



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 21, 2016 – 04:35 AM EDT

PDB ID : 4Z7O
Title : Integrin alphaIIb beta3 in complex with AGDV peptide
Authors : Lin, F.Y.; Zhu, J.; Springer, T.A.
Deposited on : 2015-04-07
Resolution : 2.85 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:

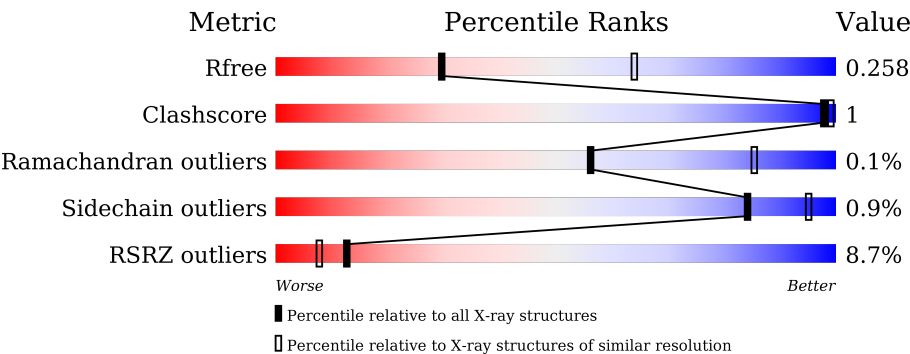
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

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 2.85 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.



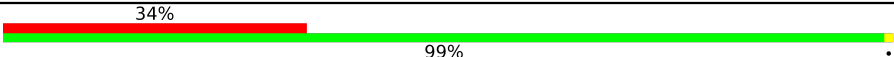
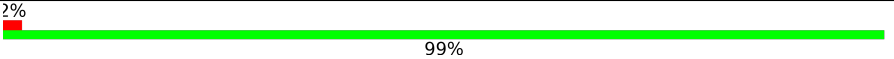

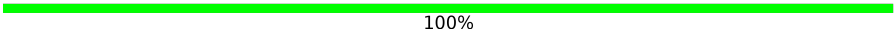
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	455	<div><div></div><div>96%</div><div></div></div>
1	C	455	<div><div>2%</div><div></div><div>96%</div><div></div></div>
2	B	469	<div><div>5%</div><div></div><div>94%</div><div>5%</div></div>
2	D	469	<div><div>9%</div><div></div><div>97%</div><div></div></div>
3	E	221	<div><div>30%</div><div></div><div>95%</div><div></div></div>
3	H	221	<div><div>9%</div><div></div><div>94%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
4	F	214	
4	L	214	
5	G	4	
5	I	4	

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	SO4	A	501	-	-	-	X
6	SO4	C	501	-	-	-	X
8	MN	B	2002	-	-	-	X
8	MN	D	2002	-	-	-	X
8	MN	D	2003	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 41839 atoms, of which 20230 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
			6886	2237	3369	607	665	8			
1	C	453	Total	C	H	N	O	S	0	1	0
			6796	2212	3315	600	661	8			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	464	Total	C	H	N	O	S	0	1	0
			7066	2230	3484	612	707	33			
2	D	469	Total	C	H	N	O	S	0	0	0
			7140	2248	3528	617	713	34			

- Molecule 3 is a protein called Monoclonal antibody 10E5 Fab heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	216	Total	C	H	N	O	S	0	0	0
			3242	1041	1600	266	329	6			
3	H	216	Total	C	H	N	O	S	0	0	0
			3243	1041	1601	266	329	6			

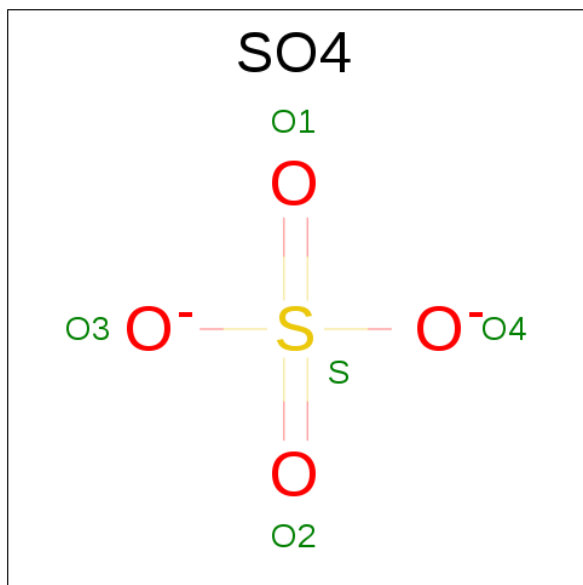
- Molecule 4 is a protein called Monoclonal antibody 10E5 Fab light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	214	Total	C	H	N	O	S	0	0	0
			3190	1019	1553	268	341	9			
4	L	214	Total	C	H	N	O	S	0	0	0
			3191	1019	1554	268	341	9			

- Molecule 5 is a protein called Tetrapeptide ALA-GLY-ASP-VAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	4	Total	C	H	N	O	0	0	0
			45	14	20	4	7			
5	I	4	Total	C	H	N	O	0	0	0
			45	14	20	4	7			

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

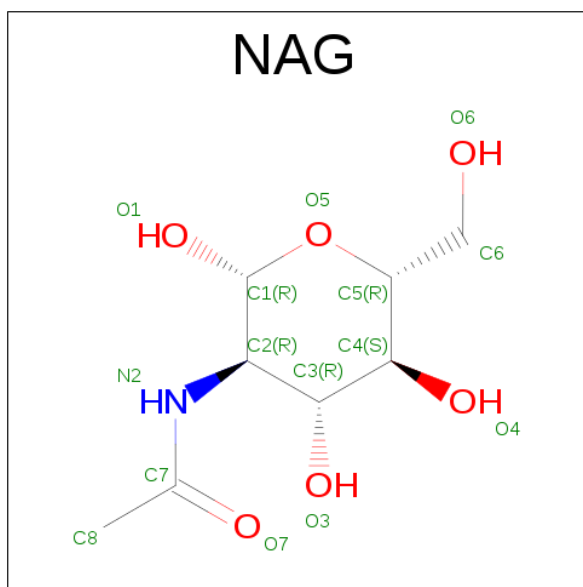
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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).

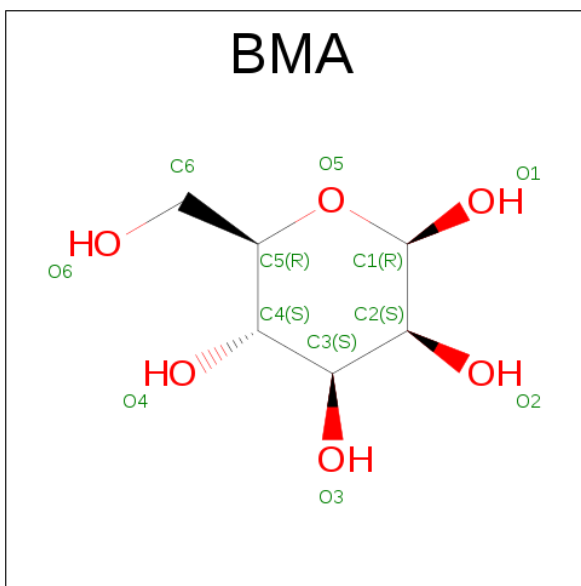
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	3	Total	Mn	0	0
			3	3		
8	D	3	Total	Mn	0	0
			3	3		

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



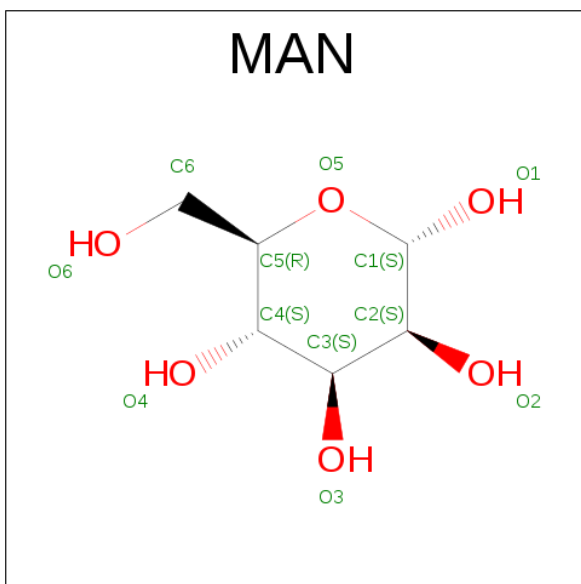
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
9	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
9	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
9	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
9	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
9	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
9	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
9	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
9	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
9	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 10 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	0	0
			20	6	9	5		
10	D	1	Total	C	H	O	0	0
			21	6	10	5		

- Molecule 11 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	H	O	0	0
			22	6	11	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	H	O	0	0
			22	6	11	5		
11	D	1	Total	C	H	O	0	0
			22	6	11	5		

- 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.

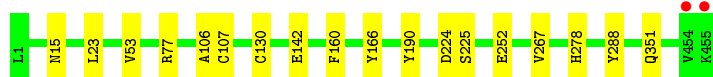
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	265	Total	O	0	0
			265	265		
13	B	117	Total	O	0	0
			117	117		
13	C	84	Total	O	0	0
			84	84		
13	D	64	Total	O	0	0
			64	64		
13	E	5	Total	O	0	0
			5	5		
13	F	9	Total	O	0	0
			9	9		
13	H	22	Total	O	0	0
			22	22		
13	L	16	Total	O	0	0
			16	16		
13	G	2	Total	O	0	0
			2	2		

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 ($\text{RSRZ} > 2$). 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.

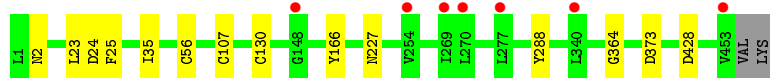
• Molecule 1: Integrin alpha-IIb

Chain A:  96%



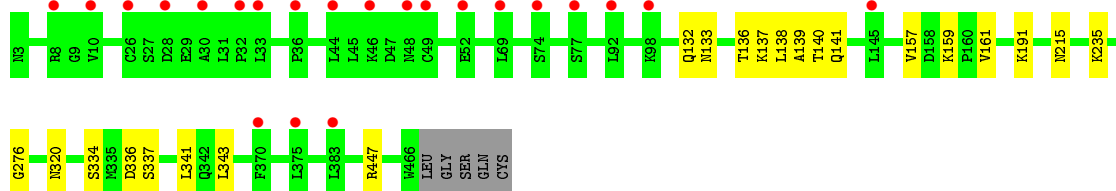
• Molecule 1: Integrin alpha-IIb

Chain C:  96%



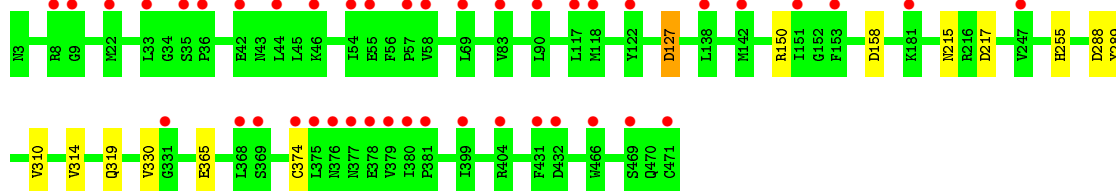
• Molecule 2: Integrin beta-3

Chain B:  94%



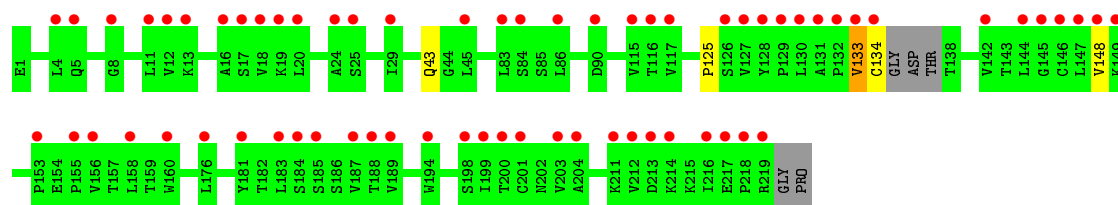
• Molecule 2: Integrin beta-3

Chain D:  97%

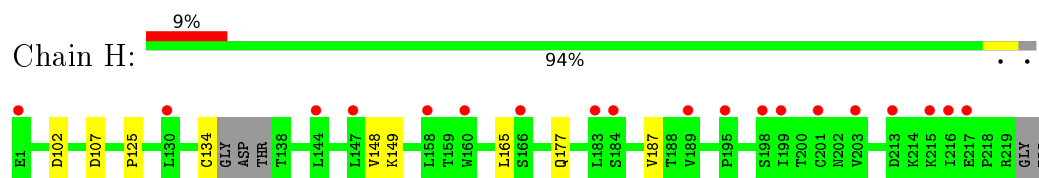


• Molecule 3: Monoclonal antibody 10E5 Fab heavy chain

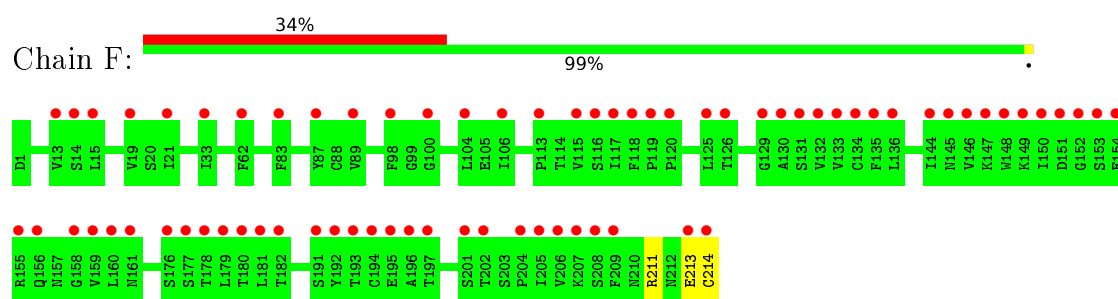
Chain E:  95%



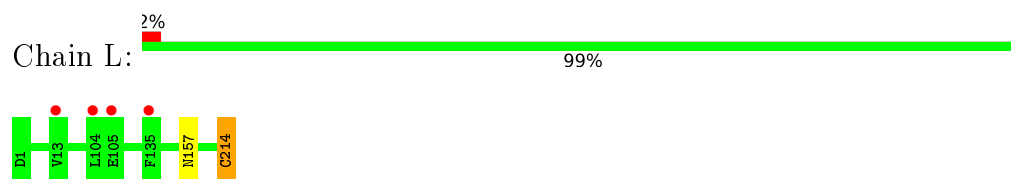
- Molecule 3: Monoclonal antibody 10E5 Fab heavy chain



- Molecule 4: Monoclonal antibody 10E5 Fab light chain



- Molecule 4: Monoclonal antibody 10E5 Fab light chain



- Molecule 5: Tetrapeptide ALA-GLY-ASP-VAL



There are no outlier residues recorded for this chain.

- Molecule 5: Tetrapeptide ALA-GLY-ASP-VAL



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	259.92Å 144.52Å 104.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 2.85 49.03 – 2.85	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.03-2.85) 84.1 (49.03-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.10 _2142: ???)	Depositor
R, R_{free}	0.223 , 0.257 0.223 , 0.258	Depositor DCC
R_{free} test set	1699 reflections (2.18%)	DCC
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 92354 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	41839	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: 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	0.29	0/3629	0.44	0/4944
1	C	0.26	0/3581	0.42	0/4880
2	B	0.26	0/3651	0.43	0/4950
2	D	0.26	0/3678	0.41	0/4986
3	E	0.25	0/1684	0.42	0/2305
3	H	0.24	0/1684	0.43	0/2305
4	F	0.25	0/1673	0.41	0/2269
4	L	0.25	0/1673	0.42	0/2269
5	G	0.19	0/24	0.45	0/30
5	I	0.25	0/24	0.48	0/30
All	All	0.26	0/21301	0.42	0/28968

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	3517	3369	3370	10	0
1	C	3481	3315	3315	8	0
2	B	3582	3484	3495	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3612	3528	3526	6	0
3	E	1642	1600	1600	3	0
3	H	1642	1601	1600	6	0
4	F	1637	1553	1553	1	0
4	L	1637	1554	1553	2	0
5	G	25	20	20	0	0
5	I	25	20	20	0	0
6	A	5	0	0	0	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	70	67	62	1	0
9	D	70	67	62	0	0
10	B	11	9	8	0	0
10	D	11	10	9	0	0
11	B	22	22	20	0	0
11	D	11	11	10	0	0
12	C	1	0	0	0	0
13	A	265	0	0	5	1
13	B	117	0	0	1	0
13	C	84	0	0	4	1
13	D	64	0	0	1	0
13	E	5	0	0	0	0
13	F	9	0	0	0	0
13	G	2	0	0	0	0
13	H	22	0	0	1	0
13	L	16	0	0	1	0
All	All	21609	20230	20223	44	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 1.

All (44) 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)
1:A:351:GLN:OE1	13:A:601:HOH:O	2.13	0.67
1:A:15[B]:ASN:OD1	13:A:602:HOH:O	2.15	0.65
4:L:157:ASN:OD1	13:L:401:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ASN:ND2	9:B:2005:NAG:O7	2.37	0.56
1:A:142:GLU:OE1	13:A:603:HOH:O	2.18	0.56
1:A:278[B]:HIS:NE2	13:A:614:HOH:O	2.34	0.53
1:C:24:ASP:OD1	1:C:25:PHE:N	2.41	0.52
1:C:428:ASP:OD2	13:C:601:HOH:O	2.19	0.50
3:H:107:ASP:O	13:H:301:HOH:O	2.20	0.49
1:A:224:ASP:OD1	1:A:225:SER:N	2.40	0.48
3:H:149:LYS:NZ	3:H:177:GLN:OE1	2.38	0.48
2:B:133:ASN:OD1	2:B:137:LYS:HG3	2.14	0.47
1:C:373:ASP:O	13:C:602:HOH:O	2.20	0.47
1:A:77:ARG:NH2	3:H:102:ASP:OD2	2.43	0.47
2:B:159:LYS:O	2:B:161:VAL:N	2.47	0.47
2:B:235:LYS:NZ	2:B:276:GLY:O	2.48	0.47
2:B:138:LEU:O	2:B:141:GLN:N	2.49	0.46
1:C:107:CYS:HA	1:C:130:CYS:HA	1.98	0.46
1:C:364:GLY:N	13:C:602:HOH:O	2.43	0.46
2:B:138:LEU:HA	2:B:341:LEU:CD1	2.46	0.45
4:F:211:ARG:O	4:F:213:GLU:N	2.47	0.45
2:D:127:ASP:N	2:D:127:ASP:OD1	2.50	0.45
3:H:165:LEU:HD21	3:H:187:VAL:HG21	2.00	0.44
1:C:227:ASN:ND2	13:C:613:HOH:O	2.49	0.44
2:D:217:ASP:OD2	2:D:255:HIS:NE2	2.50	0.44
1:A:160:PHE:O	13:A:605:HOH:O	2.21	0.44
1:A:53:VAL:HG21	1:A:106:ALA:CB	2.47	0.44
2:B:138:LEU:O	2:B:140:THR:N	2.51	0.43
2:D:288:ASP:OD1	2:D:289:TYR:N	2.43	0.43
1:C:35:ILE:O	1:C:56:CYS:N	2.46	0.43
3:E:43:GLN:N	3:E:43:GLN:OE1	2.48	0.43
3:E:125:PRO:HB2	3:E:148:VAL:HG13	2.01	0.43
3:H:125:PRO:HB2	3:H:148:VAL:HG13	2.01	0.43
1:C:2:ASN:N	1:C:2:ASN:OD1	2.51	0.42
2:D:310:VAL:HB	2:D:314:VAL:HG23	2.02	0.42
2:B:133:ASN:OD1	2:B:137:LYS:HE3	2.20	0.42
2:D:150:ARG:NH1	13:D:2111:HOH:O	2.44	0.42
2:B:334:SER:O	2:B:336:ASP:N	2.49	0.42
2:B:191:LYS:NZ	13:B:2119:HOH:O	2.49	0.41
1:A:107:CYS:HA	1:A:130:CYS:HA	2.02	0.41
2:D:319:GLN:HA	2:D:330:VAL:HG21	2.03	0.40
3:H:134:CYS:HB2	4:L:214:CYS:OXT	2.21	0.40
3:E:133:VAL:O	3:E:134:CYS:SG	2.80	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:833:HOH:O	13:C:650:HOH:O[1_554]	2.14	0.06

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	458/455 (101%)	432 (94%)	26 (6%)	0	100	100
1	C	452/455 (99%)	429 (95%)	23 (5%)	0	100	100
2	B	463/469 (99%)	435 (94%)	26 (6%)	2 (0%)	39	71
2	D	467/469 (100%)	438 (94%)	28 (6%)	1 (0%)	52	82
3	E	212/221 (96%)	198 (93%)	13 (6%)	1 (0%)	34	67
3	H	212/221 (96%)	202 (95%)	10 (5%)	0	100	100
4	F	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
4	L	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
5	G	2/4 (50%)	2 (100%)	0	0	100	100
5	I	2/4 (50%)	2 (100%)	0	0	100	100
All	All	2692/2726 (99%)	2545 (94%)	143 (5%)	4 (0%)	56	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	133	VAL
2	B	139	ALA
2	D	374	CYS
2	B	157	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	368/363 (101%)	362 (98%)	6 (2%)	70	90
1	C	362/363 (100%)	359 (99%)	3 (1%)	86	96
2	B	411/415 (99%)	405 (98%)	6 (2%)	72	91
2	D	415/415 (100%)	411 (99%)	4 (1%)	82	94
3	E	187/190 (98%)	187 (100%)	0	100	100
3	H	187/190 (98%)	187 (100%)	0	100	100
4	F	188/188 (100%)	187 (100%)	1 (0%)	92	97
4	L	188/188 (100%)	187 (100%)	1 (0%)	92	97
5	G	2/2 (100%)	2 (100%)	0	100	100
5	I	2/2 (100%)	2 (100%)	0	100	100
All	All	2310/2316 (100%)	2289 (99%)	21 (1%)	84	95

All (21) 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	252	GLU
1	A	267	VAL
1	A	288	TYR
2	B	132	GLN
2	B	136	THR
2	B	215	ASN
2	B	337	SER
2	B	343	LEU
2	B	447	ARG
1	C	23	LEU
1	C	166	TYR
1	C	288	TYR
2	D	127	ASP

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Mol	Chain	Res	Type
2	D	158	ASP
2	D	215	ASN
2	D	365	GLU
4	F	214	CYS
4	L	214	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	132	GLN
2	D	280	HIS

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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 15 are monoatomic - leaving 18 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	501	-	4,4,4	0.27	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	B	2004	2	14,14,15	0.55	0	15,19,21	0.70	1 (6%)
9	NAG	B	2005	9,2	14,14,15	0.38	0	15,19,21	0.57	0
9	NAG	B	2006	9,10	14,14,15	0.23	0	15,19,21	0.40	0
10	BMA	B	2007	9,11	11,11,12	0.61	0	15,15,17	1.06	0
11	MAN	B	2008	10	11,11,12	0.48	0	15,15,17	0.90	1 (6%)
11	MAN	B	2009	10	11,11,12	0.62	0	15,15,17	1.25	2 (13%)
9	NAG	B	2010	9,2	14,14,15	0.48	0	15,19,21	0.37	0
9	NAG	B	2011	9	14,14,15	0.16	0	15,19,21	0.37	0
6	SO4	C	501	-	4,4,4	0.25	0	6,6,6	0.07	0
9	NAG	D	2004	2	14,14,15	0.36	0	15,19,21	0.50	0
9	NAG	D	2005	9,2	14,14,15	0.57	0	15,19,21	0.42	0
9	NAG	D	2006	9,10	14,14,15	0.34	0	15,19,21	0.45	0
10	BMA	D	2007	9,11	11,11,12	0.68	0	15,15,17	0.82	0
11	MAN	D	2008	10	11,11,12	0.51	0	15,15,17	1.03	2 (13%)
9	NAG	D	2009	9,2	14,14,15	0.41	0	15,19,21	0.47	0
9	NAG	D	2010	9	14,14,15	0.28	0	15,19,21	0.37	0
6	SO4	L	301	-	4,4,4	0.26	0	6,6,6	0.06	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	501	-	-	0/0/0/0	0/0/0/0
9	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
9	NAG	B	2005	9,2	-	0/6/23/26	0/1/1/1
9	NAG	B	2006	9,10	-	0/6/23/26	0/1/1/1
10	BMA	B	2007	9,11	-	0/2/19/22	0/1/1/1
11	MAN	B	2008	10	-	0/2/19/22	0/1/1/1
11	MAN	B	2009	10	-	0/2/19/22	0/1/1/1
9	NAG	B	2010	9,2	-	0/6/23/26	0/1/1/1
9	NAG	B	2011	9	-	0/6/23/26	0/1/1/1
6	SO4	C	501	-	-	0/0/0/0	0/0/0/0
9	NAG	D	2004	2	-	0/6/23/26	0/1/1/1
9	NAG	D	2005	9,2	-	0/6/23/26	0/1/1/1
9	NAG	D	2006	9,10	-	0/6/23/26	0/1/1/1
10	BMA	D	2007	9,11	-	0/2/19/22	0/1/1/1
11	MAN	D	2008	10	-	0/2/19/22	0/1/1/1
9	NAG	D	2009	9,2	-	0/6/23/26	0/1/1/1
9	NAG	D	2010	9	-	0/6/23/26	0/1/1/1
6	SO4	L	301	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
11	B	2009	MAN	O2-C2-C3	-2.26	105.63	110.19
11	D	2008	MAN	O2-C2-C3	-2.18	105.79	110.19
11	B	2008	MAN	O2-C2-C3	-2.06	106.03	110.19
9	B	2004	NAG	C1-O5-C5	2.36	115.60	112.14
11	D	2008	MAN	C1-O5-C5	2.66	116.05	112.14
11	B	2009	MAN	C1-O5-C5	3.54	117.35	112.14

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
9	B	2005	NAG	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	455/455 (100%)	0.29	2 (0%) 93 92	47, 67, 100, 194	0
1	C	453/455 (99%)	0.41	7 (1%) 76 73	60, 95, 134, 174	0
2	B	464/469 (98%)	0.38	22 (4%) 35 29	52, 103, 182, 241	0
2	D	469/469 (100%)	0.64	43 (9%) 11 7	73, 128, 183, 256	0
3	E	216/221 (97%)	1.51	66 (30%) 1 0	113, 178, 252, 271	0
3	H	216/221 (97%)	0.40	19 (8%) 12 7	74, 130, 191, 221	0
4	F	214/214 (100%)	1.55	72 (33%) 0 0	115, 171, 252, 305	0
4	L	214/214 (100%)	0.17	4 (1%) 70 66	79, 118, 150, 227	0
5	G	4/4 (100%)	0.58	0 100 100	60, 84, 89, 93	0
5	I	4/4 (100%)	0.64	0 100 100	91, 100, 111, 123	0
All	All	2709/2726 (99%)	0.58	235 (8%) 13 8	47, 112, 207, 305	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	193	THR	16.9
4	F	181	LEU	12.2
4	F	180	THR	9.1
1	A	455	LYS	9.0
3	E	144	LEU	8.9
3	E	142	VAL	7.8
3	E	189	VAL	7.6
3	E	148	VAL	7.6
3	E	212	VAL	6.8
3	E	19	LYS	6.6
3	E	132	PRO	6.4
4	F	132	VAL	6.0
4	F	147	LYS	6.0

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Mol	Chain	Res	Type	RSRZ
4	F	130	ALA	5.9
4	F	208	SER	5.8
2	B	33	LEU	5.8
4	F	192	TYR	5.6
4	F	214	CYS	5.6
4	F	206	VAL	5.6
3	E	127	VAL	5.5
4	F	133	VAL	5.4
4	F	194	CYS	5.4
2	D	55	GLU	5.4
3	E	130	LEU	5.3
3	E	145	GLY	5.2
4	F	148	TRP	5.2
3	E	17	SER	5.2
3	E	128	TYR	5.2
4	F	150	ILE	5.2
4	F	195	GLU	5.2
4	F	159	VAL	5.2
2	D	375	LEU	5.1
3	E	183	LEU	5.1
4	F	134	CYS	5.1
2	D	35	SER	5.1
3	E	149	LYS	5.0
2	D	22	MET	5.0
3	E	194	TRP	5.0
2	B	36	PRO	4.9
2	D	44	LEU	4.8
4	F	117	ILE	4.8
2	D	469	SER	4.7
1	C	340	LEU	4.7
4	F	207	LYS	4.7
3	E	147	LEU	4.6
4	F	146	VAL	4.6
4	F	205	ILE	4.6
3	E	204	ALA	4.5
3	E	156	VAL	4.4
2	D	376	ASN	4.4
4	F	149	LYS	4.4
4	F	155	ARG	4.4
3	E	11	LEU	4.3
3	H	215	LYS	4.3
2	D	151	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
3	E	211	LYS	4.3
3	E	216	ILE	4.3
3	E	131	ALA	4.2
4	F	202	THR	4.2
4	F	179	LEU	4.2
4	F	115	VAL	4.1
2	B	48	ASN	4.1
3	E	199	ILE	4.1
4	F	116	SER	4.1
4	F	118	PHE	4.1
4	F	135	PHE	4.1
3	E	134	CYS	4.0
4	F	161	ASN	4.0
2	D	58	VAL	4.0
3	E	203	VAL	3.9
2	D	379	VAL	3.9
2	D	83	VAL	3.9
4	F	158	GLY	3.8
3	E	133	VAL	3.8
3	E	117	VAL	3.8
1	C	269	ILE	3.7
3	E	83	LEU	3.7
4	F	119	PRO	3.7
4	F	209	PHE	3.7
4	F	152	GLY	3.7
4	F	153	SER	3.7
4	F	176	SER	3.7
3	H	216	ILE	3.6
4	F	83	PHE	3.6
3	H	158	LEU	3.6
4	F	196	ALA	3.6
2	D	378	GLU	3.5
2	B	77	SER	3.5
4	F	104	LEU	3.5
2	D	142	MET	3.5
3	H	130	LEU	3.5
3	E	198	SER	3.4
2	D	181	LYS	3.4
3	H	144	LEU	3.4
3	E	176	LEU	3.4
3	E	12	VAL	3.4
4	F	156	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
3	E	155	PRO	3.4
4	F	177	SER	3.3
2	D	377	ASN	3.3
3	E	20	LEU	3.3
3	H	198	SER	3.3
3	E	129	PRO	3.3
3	E	200	THR	3.2
4	F	113	PRO	3.2
2	B	28	ASP	3.2
4	F	178	THR	3.2
4	F	131	SER	3.2
2	B	383	LEU	3.1
3	E	153	PRO	3.1
4	F	125	LEU	3.1
4	F	204	PRO	3.1
2	D	153	PHE	3.0
3	E	219	ARG	3.0
3	E	146	CYS	3.0
3	E	4	LEU	3.0
2	D	118	MET	3.0
3	H	201	CYS	3.0
2	D	368	LEU	2.9
3	E	18	VAL	2.9
3	E	214	LYS	2.9
3	E	217	GLU	2.9
3	E	158	LEU	2.9
2	D	381	PRO	2.9
4	L	104	LEU	2.9
3	E	115	VAL	2.9
4	F	129	GLY	2.8
4	F	197	THR	2.8
2	D	122	TYR	2.8
4	F	145	ASN	2.8
4	F	213	GLU	2.8
2	B	92	LEU	2.8
3	E	213	ASP	2.8
1	A	454	VAL	2.8
3	E	126	SER	2.8
4	F	144	ILE	2.8
3	H	217	GLU	2.8
2	D	380	ILE	2.7
4	F	160	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	191	SER	2.7
4	F	126	THR	2.7
2	D	431	PHE	2.7
1	C	148	GLY	2.7
2	B	52	GLU	2.7
3	H	199	ILE	2.6
3	H	203	VAL	2.6
2	D	54	ILE	2.6
2	D	369	SER	2.6
3	E	187	VAL	2.6
2	D	46	LYS	2.6
2	D	9	GLY	2.6
2	B	26	CYS	2.6
2	D	42	GLU	2.6
3	E	116	THR	2.5
4	L	13	VAL	2.5
3	E	5	GLN	2.5
2	B	30	ALA	2.5
2	D	33	LEU	2.5
2	D	466	TRP	2.5
1	C	277	LEU	2.5
2	D	57	PRO	2.4
3	E	184	SER	2.4
4	F	120	PRO	2.4
2	B	49	CYS	2.4
2	D	432	ASP	2.4
3	E	218	PRO	2.4
3	H	189	VAL	2.4
4	F	13	VAL	2.4
4	F	21	ILE	2.4
2	B	370	PHE	2.4
2	D	331	GLY	2.4
2	D	399	ILE	2.4
3	E	25	SER	2.4
4	L	105	GLU	2.3
2	D	36	PRO	2.3
4	F	182	THR	2.3
4	F	100	GLY	2.3
1	C	453	VAL	2.3
3	E	188	THR	2.3
3	E	160	TRP	2.3
4	F	14	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	32	PRO	2.3
4	F	98	PHE	2.3
4	F	19	VAL	2.3
3	H	1	GLU	2.3
4	F	151	ASP	2.3
2	B	145	LEU	2.3
3	E	45	LEU	2.3
4	F	33	ILE	2.3
1	C	254	VAL	2.3
2	B	10	VAL	2.3
4	F	136	LEU	2.3
2	D	90	LEU	2.3
3	E	24	ALA	2.3
2	D	247	VAL	2.2
3	E	185	SER	2.2
1	C	270	LEU	2.2
2	D	69	LEU	2.2
4	F	106	ILE	2.2
2	D	8	ARG	2.2
2	B	46	LYS	2.2
2	B	98	LYS	2.2
2	D	471	CYS	2.2
3	H	183	LEU	2.2
3	H	184	SER	2.2
2	B	8	ARG	2.2
3	E	201	CYS	2.2
2	D	404	ARG	2.2
3	H	160	TRP	2.1
4	F	62	PHE	2.1
3	H	213	ASP	2.1
4	L	135	PHE	2.1
2	D	117	LEU	2.1
3	E	13	LYS	2.1
4	F	15	LEU	2.1
4	F	154	GLU	2.1
3	E	90	ASP	2.1
2	D	138	LEU	2.1
3	E	181	TYR	2.1
3	H	147	LEU	2.1
2	D	374	CYS	2.1
4	F	201	SER	2.1
4	F	87	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	44	LEU	2.0
3	H	166	SER	2.0
3	E	16	ALA	2.0
2	B	69	LEU	2.0
2	B	375	LEU	2.0
3	E	86	LEU	2.0
3	E	29	ILE	2.0
3	H	195	PRO	2.0
3	E	8	GLY	2.0
2	B	74	SER	2.0
3	E	84	SER	2.0
4	F	89	VAL	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](#)

There are no carbohydrates in this entry.

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, 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
8	MN	D	2002	1/1	0.62	0.57	5.16	431,431,431,431	0
8	MN	D	2003	1/1	0.65	0.36	4.36	216,216,216,216	0
6	SO4	C	501	5/5	0.78	0.38	3.68	184,193,196,198	0
8	MN	B	2002	1/1	0.49	0.33	3.46	361,361,361,361	0
6	SO4	A	501	5/5	0.95	0.31	3.24	118,124,133,142	0
7	CA	C	506	1/1	0.92	0.20	1.17	108,108,108,108	0
8	MN	B	2003	1/1	0.95	0.25	0.64	90,90,90,90	0
8	MN	B	2001	1/1	0.97	0.24	0.61	57,57,57,57	0
7	CA	A	503	1/1	0.97	0.18	0.31	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	CA	C	503	1/1	0.76	0.22	0.25	197,197,197,197	0
7	CA	C	505	1/1	0.79	0.16	0.06	99,99,99,99	0
12	CL	C	502	1/1	0.82	0.25	0.03	85,85,85,85	0
9	NAG	B	2010	14/15	0.82	0.23	-0.08	106,133,156,160	0
7	CA	A	502	1/1	0.95	0.14	-0.23	77,77,77,77	0
8	MN	D	2001	1/1	0.81	0.20	-0.36	121,121,121,121	0
7	CA	A	505	1/1	0.96	0.21	-0.37	66,66,66,66	0
6	SO4	L	301	5/5	0.90	0.13	-0.44	151,154,159,161	0
7	CA	A	504	1/1	0.91	0.19	-0.52	57,57,57,57	0
7	CA	C	504	1/1	0.72	0.15	-0.74	168,168,168,168	0
9	NAG	D	2009	14/15	0.88	0.23	-0.87	120,141,169,170	0
9	NAG	D	2005	14/15	0.90	0.14	-1.44	94,125,155,157	0
11	MAN	B	2009	11/12	0.78	0.18	-	103,138,164,166	0
9	NAG	D	2006	14/15	0.83	0.20	-	127,139,163,173	0
10	BMA	B	2007	11/12	0.84	0.14	-	98,134,169,169	0
11	MAN	D	2008	11/12	0.89	0.28	-	129,155,171,179	0
9	NAG	B	2006	14/15	0.92	0.20	-	87,116,134,159	0
11	MAN	B	2008	11/12	0.92	0.13	-	115,133,147,159	0
9	NAG	B	2005	14/15	0.93	0.18	-	69,90,110,110	0
9	NAG	B	2004	14/15	0.89	0.27	-	118,139,166,167	0
9	NAG	B	2011	14/15	0.88	0.25	-	135,155,178,186	0
9	NAG	D	2004	14/15	0.83	0.23	-	114,142,170,175	0
10	BMA	D	2007	11/12	0.78	0.18	-	118,147,176,179	0
9	NAG	D	2010	14/15	0.84	0.24	-	119,154,187,187	0

6.5 Other polymers [i](#)

There are no such residues in this entry.