	0.98	0.17	-1.55	104,104,104,104	0
7	CA	C	2005	1/1	0.97	0.08	-2.39	90,90,90,90	0
9	NAG	B	3099	14/15	0.90	0.35	-	114,153,183,188	0
6	SO4	A	1456	5/5	0.93	0.17	-	75,98,98,117	0

6.5 Other polymers (i)

There are no such residues in this entry.