



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2016 – 03:16 AM EDT

PDB ID : 5HDB
Title : Integrin alphaIIb beta3 in complex with Ro-435054
Authors : Lin, F.Y.
Deposited on : 2016-01-05
Resolution : 2.70 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

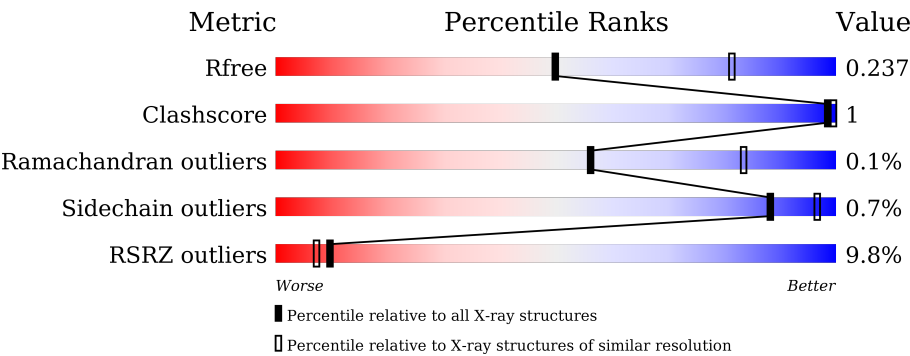
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



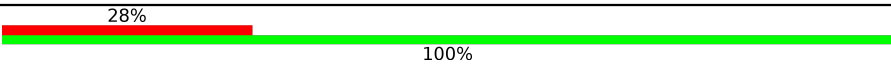
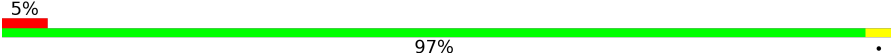
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	454	<div><div></div><div>97%</div><div></div></div>
1	C	454	<div><div>2%</div><div></div><div>96%</div><div></div></div>
2	B	471	<div><div>10%</div><div></div><div>96%</div><div></div></div>
2	D	471	<div><div>8%</div><div></div><div>97%</div><div></div></div>
3	E	219	<div><div>37%</div><div></div><div>95%</div><div></div></div>
3	H	219	<div><div>9%</div><div></div><div>97%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
4	F	214	
4	L	214	

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
5	SO4	A	501	-	-	-	X
5	SO4	A	502	-	-	-	X
5	SO4	C	501	-	-	-	X
6	GOL	A	504	-	-	-	X
7	CA	A	506	-	-	-	X
7	CA	A	507	-	-	-	X
7	CA	D	503	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 42246 atoms, of which 20351 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	0	9	0
			6908	2242	3381	610	667	8			
1	C	453	Total	C	H	N	O	S	0	6	0
			6840	2224	3338	604	666	8			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	466	Total	C	H	N	O	S	24	8	0
			7184	2260	3556	619	715	34			
2	D	471	Total	C	H	N	O	S	28	2	0
			7182	2260	3551	620	716	35			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	214	Total	C	H	N	O	S	0	0	0
			3221	1035	1590	264	326	6			
3	H	216	Total	C	H	N	O	S	0	0	0
			3242	1041	1600	266	329	6			

- Molecule 4 is a protein called Monoclonal antibody 10E5 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
			3190	1019	1553	268	341	9			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- 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		

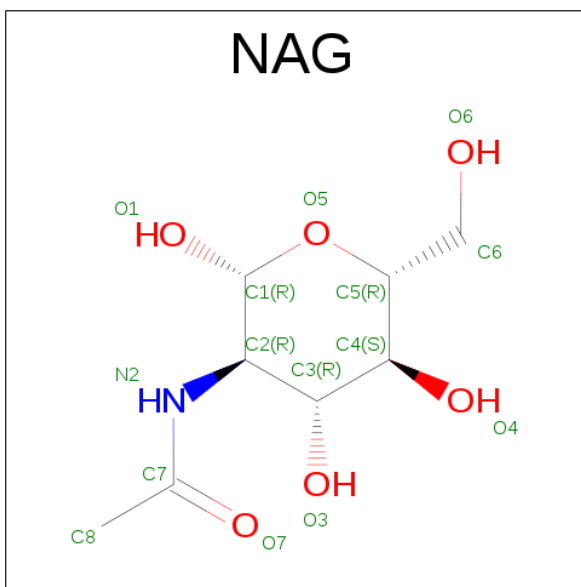
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	4	Total	Ca	0	0
			4	4		
7	D	2	Total	Ca	0	0
			2	2		
7	C	4	Total	Ca	0	0
			4	4		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

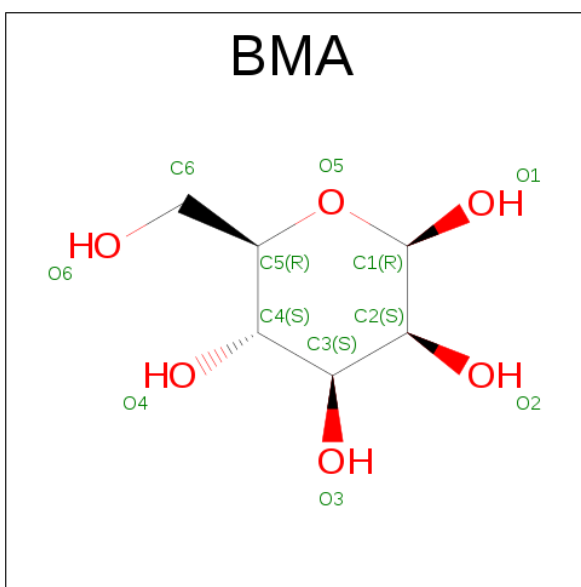
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		

- Molecule 9 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



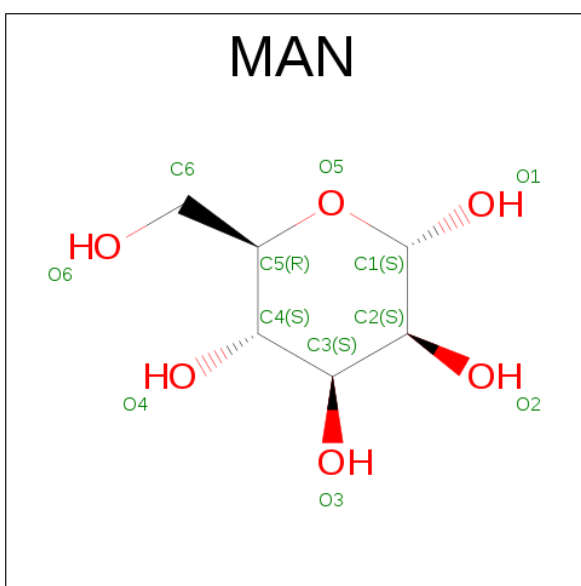
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
9	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
9	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
9	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
9	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
9	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
9	D	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
9	D	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
9	D	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
9	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 10 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	0	0
			19	6	8	5		
10	D	1	Total	C	H	O	0	0
			20	6	9	5		

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



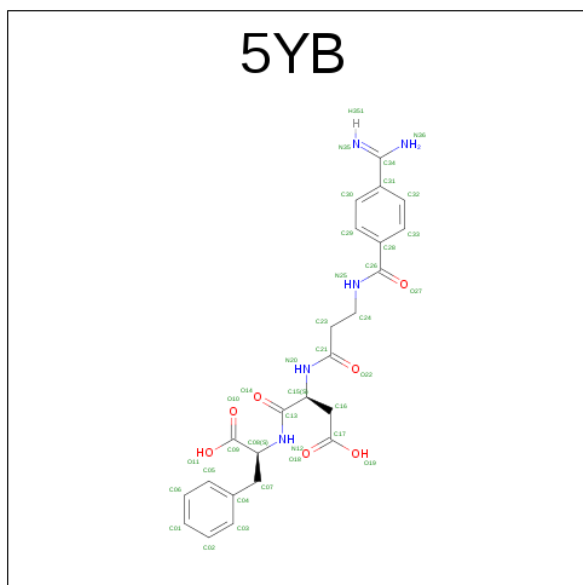
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	H	O	0	0
			21	6	10	5		
11	B	1	Total	C	H	O	0	0
			21	6	10	5		

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

- Molecule 12 is N-(4-carbamimidoylbenzoyl)-beta-alanyl-L-alpha-aspartyl-L-phenylalanine (three-letter code: 5YB) (formula: C₂₄H₂₇N₅O₇).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	H	N	O	0	0
			61	24	25	5	7		
12	D	1	Total	C	H	N	O	0	0
			61	24	25	5	7		

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	2	Total	Cl	0	0
			2	2		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	303	Total	O	0	0
			303	303		
14	B	175	Total	O	0	0
			175	175		

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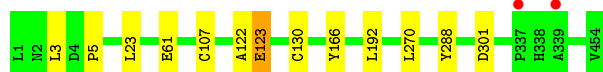
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	80	Total 80	O 80	0	0
14	D	96	Total 96	O 96	0	0
14	E	10	Total 10	O 10	0	0
14	F	13	Total 13	O 13	0	0
14	H	24	Total 24	O 24	0	0
14	L	41	Total 41	O 41	0	0

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:  97%



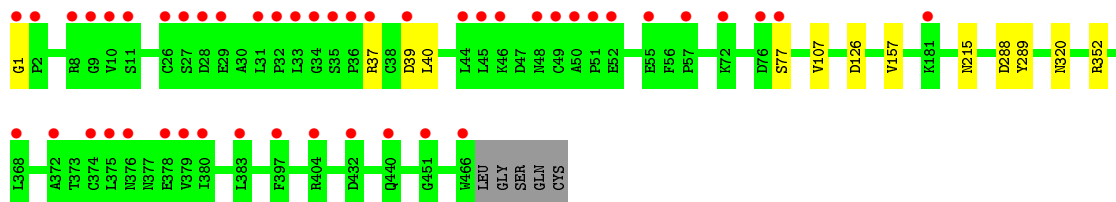
- Molecule 1: Integrin alpha-IIb

Chain C:  96%



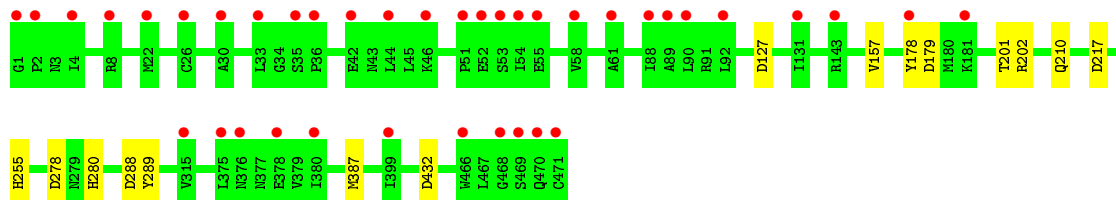
- Molecule 2: Integrin beta-3

Chain B:  96%



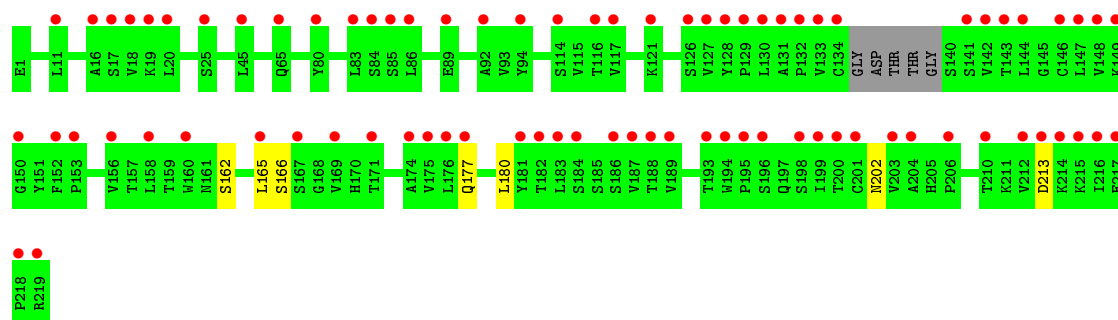
- Molecule 2: Integrin beta-3

Chain D:  97%

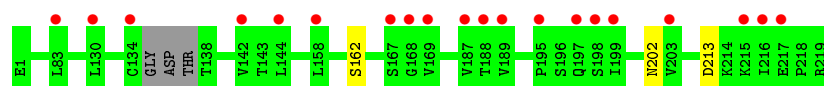


- Molecule 3: Monoclonal antibody 10E5 heavy chain

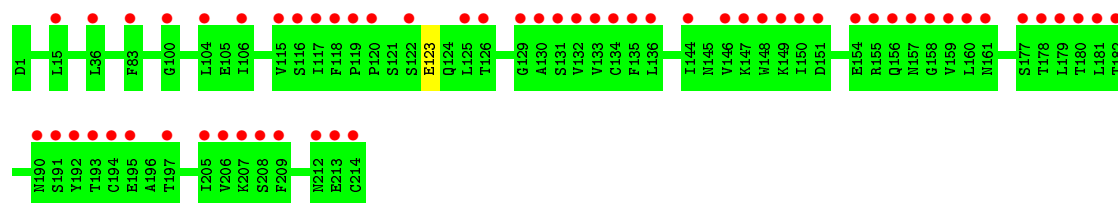
Chain E:  95%



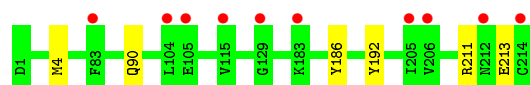
- Molecule 3: Monoclonal antibody 10E5 heavy chain



- Molecule 4: Monoclonal antibody 10E5 light chain



- Molecule 4: Monoclonal antibody 10E5 light 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	259.35Å 144.44Å 104.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.01 – 2.70 49.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.01-2.70) 85.7 (49.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.212 , 0.237 0.211 , 0.237	Depositor DCC
R_{free} test set	1769 reflections (1.90%)	DCC
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 107062 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	42246	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, BMA, NAG, CL, CA, 5YB, 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	0.27	0/3651	0.44	0/4975
1	C	0.25	0/3618	0.43	0/4930
2	B	0.24	0/3726	0.42	0/5051
2	D	0.24	0/3710	0.41	0/5029
3	E	0.24	0/1673	0.43	0/2290
3	H	0.24	0/1684	0.43	0/2305
4	F	0.24	0/1673	0.41	0/2269
4	L	0.24	0/1673	0.43	0/2269
All	All	0.25	0/21408	0.43	0/29118

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 [i](#)

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	3527	3381	3365	5	0
1	C	3502	3338	3320	8	0
2	B	3628	3556	3525	6	0
2	D	3631	3551	3539	8	0
3	E	1631	1590	1590	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	1600	1600	2	0
4	F	1637	1553	1553	1	0
4	L	1637	1553	1553	3	0
5	A	15	0	0	0	0
5	C	10	0	0	0	0
5	L	5	0	0	0	0
6	A	6	8	8	0	0
7	A	4	0	0	0	0
7	B	1	0	0	0	0
7	C	4	0	0	0	0
7	D	2	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	B	70	62	62	1	0
9	D	70	62	62	0	0
10	B	11	8	8	0	0
10	D	11	9	9	0	0
11	B	22	20	20	0	0
11	D	11	10	10	0	0
12	B	36	25	24	1	0
12	D	36	25	24	1	0
13	C	2	0	0	0	0
14	A	303	0	0	1	1
14	B	175	0	0	3	0
14	C	80	0	0	1	1
14	D	96	0	0	4	0
14	E	10	0	0	0	0
14	F	13	0	0	0	0
14	H	24	0	0	0	0
14	L	41	0	0	0	0
All	All	21895	20351	20272	38	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 (38) 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:387:MET:O	14:D:2101:HOH:O	2.01	0.79
2:B:126[B]:ASP:OD1	14:B:2101:HOH:O	2.07	0.70
2:D:280:HIS:O	14:D:2102:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:ASP:OD2	14:C:601:HOH:O	2.16	0.61
1:A:301:ASP:OD2	14:A:601:HOH:O	2.17	0.60
2:B:1:GLY:O	14:B:2102:HOH:O	2.17	0.55
1:C:1:LEU:N	1:C:2:ASN:HA	2.25	0.51
1:C:224:ASP:OD1	1:C:225:SER:N	2.40	0.49
2:D:288:ASP:OD1	2:D:289:TYR:N	2.41	0.49
2:B:320:ASN:OD1	14:B:2103:HOH:O	2.20	0.48
2:D:178:TYR:CG	2:D:179:ASP:N	2.81	0.48
4:L:211:ARG:O	4:L:213:GLU:N	2.43	0.47
1:A:122:ALA:O	1:A:123:GLU:HB2	2.15	0.47
9:B:2009:NAG:O4	9:B:2010:NAG:H83	2.15	0.46
4:L:4:MET:HE1	4:L:90:GLN:HB3	1.97	0.46
2:B:288:ASP:OD1	2:B:289:TYR:N	2.44	0.46
2:D:210:GLN:OE1	14:D:2103:HOH:O	2.21	0.45
1:C:231:PHE:CE1	12:D:501:5YB:H321	2.51	0.45
2:B:107:VAL:O	2:B:352:ARG:NH2	2.46	0.45
2:D:201:THR:OG1	14:D:2104:HOH:O	2.21	0.45
4:L:186:TYR:O	4:L:192:TYR:OH	2.34	0.44
1:C:3:LEU:O	1:C:405:GLN:NE2	2.41	0.44
1:A:192:LEU:HD11	12:B:2011:5YB:H321	1.99	0.43
2:B:39:ASP:OD1	2:B:40:LEU:N	2.51	0.43
1:C:35:ILE:O	1:C:56:CYS:N	2.51	0.43
3:H:213:ASP:N	3:H:213:ASP:OD1	2.52	0.43
3:E:162:SER:N	3:E:202:ASN:OD1	2.52	0.43
3:E:165:LEU:HD12	3:E:166:SER:N	2.34	0.42
3:E:177:GLN:N	3:E:180:LEU:O	2.48	0.42
2:D:217:ASP:OD2	2:D:255:HIS:NE2	2.45	0.42
4:F:123:GLU:OE1	4:F:123:GLU:N	2.48	0.42
1:C:303:ARG:NH1	1:C:335:ARG:HD3	2.35	0.41
1:A:107:CYS:HA	1:A:130:CYS:HA	2.02	0.41
1:C:107:CYS:HA	1:C:130:CYS:HA	2.03	0.41
2:D:278:ASP:OD2	2:D:280:HIS:HB2	2.21	0.41
3:E:213:ASP:N	3:E:213:ASP:OD1	2.55	0.40
3:H:162:SER:N	3:H:202:ASN:OD1	2.48	0.40
1:A:3:LEU:O	1:A:5:PRO:HD3	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:882:HOH:O	14:C:678:HOH:O[1_554]	1.96	0.24

5.3 Torsion angles

5.3.1 Protein backbone

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	461/454 (102%)	441 (96%)	19 (4%)	1 (0%)	52	80
1	C	457/454 (101%)	433 (95%)	23 (5%)	1 (0%)	52	80
2	B	472/471 (100%)	451 (96%)	20 (4%)	1 (0%)	52	80
2	D	471/471 (100%)	453 (96%)	17 (4%)	1 (0%)	52	80
3	E	210/219 (96%)	199 (95%)	11 (5%)	0	100	100
3	H	212/219 (97%)	200 (94%)	12 (6%)	0	100	100
4	F	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
4	L	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
All	All	2707/2716 (100%)	2580 (95%)	123 (4%)	4 (0%)	56	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	C	123	GLU
2	D	157	VAL
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	370/362 (102%)	365 (99%)	5 (1%)	74	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	366/362 (101%)	362 (99%)	4 (1%)	80	94
2	B	420/416 (101%)	417 (99%)	3 (1%)	88	96
2	D	418/416 (100%)	415 (99%)	3 (1%)	88	96
3	E	186/189 (98%)	186 (100%)	0	100	100
3	H	187/189 (99%)	187 (100%)	0	100	100
4	F	188/188 (100%)	188 (100%)	0	100	100
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2323/2310 (101%)	2308 (99%)	15 (1%)	88	97

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	61	GLU
1	A	166	TYR
1	A	270	LEU
1	A	288	TYR
2	B	37	ARG
2	B	77	SER
2	B	215	ASN
1	C	23	LEU
1	C	166	TYR
1	C	272	SER
1	C	288	TYR
2	D	127	ASP
2	D	202	ARG
2	D	432	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 15 are monoatomic - leaving 24 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$
5	SO4	A	501	-	4,4,4	0.21	0	6,6,6	0.10	0
5	SO4	A	502	-	4,4,4	0.20	0	6,6,6	0.06	0
5	SO4	A	503	-	4,4,4	0.23	0	6,6,6	0.15	0
6	GOL	A	504	-	5,5,5	0.37	0	5,5,5	0.22	0
9	NAG	B	2003	2	14,14,15	0.27	0	15,19,21	0.35	0
9	NAG	B	2004	9,2	14,14,15	0.37	0	15,19,21	0.41	0
9	NAG	B	2005	9,10	14,14,15	0.23	0	15,19,21	0.39	0
10	BMA	B	2006	9,11	11,11,12	0.76	0	15,15,17	0.94	1 (6%)
11	MAN	B	2007	10	11,11,12	0.61	0	15,15,17	0.93	1 (6%)
11	MAN	B	2008	10	11,11,12	0.60	0	15,15,17	1.08	2 (13%)
9	NAG	B	2009	9,2	14,14,15	0.31	0	15,19,21	0.40	0
9	NAG	B	2010	9	14,14,15	0.25	0	15,19,21	0.55	0
12	5YB	B	2011	8	31,37,37	2.51	8 (25%)	39,49,49	1.16	3 (7%)
5	SO4	C	501	-	4,4,4	0.18	0	6,6,6	0.12	0
5	SO4	C	502	-	4,4,4	0.18	0	6,6,6	0.10	0
12	5YB	D	501	8	31,37,37	2.54	7 (22%)	39,49,49	1.14	3 (7%)
9	NAG	D	505	2	14,14,15	0.40	0	15,19,21	0.47	0
9	NAG	D	506	9,2	14,14,15	0.38	0	15,19,21	0.56	0
9	NAG	D	507	9,10	14,14,15	0.32	0	15,19,21	0.30	0
10	BMA	D	508	9,11	11,11,12	0.61	0	15,15,17	0.78	0
11	MAN	D	509	10	11,11,12	0.68	0	15,15,17	1.05	2 (13%)
9	NAG	D	510	9,2	14,14,15	0.35	0	15,19,21	0.35	0
9	NAG	D	511	9	14,14,15	0.11	0	15,19,21	0.41	0
5	SO4	L	301	-	4,4,4	0.20	0	6,6,6	0.09	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
5	SO4	A	501	-	-	0/0/0/0	0/0/0/0
5	SO4	A	502	-	-	0/0/0/0	0/0/0/0
5	SO4	A	503	-	-	0/0/0/0	0/0/0/0
6	GOL	A	504	-	-	0/4/4/4	0/0/0/0
9	NAG	B	2003	2	-	0/6/23/26	0/1/1/1
9	NAG	B	2004	9,2	-	0/6/23/26	0/1/1/1
9	NAG	B	2005	9,10	-	0/6/23/26	0/1/1/1
10	BMA	B	2006	9,11	-	0/2/19/22	0/1/1/1
11	MAN	B	2007	10	-	0/2/19/22	0/1/1/1
11	MAN	B	2008	10	-	0/2/19/22	0/1/1/1
9	NAG	B	2009	9,2	-	0/6/23/26	0/1/1/1
9	NAG	B	2010	9	-	0/6/23/26	0/1/1/1
12	5YB	B	2011	8	-	0/32/38/38	0/2/2/2
5	SO4	C	501	-	-	0/0/0/0	0/0/0/0
5	SO4	C	502	-	-	0/0/0/0	0/0/0/0
12	5YB	D	501	8	-	0/32/38/38	0/2/2/2
9	NAG	D	505	2	-	0/6/23/26	0/1/1/1
9	NAG	D	506	9,2	-	0/6/23/26	0/1/1/1
9	NAG	D	507	9,10	-	0/6/23/26	0/1/1/1
10	BMA	D	508	9,11	-	0/2/19/22	0/1/1/1
11	MAN	D	509	10	-	0/2/19/22	0/1/1/1
9	NAG	D	510	9,2	-	0/6/23/26	0/1/1/1
9	NAG	D	511	9	-	0/6/23/26	0/1/1/1
5	SO4	L	301	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2011	5YB	O22-C21	-2.00	1.19	1.23
12	D	501	5YB	C07-C04	2.68	1.57	1.51
12	B	2011	5YB	C07-C04	2.72	1.58	1.51
12	B	2011	5YB	C31-C34	3.10	1.52	1.47
12	D	501	5YB	C31-C34	3.40	1.53	1.47
12	B	2011	5YB	C34-N36	3.99	1.43	1.33
12	D	501	5YB	C34-N36	4.01	1.43	1.33
12	B	2011	5YB	C23-C21	4.54	1.60	1.51
12	D	501	5YB	C23-C21	4.56	1.60	1.51
12	B	2011	5YB	C26-N25	5.16	1.44	1.33
12	D	501	5YB	C26-N25	5.29	1.45	1.33
12	B	2011	5YB	C21-N20	6.28	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	501	5YB	C21-N20	6.45	1.47	1.34
12	D	501	5YB	C13-N12	7.15	1.50	1.34
12	B	2011	5YB	C13-N12	7.16	1.50	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	509	MAN	O2-C2-C3	-2.25	105.64	110.19
11	B	2007	MAN	O2-C2-C3	-2.21	105.74	110.19
11	B	2008	MAN	O2-C2-C3	-2.19	105.77	110.19
12	B	2011	5YB	O22-C21-N20	-2.19	119.28	122.96
12	B	2011	5YB	C08-N12-C13	-2.11	119.69	123.43
12	D	501	5YB	C08-N12-C13	-2.05	119.80	123.43
10	B	2006	BMA	C3-C4-C5	2.06	113.90	110.23
12	D	501	5YB	C28-C26-N25	2.19	122.12	117.19
11	D	509	MAN	C1-O5-C5	2.82	116.29	112.14
12	D	501	5YB	C23-C21-N20	2.87	120.66	115.85
11	B	2008	MAN	C1-O5-C5	2.97	116.51	112.14
12	B	2011	5YB	C23-C21-N20	3.04	120.95	115.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	2009	NAG	1	0
9	B	2010	NAG	1	0
12	B	2011	5YB	1	0
12	D	501	5YB	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	454/454 (100%)	0.32	2 (0%) 93 94	35, 49, 78, 127	0
1	C	453/454 (99%)	0.39	8 (1%) 71 72	45, 71, 105, 148	0
2	B	466/471 (98%)	0.57	47 (10%) 9 7	39, 81, 171, 207	1 (0%)
2	D	471/471 (100%)	0.65	39 (8%) 14 11	54, 96, 146, 220	1 (0%)
3	E	214/219 (97%)	1.79	80 (37%) 0 0	82, 145, 210, 246	0
3	H	216/219 (98%)	0.48	20 (9%) 11 8	56, 108, 164, 212	0
4	F	214/214 (100%)	1.54	59 (27%) 1 1	88, 138, 210, 235	0
4	L	214/214 (100%)	0.44	10 (4%) 35 34	63, 96, 126, 196	0
All	All	2702/2716 (99%)	0.67	265 (9%) 10 7	35, 87, 174, 246	2 (0%)

All (265) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	193	THR	12.7
3	E	147	LEU	8.9
4	F	130	ALA	8.7
2	D	469	SER	8.5
3	E	183	LEU	8.2
2	B	33	LEU	8.1
4	F	132	VAL	7.7
3	E	133	VAL	7.6
4	F	181	LEU	7.5
4	F	206	VAL	7.4
3	E	194	TRP	7.3
3	E	216	ILE	7.2
3	E	201	CYS	7.1
4	F	135	PHE	6.6
4	F	159	VAL	6.6
4	F	180	THR	6.4

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Mol	Chain	Res	Type	RSRZ
4	F	178	THR	6.3
3	E	219	ARG	6.3
3	E	156	VAL	6.0
4	F	115	VAL	5.9
4	F	214	CYS	5.9
4	F	125	LEU	5.7
3	E	142	VAL	5.5
3	E	210	THR	5.4
3	E	134	CYS	5.4
4	F	194	CYS	5.4
3	E	149	LYS	5.3
3	E	212	VAL	5.2
4	F	147	LYS	5.2
4	F	179	LEU	5.2
2	B	1	GLY	5.1
3	E	148	VAL	5.1
4	F	148	TRP	5.0
2	D	181	LYS	5.0
4	F	208	SER	5.0
2	D	471	CYS	4.9
3	E	127	VAL	4.9
2	B	51	PRO	4.9
3	E	129	PRO	4.9
4	F	191	SER	4.9
2	B	34	GLY	4.9
3	E	217	GLU	4.8
3	E	187	VAL	4.7
3	E	16	ALA	4.6
2	D	376	ASN	4.6
3	E	132	PRO	4.6
4	F	131	SER	4.6
4	F	160	LEU	4.5
4	F	146	VAL	4.5
2	B	10	VAL	4.4
2	D	44	LEU	4.4
3	E	198	SER	4.4
3	E	144	LEU	4.4
4	F	117	ILE	4.4
4	F	192	TYR	4.4
3	E	184	SER	4.3
2	D	375	LEU	4.3
3	E	128	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	36	PRO	4.3
2	D	54	ILE	4.3
3	E	196	SER	4.3
2	B	375	LEU	4.2
4	F	190	ASN	4.2
2	D	58	VAL	4.1
4	L	214	CYS	4.1
4	F	133	VAL	4.1
3	H	144	LEU	4.1
2	B	383	LEU	4.0
4	F	209	PHE	4.0
3	E	204	ALA	4.0
3	E	169	VAL	4.0
3	E	160	TRP	4.0
3	E	130	LEU	4.0
3	E	195	PRO	4.0
3	H	216	ILE	3.9
2	D	33	LEU	3.9
2	B	50	ALA	3.9
3	E	203	VAL	3.9
4	F	157	ASN	3.8
2	B	44	LEU	3.8
3	E	189	VAL	3.8
2	B	2	PRO	3.8
3	E	200	THR	3.8
4	F	213	GLU	3.8
3	E	20	LEU	3.8
3	E	188	THR	3.8
4	F	136	LEU	3.7
3	E	131	ALA	3.7
3	E	153	PRO	3.6
3	E	176	LEU	3.6
1	C	453	VAL	3.5
3	E	175	VAL	3.5
2	D	36	PRO	3.5
3	E	83	LEU	3.5
3	E	158	LEU	3.5
2	B	8	ARG	3.5
4	F	134	CYS	3.4
4	F	151	ASP	3.4
3	H	130	LEU	3.4
4	F	207	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
3	E	11	LEU	3.4
4	F	212	ASN	3.3
3	H	168	GLY	3.3
2	D	35	SER	3.3
2	B	379	VAL	3.3
4	F	116	SER	3.3
2	B	378	GLU	3.3
2	D	178	TYR	3.2
2	D	52	GLU	3.2
3	E	121	LYS	3.2
4	F	158	GLY	3.2
4	F	126	THR	3.2
3	E	146	CYS	3.2
2	D	399	ILE	3.1
4	F	119	PRO	3.1
4	F	15	LEU	3.1
2	B	181	LYS	3.1
3	E	85	SER	3.1
3	E	150	GLY	3.1
3	H	158	LEU	3.1
4	F	36	LEU	3.1
2	D	8	ARG	3.1
4	F	182	THR	3.1
2	B	404	ARG	3.1
1	A	339	ALA	3.0
4	L	205	ILE	3.0
2	B	9	GLY	3.0
4	F	120	PRO	3.0
4	F	149	LYS	3.0
4	F	195	GLU	3.0
3	E	214	LYS	2.9
3	E	167	SER	2.9
4	F	150	ILE	2.9
3	E	182	THR	2.9
2	B	466	TRP	2.9
2	B	11	SER	2.9
3	E	174	ALA	2.9
3	H	142	VAL	2.9
2	B	45	LEU	2.8
2	B	52	GLU	2.8
2	B	380	ILE	2.8
4	F	161	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	337	PRO	2.8
3	E	199	ILE	2.8
3	E	193	THR	2.8
3	E	218	PRO	2.8
3	E	177	GLN	2.8
2	D	1	GLY	2.8
4	L	115	VAL	2.7
3	E	165	LEU	2.7
2	B	72	LYS	2.7
4	F	118	PHE	2.7
4	F	144	ILE	2.7
3	E	92	ALA	2.7
3	E	215	LYS	2.7
2	B	37	ARG	2.7
3	E	152	PHE	2.7
2	D	380	ILE	2.7
2	D	46	LYS	2.7
2	D	2	PRO	2.7
2	D	61	ALA	2.7
2	B	451	GLY	2.7
4	F	205	ILE	2.7
4	F	129	GLY	2.7
4	F	156	GLN	2.7
2	D	30	ALA	2.7
4	F	155	ARG	2.7
2	B	376	ASN	2.6
3	E	45	LEU	2.6
2	B	46	LYS	2.6
3	E	86	LEU	2.6
2	D	466	TRP	2.6
4	L	183	LYS	2.6
4	F	177	SER	2.6
2	B	55	GLU	2.6
2	D	55	GLU	2.6
4	L	206	VAL	2.6
1	C	340	LEU	2.6
3	E	213	ASP	2.6
2	D	378	GLU	2.6
1	C	336	GLY	2.6
3	E	19	LYS	2.5
3	E	116	THR	2.5
4	F	154	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
3	H	134	CYS	2.5
3	H	217	GLU	2.5
2	B	49	CYS	2.5
4	L	105	GLU	2.5
2	B	397	PHE	2.5
2	B	27	SER	2.5
4	F	197	THR	2.5
3	E	18	VAL	2.5
2	D	53	SER	2.5
3	E	17	SER	2.5
2	B	26	CYS	2.5
3	H	83	LEU	2.4
3	E	126	SER	2.4
2	B	32	PRO	2.4
2	B	35	SER	2.4
1	C	278[A]	HIS	2.4
2	B	372	ALA	2.4
3	H	188	THR	2.4
4	F	104	LEU	2.4
3	H	167	SER	2.4
3	E	94	TYR	2.4
3	E	143	THR	2.4
2	D	470	GLN	2.4
4	L	212	ASN	2.3
2	D	51	PRO	2.3
2	B	374	CYS	2.3
3	H	198	SER	2.3
2	D	26	CYS	2.3
2	D	90	LEU	2.3
2	B	77	SER	2.3
3	E	181	TYR	2.3
2	B	368	LEU	2.3
2	B	39	ASP	2.3
2	B	432	ASP	2.3
1	C	244	PHE	2.2
3	E	65	GLN	2.2
4	F	122	SER	2.2
2	B	48	ASN	2.2
3	E	89	GLU	2.2
4	F	100	GLY	2.2
3	E	141	SER	2.2
2	B	57	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	84	SER	2.2
2	B	31	LEU	2.2
3	H	187	VAL	2.2
4	F	106	ILE	2.1
2	B	440	GLN	2.1
4	L	104	LEU	2.1
3	H	215	LYS	2.1
1	C	213	LEU	2.1
2	D	468	GLY	2.1
1	C	335	ARG	2.1
2	B	28	ASP	2.1
3	H	195	PRO	2.1
3	E	171	THR	2.1
2	D	131	ILE	2.1
3	E	80	TYR	2.1
3	H	199	ILE	2.1
2	D	89	ALA	2.1
2	D	4	ILE	2.1
3	H	189	VAL	2.1
3	E	25	SER	2.1
2	B	76	ASP	2.1
2	D	42	GLU	2.1
3	E	186	SER	2.1
4	L	83	PHE	2.1
2	D	92	LEU	2.0
3	H	197	GLN	2.0
2	D	88	ILE	2.0
3	E	206	PRO	2.0
1	C	130	CYS	2.0
2	D	22	MET	2.0
3	E	114	SER	2.0
3	E	117	VAL	2.0
3	H	203	VAL	2.0
4	L	129	GLY	2.0
2	D	143	ARG	2.0
3	H	169	VAL	2.0
4	F	83	PHE	2.0
2	B	29	GLU	2.0
2	D	315	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
5	SO4	A	501	5/5	0.83	0.50	14.04	169,171,181,184	0
6	GOL	A	504	6/6	0.89	0.32	11.21	86,104,123,124	0
5	SO4	C	501	5/5	0.86	0.41	9.37	176,179,182,182	0
5	SO4	A	502	5/5	0.93	0.36	9.16	134,139,148,154	0
7	CA	A	507	1/1	0.92	0.38	7.84	79,79,79,79	0
7	CA	D	503	1/1	0.70	0.48	5.93	210,210,210,210	0
7	CA	A	506	1/1	0.85	0.23	2.48	68,68,68,68	0
12	5YB	B	2011	36/36	0.92	0.26	1.34	34,77,107,118	0
9	NAG	B	2003	14/15	0.89	0.29	0.90	111,144,173,174	0
8	MG	B	2001	1/1	0.91	0.22	0.71	31,31,31,31	0
12	5YB	D	501	36/36	0.94	0.23	0.54	45,85,116,122	0
9	NAG	B	2004	14/15	0.96	0.20	0.15	55,79,95,98	0
7	CA	C	505	1/1	0.02	0.20	0.13	174,174,174,174	0
9	NAG	B	2009	14/15	0.89	0.24	0.08	105,134,169,169	0
9	NAG	D	505	14/15	0.85	0.24	-0.08	104,142,170,170	0
7	CA	C	508	1/1	0.99	0.15	-0.28	62,62,62,62	0
7	CA	A	508	1/1	1.00	0.19	-0.30	38,38,38,38	0
9	NAG	D	510	14/15	0.90	0.21	-0.59	102,140,174,174	0
7	CA	A	505	1/1	0.91	0.11	-0.82	62,62,62,62	0
9	NAG	D	506	14/15	0.92	0.17	-0.87	81,115,156,158	0
8	MG	D	502	1/1	0.95	0.15	-1.31	47,47,47,47	0
7	CA	D	504	1/1	0.99	0.17	-1.46	50,50,50,50	0
7	CA	C	507	1/1	0.93	0.12	-1.79	56,56,56,56	0
7	CA	C	506	1/1	0.93	0.05	-2.84	67,67,67,67	0
7	CA	B	2002	1/1	0.99	0.15	-4.40	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	MAN	D	509	11/12	0.89	0.19	-	125,145,174,175	0
11	MAN	B	2008	11/12	0.78	0.22	-	118,137,164,166	0
5	SO4	C	502	5/5	0.88	0.22	-	188,191,193,193	0
10	BMA	D	508	11/12	0.83	0.24	-	118,141,169,169	0
9	NAG	D	511	14/15	0.82	0.21	-	128,154,185,204	0
5	SO4	A	503	5/5	0.95	0.22	-	97,111,113,122	0
11	MAN	B	2007	11/12	0.89	0.18	-	109,130,153,158	0
10	BMA	B	2006	11/12	0.80	0.15	-	110,142,177,177	0
5	SO4	L	301	5/5	0.93	0.16	-	176,178,179,181	0
13	CL	C	504	1/1	0.66	0.17	-	100,100,100,100	0
9	NAG	D	507	14/15	0.91	0.22	-	108,141,179,183	0
13	CL	C	503	1/1	0.83	0.20	-	81,81,81,81	0
9	NAG	B	2010	14/15	0.85	0.25	-	126,160,184,202	0
9	NAG	B	2005	14/15	0.88	0.23	-	104,134,157,176	0

6.5 Other polymers [i](#)

There are no such residues in this entry.