



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:10 PM GMT

PDB ID : 3T3P
Title : A Novel High Affinity Integrin α IIb β 3 Receptor Antagonist That Unexpectedly Displaces Mg²⁺ from the β 3 MIDAS
Authors : Zhu, J.; Zhu, J.; Springer, T.A.
Deposited on : 2011-07-25
Resolution : 2.20 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

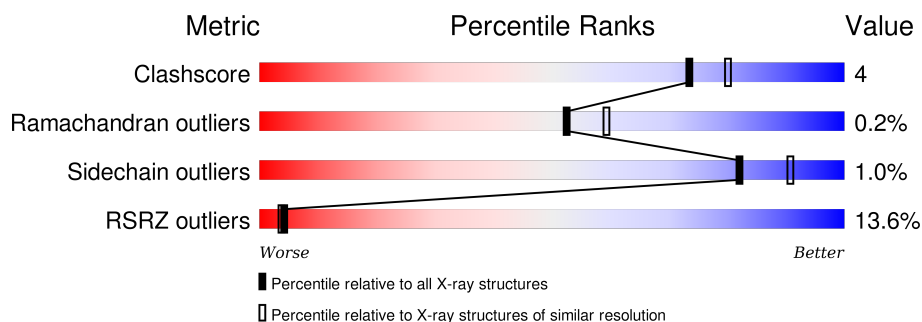
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



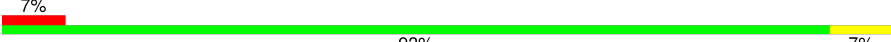
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	457	<div> <div>2%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
1	C	457	<div> <div>3%</div> <div>91%</div> <div>8%</div> <div>..</div> </div>
2	B	472	<div> <div>11%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
2	D	472	<div> <div>10%</div> <div>91%</div> <div>9%</div> </div>
3	E	221	<div> <div>40%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
3	H	221	<div> <div>19%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
4	F	214	<div> <div>46%</div> <div>83%</div> <div>17%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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
12	NAG	D	3371	-	-	-	X
5	SO4	A	459	-	-	-	X
5	SO4	C	460	-	-	-	X
6	GOL	A	461	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22411 atoms, of which 0 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	N	O	S	0	8	0
			3532	2245	611	668	8			
1	C	453	Total	C	N	O	S	0	4	0
			3502	2224	604	666	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	4	7	0
			3643	2269	622	718	34			
2	D	471	Total	C	N	O	S	3	2	0
			3642	2270	621	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	N	O	S	0	0	0
			1631	1035	264	326	6			
3	H	216	Total	C	N	O	S	0	0	0
			1642	1041	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	N	O	S	0	0	0
			1637	1019	268	341	9			
4	L	214	Total	C	N	O	S	0	0	0
			1637	1019	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	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	O	0	0
			6	3	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
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		

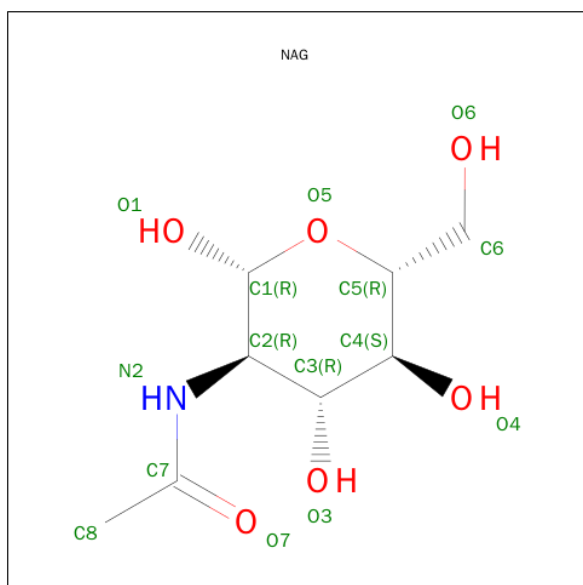
- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		
8	D	1	Total	Cl	0	0
			1	1		
8	C	2	Total	Cl	0	0
			2	2		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 10 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C N O 14 8 1 5	0	0
10	D	1	Total C N O 14 8 1 5	0	0

- Molecule 11 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	5	Total C N O 61 34 2 25	0	0

- Molecule 12 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	2	Total C N O 28 16 2 10	0	0
12	D	2	Total C N O 28 16 2 10	0	0

- Molecule 13 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	D	4	Total	C	N	O	0	0
			50	28	2	20		

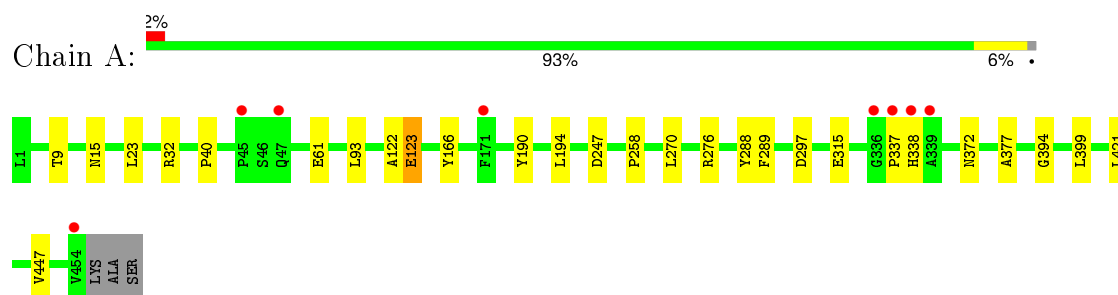
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	463	Total	O	0	0
			463	463		
14	B	249	Total	O	0	0
			249	249		
14	C	274	Total	O	0	0
			274	274		
14	D	200	Total	O	0	0
			200	200		
14	E	17	Total	O	0	0
			17	17		
14	F	13	Total	O	0	0
			13	13		
14	H	29	Total	O	0	0
			29	29		
14	L	46	Total	O	0	0
			46	46		

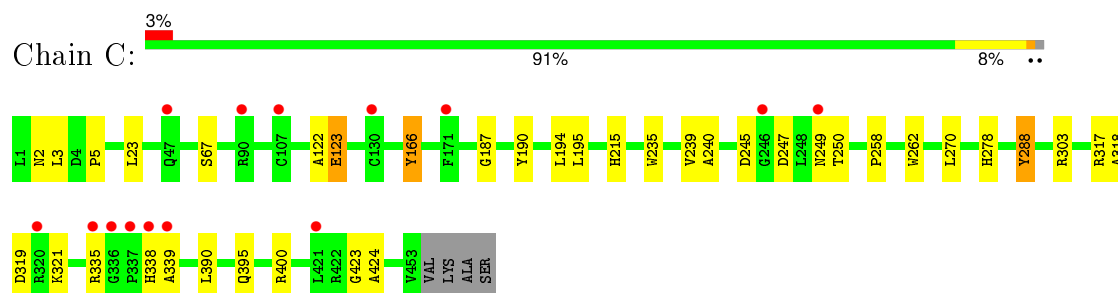
3 Residue-property plots [i](#)

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.

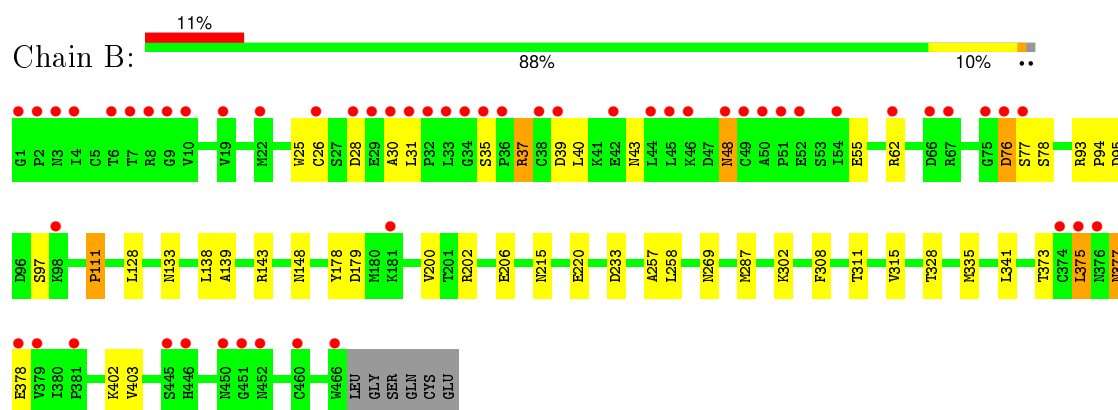
• Molecule 1: Integrin alpha-IIb

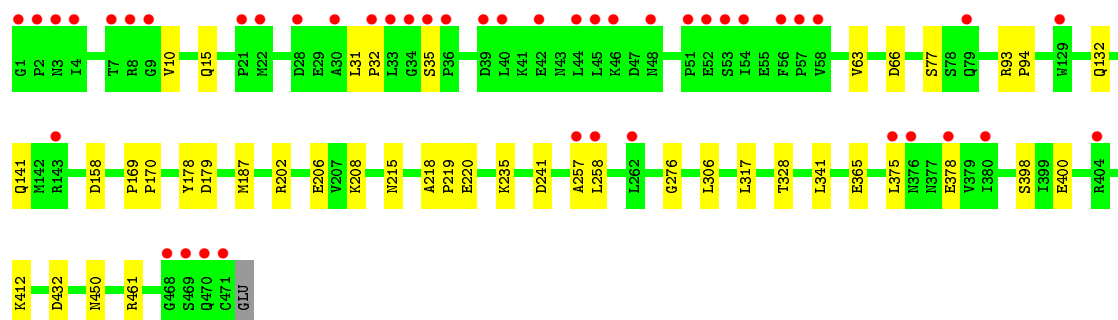


• Molecule 1: Integrin alpha-IIb

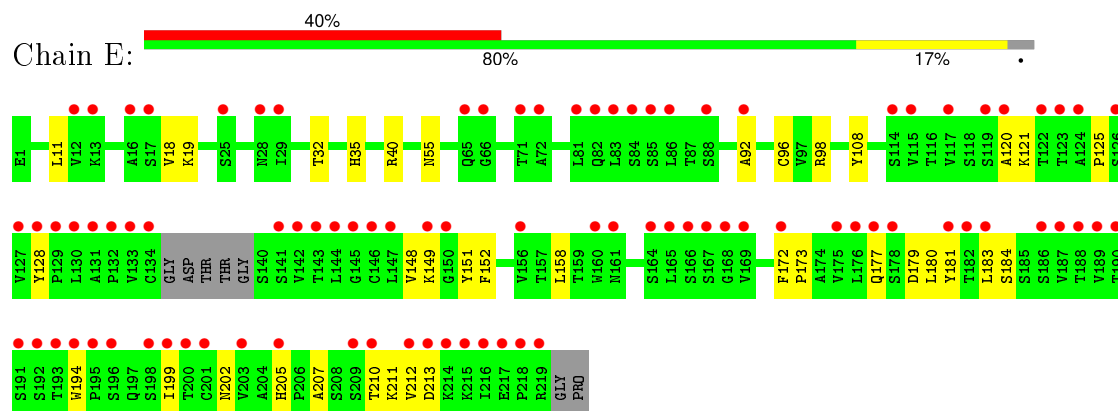


• Molecule 2: Integrin beta-3

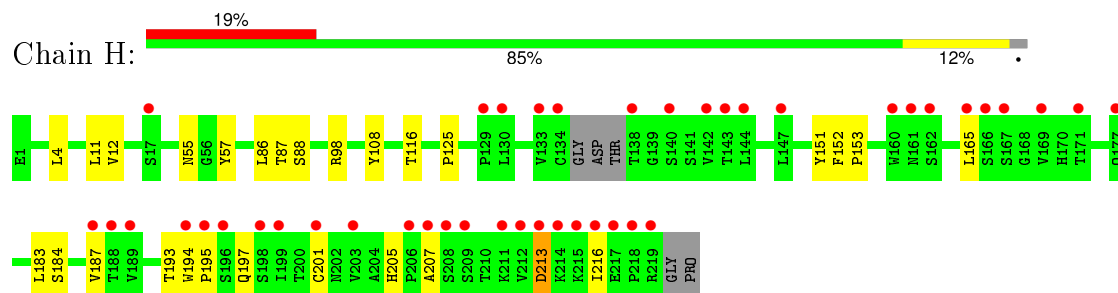




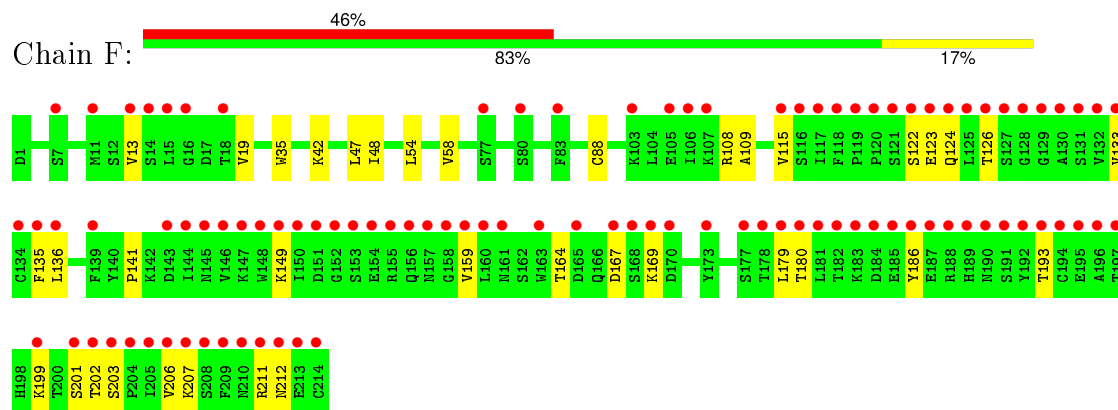
- Molecule 3: Monoclonal antibody 10E5 heavy chain



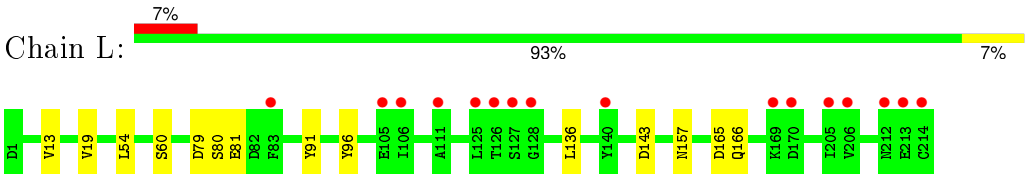
- Molecule 3: Monoclonal antibody 10E5 heavy chain



- 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 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	259.53 Å 145.26 Å 104.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 2.20 48.39 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.39-2.20) 99.3 (48.39-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.20 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.189 , 0.220 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.4	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	0 of 199292 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22411	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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, 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	0.36	0/3647	0.53	0/4969
1	C	0.31	0/3605	0.47	0/4912
2	B	0.32	0/3716	0.49	0/5037
2	D	0.29	0/3714	0.45	0/5036
3	E	0.22	0/1673	0.40	0/2290
3	H	0.26	0/1684	0.44	0/2305
4	F	0.24	0/1673	0.40	0/2269
4	L	0.27	0/1673	0.44	0/2269
All	All	0.30	0/21385	0.46	0/29087

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	3532	0	3383	14	0
1	C	3502	0	3334	20	0
2	B	3643	0	3566	31	0
2	D	3642	0	3558	31	0
3	E	1631	0	1590	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	18	0
4	F	1637	0	1553	25	0
4	L	1637	0	1553	8	0
5	A	15	0	0	1	0
5	C	15	0	0	0	0
5	L	5	0	0	0	0
6	A	6	0	8	0	0
7	A	4	0	0	0	0
7	B	2	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	C	2	0	0	0	0
8	D	1	0	0	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	B	14	0	13	0	0
10	D	14	0	13	0	0
11	B	61	0	52	0	0
12	B	28	0	25	0	0
12	D	28	0	25	2	0
13	D	50	0	43	0	0
14	A	463	0	0	4	0
14	B	249	0	0	6	0
14	C	274	0	0	0	0
14	D	200	0	0	2	0
14	E	17	0	0	0	0
14	F	13	0	0	0	0
14	H	29	0	0	0	0
14	L	46	0	0	1	0
All	All	22411	0	20316	171	0

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 4.

All (171) 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)
5:A:460:SO4:O4	14:A:691:HOH:O	2.14	0.65
1:A:122:ALA:O	1:A:123:GLU:HB2	1.99	0.62
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:202:ASN:HA	3:E:213:ASP:HB3	1.83	0.60
2:D:178:TYR:CG	2:D:179:ASP:N	2.70	0.59
2:D:375:LEU:O	2:D:378:GLU:HG2	2.03	0.59
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.84	0.59
3:H:87:THR:HG22	3:H:88:SER:N	2.19	0.57
1:C:122:ALA:O	1:C:123:GLU:HB2	2.04	0.57
2:D:400:GLU:HB2	12:D:3371:NAG:H83	1.86	0.56
1:A:337:PRO:O	1:A:338:HIS:CG	2.59	0.56
3:E:173:PRO:HD3	4:F:164:THR:HG22	1.88	0.56
4:F:193:THR:HG23	4:F:206:VAL:HG13	1.89	0.55
2:D:257:ALA:O	2:D:258:LEU:HB2	2.08	0.54
2:D:235:LYS:HE3	2:D:276:GLY:O	2.08	0.54
3:H:4:LEU:N	3:H:4:LEU:HD12	2.24	0.53
3:E:177:GLN:N	3:E:180:LEU:O	2.37	0.53
2:D:202:ARG:NH2	2:D:206:GLU:OE2	2.39	0.53
2:B:62:ARG:HD3	14:B:1066:HOH:O	2.09	0.53
2:B:26:CYS:O	2:B:37:ARG:NH1	2.42	0.53
3:H:194:TRP:CG	3:H:195:PRO:HA	2.44	0.52
3:E:125:PRO:HB2	3:E:148:VAL:HG13	1.92	0.52
3:E:98:ARG:HG3	3:E:108:TYR:HB2	1.91	0.52
4:F:159:VAL:HG22	4:F:179:LEU:HD13	1.91	0.52
3:H:193:THR:O	3:H:197:GLN:N	2.35	0.51
4:F:141:PRO:HD3	4:F:199:LYS:HD3	1.93	0.51
1:C:2:ASN:OD1	1:C:2:ASN:N	2.42	0.51
4:L:136:LEU:N	4:L:136:LEU:HD12	2.26	0.51
4:F:201:SER:OG	4:F:203:SER:O	2.19	0.51
1:C:245:ASP:OD1	1:C:250:THR:OG1	2.29	0.51
3:E:40:ARG:CG	3:E:92:ALA:HB2	2.41	0.51
2:B:335:MET:HE2	14:B:518:HOH:O	2.10	0.51
4:F:47:LEU:HA	4:F:58:VAL:HG21	1.93	0.50
3:E:205:HIS:CE1	3:E:207:ALA:HB3	2.46	0.50
4:F:136:LEU:N	4:F:136:LEU:HD12	2.26	0.50
1:C:303:ARG:NH1	1:C:335:ARG:HD3	2.27	0.50
4:F:149:LYS:HB2	4:F:193:THR:HB	1.93	0.50
2:D:202:ARG:HD3	14:D:754:HOH:O	2.12	0.50
3:E:149:LYS:NZ	4:F:180:THR:HG21	2.26	0.50
4:F:108:ARG:NE	4:F:109:ALA:O	2.43	0.50
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.94	0.49
1:A:194:LEU:C	1:A:194:LEU:HD12	2.32	0.49
3:E:120:ALA:HB2	3:E:179:ASP:HB3	1.93	0.49
4:F:167:ASP:OD1	4:F:169:LYS:HB3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.94	0.48
2:D:178:TYR:CZ	2:D:179:ASP:HB3	2.48	0.48
2:D:93:ARG:HB2	2:D:94:PRO:HD2	1.95	0.48
1:A:270:LEU:HD23	1:A:276:ARG:HA	1.96	0.48
2:B:95:ASP:HA	2:B:403:VAL:O	2.14	0.47
3:H:87:THR:CG2	3:H:88:SER:N	2.76	0.47
2:D:306:LEU:HB3	2:D:328:THR:HG22	1.95	0.47
3:H:11:LEU:HD12	3:H:116:THR:HB	1.97	0.47
4:L:157:ASN:ND2	14:L:1197:HOH:O	2.47	0.47
1:A:15[B]:ASN:ND2	14:A:1000:HOH:O	2.34	0.47
2:D:218:ALA:HB3	2:D:219:PRO:HD3	1.95	0.47
4:F:141:PRO:CD	4:F:199:LYS:HD3	2.45	0.47
2:B:178:TYR:CG	2:B:179:ASP:N	2.83	0.47
1:C:215:HIS:CE1	3:E:32:THR:HG22	2.50	0.47
1:A:32[A]:ARG:HD2	14:A:980:HOH:O	2.15	0.47
4:F:206:VAL:HG12	4:F:207:LYS:N	2.29	0.46
2:B:76:ASP:OD2	2:B:76:ASP:N	2.47	0.46
1:A:247:ASP:OD2	1:A:247:ASP:C	2.54	0.46
2:B:133[A]:ASN:OD1	14:B:1138:HOH:O	2.21	0.46
3:E:128:TYR:CZ	4:F:124:GLN:HA	2.51	0.46
2:D:141:GLN:HG3	2:D:341:LEU:HD21	1.97	0.46
1:C:194:LEU:HD12	1:C:194:LEU:C	2.36	0.46
1:C:122:ALA:O	1:C:123:GLU:CB	2.63	0.46
4:L:79:ASP:OD1	4:L:80:SER:N	2.48	0.46
2:B:375:LEU:HB2	14:B:932:HOH:O	2.15	0.46
2:D:398:SER:OG	12:D:3371:NAG:O7	2.26	0.46
3:E:158:LEU:C	3:E:158:LEU:HD23	2.36	0.46
1:A:315:GLU:OE2	14:A:532:HOH:O	2.21	0.46
4:F:35:TRP:CZ3	4:F:88:CYS:HB3	2.51	0.46
2:B:138:LEU:HA	2:B:341:LEU:CD1	2.45	0.46
2:D:63:VAL:HG11	2:D:66:ASP:HB2	1.98	0.46
4:F:115:VAL:HG12	4:F:207:LYS:HG3	1.97	0.46
3:H:201:CYS:O	3:H:213:ASP:HA	2.15	0.46
1:C:390:LEU:HD12	1:C:390:LEU:N	2.31	0.45
2:B:97:SER:HB3	2:B:402:LYS:HG2	1.98	0.45
1:C:318:ALA:O	1:C:319:ASP:HB2	2.17	0.45
1:A:258:PRO:HA	1:A:289:PHE:O	2.15	0.45
2:D:365:GLU:OE2	2:D:412:LYS:NZ	2.48	0.45
2:B:378:GLU:HB3	14:B:932:HOH:O	2.15	0.45
2:D:158:ASP:H	2:D:187[B]:MET:HE3	1.82	0.45
3:E:125:PRO:HB2	3:E:148:VAL:CG1	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:ARG:HB2	2:B:94:PRO:CD	2.47	0.45
2:D:341:LEU:HD23	2:D:341:LEU:C	2.37	0.45
3:E:194:TRP:CD1	3:E:199:ILE:HD12	2.52	0.45
3:E:205:HIS:HB3	3:E:210:THR:CG2	2.47	0.45
3:E:183:LEU:HD23	3:E:183:LEU:C	2.37	0.45
1:A:9:THR:HB	1:A:447:VAL:HB	1.98	0.45
2:B:233:ASP:OD1	2:B:302:LYS:HD2	2.17	0.45
3:E:205:HIS:HB3	3:E:210:THR:HG22	1.99	0.45
3:E:212:VAL:HG12	3:E:213:ASP:N	2.31	0.44
2:D:10:VAL:HA	2:D:15:GLN:NE2	2.32	0.44
2:B:31:LEU:CD2	2:B:35:SER:HB2	2.47	0.44
4:F:122:SER:O	4:F:126:THR:HG23	2.17	0.44
1:A:394:GLY:HA2	1:A:399:LEU:HD23	1.99	0.44
3:E:213:ASP:OD1	3:E:213:ASP:N	2.51	0.44
1:C:278[A]:HIS:CE1	1:C:339:ALA:HB1	2.52	0.44
2:B:39:ASP:OD2	2:B:43:ASN:ND2	2.51	0.44
2:D:158:ASP:N	2:D:187[B]:MET:HE3	2.33	0.44
3:E:172:PHE:CD1	4:F:164:THR:HG23	2.53	0.44
4:F:186:TYR:CE2	4:F:211:ARG:HG3	2.53	0.44
4:L:54:LEU:HD21	4:L:60:SER:HA	1.99	0.44
1:C:317:ARG:HB2	1:C:321:LYS:HB2	1.99	0.44
2:B:39:ASP:OD2	2:B:40:LEU:N	2.51	0.44
4:F:133:VAL:HG11	4:F:135:PHE:CZ	2.52	0.44
2:D:77:SER:HB2	2:D:241:ASP:CG	2.38	0.44
4:F:123:GLU:O	4:F:126:THR:OG1	2.35	0.43
2:B:373:THR:CG2	2:B:377:ASN:HA	2.49	0.43
2:B:220:GLU:HA	2:B:220:GLU:OE1	2.17	0.43
3:E:210:THR:C	3:E:211:LYS:HG3	2.38	0.43
2:D:132:GLN:OE1	2:D:208:LYS:HG2	2.18	0.43
1:C:166:TYR:O	1:C:187:GLY:HA3	2.18	0.43
3:H:183:LEU:HD23	3:H:183:LEU:C	2.38	0.43
3:H:165:LEU:HD21	3:H:187:VAL:HG21	2.00	0.43
2:B:308:PHE:CE2	2:B:328:THR:HG21	2.54	0.43
3:H:55:ASN:CG	3:H:57:TYR:HD2	2.22	0.43
2:D:450:ASN:ND2	2:D:450:ASN:O	2.51	0.43
3:H:98:ARG:HG3	3:H:108:TYR:HB2	2.00	0.43
3:H:194:TRP:CZ2	3:H:216:ILE:HG22	2.54	0.43
1:C:3:LEU:O	1:C:5:PRO:HD3	2.19	0.43
3:H:205:HIS:CE1	3:H:207:ALA:HB3	2.54	0.43
1:C:258:PRO:HB2	1:C:288:TYR:CD1	2.54	0.42
3:E:11:LEU:N	3:E:11:LEU:HD12	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:121:LYS:HD2	3:E:121:LYS:N	2.34	0.42
3:E:40:ARG:HG3	3:E:92:ALA:HB2	2.01	0.42
1:A:297:ASP:O	1:A:372:ASN:HB2	2.19	0.42
1:A:40:PRO:HA	1:A:93:LEU:O	2.20	0.42
4:F:48:ILE:CD1	4:F:54:LEU:HD23	2.50	0.42
3:E:18:VAL:HG22	3:E:19:LYS:N	2.34	0.42
1:C:247:ASP:OD2	1:C:249:ASN:HB2	2.19	0.42
2:D:31:LEU:HD12	2:D:32:PRO:HD2	2.02	0.42
4:F:13:VAL:HG11	4:F:19:VAL:HG11	2.01	0.42
3:H:183:LEU:HD23	3:H:184:SER:N	2.35	0.42
2:B:28:ASP:OD2	2:B:30:ALA:N	2.53	0.42
2:D:461:ARG:NE	14:D:880:HOH:O	2.47	0.41
3:H:12:VAL:HG21	3:H:86:LEU:CD1	2.50	0.41
4:L:13:VAL:HG11	4:L:19:VAL:HG11	2.02	0.41
1:C:262:TRP:HB3	2:D:317:LEU:HD13	2.02	0.41
2:D:220:GLU:HA	2:D:220:GLU:OE1	2.20	0.41
4:F:202:THR:HG22	4:F:202:THR:O	2.20	0.41
4:L:81:GLU:N	4:L:81:GLU:OE1	2.54	0.41
1:C:423:GLY:O	1:C:424:ALA:HB3	2.20	0.41
2:B:139:ALA:HB2	2:B:200:VAL:HG11	2.02	0.41
1:C:395:GLN:OE1	1:C:400:ARG:HD3	2.21	0.41
3:H:152:PHE:CD1	3:H:153:PRO:HA	2.55	0.41
1:A:377:ALA:HB2	1:A:421:LEU:HD11	2.03	0.41
2:D:93:ARG:HB2	2:D:94:PRO:CD	2.51	0.41
4:F:42:LYS:N	4:F:42:LYS:HD2	2.35	0.41
2:B:77:SER:O	2:B:78:SER:OG	2.29	0.41
2:D:169:PRO:CB	2:D:170:PRO:CD	2.99	0.41
1:C:239:VAL:HG22	1:C:240:ALA:N	2.36	0.41
3:E:183:LEU:HD23	3:E:184:SER:N	2.37	0.40
2:D:32:PRO:O	2:D:35:SER:HB3	2.21	0.40
4:L:91:TYR:HB2	4:L:96:TYR:CZ	2.55	0.40
2:B:311:THR:O	2:B:315[B]:VAL:HG23	2.20	0.40
2:B:111:PRO:HB3	2:B:148:ASN:HB3	2.03	0.40
2:B:25:TRP:HB3	2:B:55:GLU:HB2	2.02	0.40
3:E:151:TYR:CZ	3:E:181:TYR:HB2	2.56	0.40
2:B:143:ARG:NH1	14:B:797:HOH:O	2.30	0.40
2:D:341:LEU:HD23	2:D:341:LEU:O	2.21	0.40
2:B:269:ASN:HA	2:B:287:MET:CG	2.51	0.40
3:E:152:PHE:CD2	3:E:152:PHE:C	2.94	0.40
4:L:165:ASP:O	4:L:166:GLN:C	2.58	0.40
3:E:35:HIS:O	3:E:96:CYS:HA	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:TRP:CZ2	1:C:270:LEU:HD11	2.56	0.40
2:B:48:ASN:N	2:B:48:ASN:OD1	2.54	0.40
2:B:257:ALA:O	2:B:258:LEU:HB2	2.22	0.40

There are no symmetry-related clashes.

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	460/457 (101%)	441 (96%)	18 (4%)	1 (0%)	52	59
1	C	455/457 (100%)	441 (97%)	13 (3%)	1 (0%)	52	59
2	B	471/472 (100%)	452 (96%)	17 (4%)	2 (0%)	39	42
2	D	471/472 (100%)	454 (96%)	17 (4%)	0	100	100
3	E	210/221 (95%)	193 (92%)	16 (8%)	1 (0%)	34	35
3	H	212/221 (96%)	197 (93%)	15 (7%)	0	100	100
4	F	212/214 (99%)	195 (92%)	16 (8%)	1 (0%)	34	35
4	L	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
All	All	2703/2728 (99%)	2577 (95%)	120 (4%)	6 (0%)	52	59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	C	123	GLU
2	B	375	LEU
4	F	212	ASN
2	B	377	ASN
3	E	55	ASN

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	370/364 (102%)	365 (99%)	5 (1%)	74	85
1	C	365/364 (100%)	358 (98%)	7 (2%)	65	77
2	B	419/417 (100%)	413 (99%)	6 (1%)	74	85
2	D	418/417 (100%)	416 (100%)	2 (0%)	92	96
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	186 (100%)	1 (0%)	92	96
4	F	188/188 (100%)	188 (100%)	0	100	100
4	L	188/188 (100%)	187 (100%)	1 (0%)	92	96
All	All	2321/2318 (100%)	2299 (99%)	22 (1%)	82	92

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	61	GLU
1	A	166	TYR
1	A	190	TYR
1	A	288	TYR
2	B	37	ARG
2	B	48	ASN
2	B	76	ASP
2	B	111	PRO
2	B	128	LEU
2	B	215	ASN
1	C	23	LEU
1	C	67	SER
1	C	166	TYR
1	C	190	TYR
1	C	195	LEU
1	C	288	TYR
1	C	338	HIS
2	D	215	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	432	ASP
3	H	213	ASP
4	L	143	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	C	197	GLN
2	D	15	GLN
2	D	450	ASN
2	D	452	ASN
4	F	27	GLN
4	F	93	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](#)

13 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	$\# Z > 2$
11	NAG	B	3320	11,2	14,14,15	0.46	0	15,19,21	0.79	0
11	NAG	B	3321	11	14,14,15	0.59	0	15,19,21	0.98	1 (6%)
11	BMA	B	3322	11	11,11,12	0.60	0	14,15,17	0.96	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	B	3323	11	11,11,12	0.56	0	14,15,17	0.79	0
11	MAN	B	3324	11	11,11,12	0.61	0	14,15,17	0.67	0
12	NAG	B	3371	2,12	14,14,15	0.57	0	15,19,21	0.78	0
12	NAG	B	3372	12	14,14,15	0.50	0	15,19,21	0.71	0
13	NAG	D	3320	13,2	14,14,15	0.58	0	15,19,21	0.72	0
13	NAG	D	3321	13	14,14,15	0.64	0	15,19,21	1.08	1 (6%)
13	BMA	D	3322	13	11,11,12	0.65	0	14,15,17	0.88	1 (7%)
13	MAN	D	3323	13	11,11,12	0.58	0	14,15,17	0.87	0
12	NAG	D	3371	12,2	14,14,15	0.62	0	15,19,21	0.60	0
12	NAG	D	3372	12	14,14,15	0.51	0	15,19,21	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	B	3320	11,2	-	0/6/23/26	0/1/1/1
11	NAG	B	3321	11	-	0/6/23/26	0/1/1/1
11	BMA	B	3322	11	-	0/2/19/22	0/1/1/1
11	MAN	B	3323	11	-	0/2/19/22	0/1/1/1
11	MAN	B	3324	11	-	0/2/19/22	0/1/1/1
12	NAG	B	3371	2,12	-	0/6/23/26	0/1/1/1
12	NAG	B	3372	12	-	0/6/23/26	0/1/1/1
13	NAG	D	3320	13,2	-	0/6/23/26	0/1/1/1
13	NAG	D	3321	13	-	0/6/23/26	0/1/1/1
13	BMA	D	3322	13	-	0/2/19/22	0/1/1/1
13	MAN	D	3323	13	-	0/2/19/22	0/1/1/1
12	NAG	D	3371	12,2	-	0/6/23/26	0/1/1/1
12	NAG	D	3372	12	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	3321	NAG	C2-N2-C7	-2.18	120.24	123.04
11	B	3322	BMA	C1-C2-C3	2.16	112.10	109.54
13	D	3322	BMA	C1-C2-C3	2.23	112.18	109.54
13	D	3321	NAG	C4-C3-C2	2.63	115.31	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	3371	NAG	2	0

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 18 are monoatomic - leaving 10 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	458	-	4,4,4	0.19	0	6,6,6	0.10	0
5	SO4	A	459	-	4,4,4	0.18	0	6,6,6	0.17	0
5	SO4	A	460	-	4,4,4	0.22	0	6,6,6	0.22	0
6	GOL	A	461	-	5,5,5	0.34	0	5,5,5	0.25	0
10	NAG	B	3099	2	14,14,15	0.54	0	15,19,21	0.90	1 (6%)
5	SO4	C	458	-	4,4,4	0.21	0	6,6,6	0.13	0
5	SO4	C	459	-	4,4,4	0.22	0	6,6,6	0.09	0
5	SO4	C	460	-	4,4,4	0.23	0	6,6,6	0.12	0
10	NAG	D	3099	2	14,14,15	0.49	0	15,19,21	0.69	0
5	SO4	L	215	-	4,4,4	0.21	0	6,6,6	0.08	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	458	-	-	0/0/0/0	0/0/0/0
5	SO4	A	459	-	-	0/0/0/0	0/0/0/0
5	SO4	A	460	-	-	0/0/0/0	0/0/0/0
6	GOL	A	461	-	-	0/4/4/4	0/0/0/0
10	NAG	B	3099	2	-	0/6/23/26	0/1/1/1
5	SO4	C	458	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	C	459	-	-	0/0/0/0	0/0/0/0
5	SO4	C	460	-	-	0/0/0/0	0/0/0/0
10	NAG	D	3099	2	-	0/6/23/26	0/1/1/1
5	SO4	L	215	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	3099	NAG	C1-O5-C5	2.58	115.52	112.25

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
5	A	460	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	454/457 (99%)	0.33	8 (1%) 71 70	3, 11, 34, 73	0
1	C	453/457 (99%)	0.26	14 (3%) 52 51	9, 24, 50, 77	0
2	B	466/472 (98%)	0.72	54 (11%) 6 6	2, 32, 90, 112	1 (0%)
2	D	471/472 (99%)	0.38	45 (9%) 10 9	11, 33, 78, 142	1 (0%)
3	E	214/221 (96%)	2.18	89 (41%) 0 0	33, 85, 137, 155	0
3	H	216/221 (97%)	0.75	43 (19%) 1 1	16, 59, 103, 118	0
4	F	214/214 (100%)	2.30	99 (46%) 0 0	33, 81, 134, 157	1 (0%)
4	L	214/214 (100%)	0.34	16 (7%) 17 17	20, 44, 70, 95	1 (0%)
All	All	2702/2728 (99%)	0.73	368 (13%) 4 4	2, 34, 109, 157	4 (0%)

All (368) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	469	SER	11.9
4	F	214	CYS	11.8
3	E	133	VAL	11.3
3	E	212	VAL	10.5
3	E	165	LEU	9.8
3	E	216	ILE	9.6
2	B	33	LEU	9.4
3	E	144	LEU	9.4
3	E	134	CYS	9.2
2	B	77	SER	9.2
3	E	142	VAL	9.1
3	E	201	CYS	8.3
2	B	36	PRO	8.3
3	E	194	TRP	8.3
4	F	181	LEU	8.1
3	E	219	ARG	8.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	L	214	CYS	8.0
3	E	210	THR	7.8
4	F	126	THR	7.7
3	E	196	SER	7.7
3	E	131	ALA	7.6
4	F	179	LEU	7.5
4	F	193	THR	7.5
4	F	212	ASN	7.2
4	F	125	LEU	7.1
3	E	129	PRO	7.0
4	F	130	ALA	7.0
3	E	128	TYR	6.9
4	F	134	CYS	6.8
4	F	213	GLU	6.8
4	F	120	PRO	6.7
4	F	182	THR	6.6
4	F	122	SER	6.6
4	F	135	PHE	6.6
4	F	148	TRP	6.5
4	F	119	PRO	6.5
3	E	160	TRP	6.4
1	A	337	PRO	6.3
3	H	133	VAL	6.3
4	F	127	SER	6.3
3	E	147	LEU	6.2
3	E	218	PRO	6.1
4	F	117	ILE	6.1
2	B	34	GLY	6.0
2	B	375	LEU	6.0
4	F	206	VAL	6.0
2	D	471	CYS	6.0
4	F	115	VAL	6.0
2	B	51	PRO	5.9
4	F	194	CYS	5.9
3	E	200	THR	5.8
4	F	150	ILE	5.8
4	F	195	GLU	5.8
2	B	10	VAL	5.7
3	H	189	VAL	5.7
4	F	118	PHE	5.6
4	F	180	THR	5.5
3	E	132	PRO	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	116	SER	5.5
3	E	199	ILE	5.4
4	F	132	VAL	5.4
2	B	30	ALA	5.3
2	B	4	ILE	5.3
3	H	134	CYS	5.3
2	B	8	ARG	5.3
4	F	210	ASN	5.3
4	L	212	ASN	5.3
2	B	44	LEU	5.3
3	E	143	THR	5.2
3	E	217	GLU	5.2
2	D	8	ARG	5.2
4	F	152	GLY	5.1
2	D	2	PRO	5.1
4	F	14	SER	5.1
3	E	215	LYS	5.1
3	H	198	SER	5.1
2	B	46	LYS	5.0
4	F	184	ASP	5.0
4	F	136	LEU	5.0
3	H	142	VAL	5.0
4	F	151	ASP	4.9
3	E	16	ALA	4.9
2	B	1	GLY	4.9
3	E	198	SER	4.9
3	E	187	VAL	4.8
3	H	160	TRP	4.8
4	F	186	TYR	4.7
3	E	167	SER	4.7
2	D	48	ASN	4.7
1	A	339	ALA	4.7
2	B	35	SER	4.7
3	E	141	SER	4.7
2	B	2	PRO	4.7
4	F	146	VAL	4.7
3	E	130	LEU	4.7
2	B	32	PRO	4.7
4	F	133	VAL	4.6
1	C	336	GLY	4.6
2	B	9	GLY	4.6
3	E	127	VAL	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	156	GLN	4.6
4	F	209	PHE	4.5
3	E	192	SER	4.5
4	F	107	LYS	4.5
2	D	4	ILE	4.4
4	F	128	GLY	4.4
3	E	29	ILE	4.4
3	E	195	PRO	4.4
3	E	83	LEU	4.4
4	F	131	SER	4.4
4	F	191	SER	4.4
3	H	188	THR	4.3
2	D	470	GLN	4.3
3	E	183	LEU	4.3
4	F	192	TYR	4.3
4	F	158	GLY	4.3
4	F	129	GLY	4.3
4	F	197	THR	4.3
4	F	147	LYS	4.2
3	E	84	SER	4.2
2	B	22	MET	4.2
2	D	51	PRO	4.2
4	F	202	THR	4.1
2	D	42	GLU	4.1
3	E	65	GLN	4.1
3	E	169	VAL	4.1
3	H	217	GLU	4.0
2	D	375	LEU	4.0
2	B	466	TRP	4.0
2	D	9	GLY	4.0
2	D	380	ILE	3.9
4	F	124	GLN	3.9
3	E	149	LYS	3.9
3	H	203	VAL	3.9
3	H	199	ILE	3.9
4	F	106	ILE	3.9
4	F	154	GLU	3.9
2	D	1	GLY	3.8
2	B	450	ASN	3.8
3	H	216	ILE	3.8
3	E	177	GLN	3.8
3	E	214	LYS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	28	ASP	3.8
2	D	404	ARG	3.7
1	A	336	GLY	3.7
4	F	169	LYS	3.7
2	D	46	LYS	3.7
3	H	211	LYS	3.7
3	E	123	THR	3.7
2	B	54	ILE	3.7
4	F	121	SER	3.7
4	F	188	ARG	3.7
3	E	189	VAL	3.7
3	E	191	SER	3.7
4	F	144	ILE	3.7
3	H	201	CYS	3.7
2	B	76	ASP	3.6
3	E	85	SER	3.6
1	A	338	HIS	3.6
3	E	13	LYS	3.6
3	H	215	LYS	3.6
4	F	183	LYS	3.6
2	B	376	ASN	3.6
3	H	213	ASP	3.6
2	D	32	PRO	3.6
2	D	52	GLU	3.6
3	E	126	SER	3.5
3	E	117	VAL	3.5
4	F	190	ASN	3.5
4	F	149	LYS	3.5
4	F	170	ASP	3.5
4	L	169	LYS	3.5
1	C	335	ARG	3.5
3	H	208	SER	3.4
3	H	209	SER	3.4
2	D	33	LEU	3.4
4	F	145	ASN	3.4
2	B	50	ALA	3.4
4	F	159	VAL	3.4
2	B	75	GLY	3.4
2	D	378	GLU	3.4
3	H	138	THR	3.4
3	E	178	SER	3.4
4	F	208	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	86	LEU	3.4
3	H	144	LEU	3.4
4	F	178	THR	3.4
4	F	80	SER	3.4
3	H	207	ALA	3.4
2	B	45	LEU	3.3
4	F	185	GLU	3.3
4	F	13	VAL	3.3
3	E	115	VAL	3.3
3	H	169	VAL	3.3
2	D	53	SER	3.3
4	F	105	GLU	3.3
2	D	54	ILE	3.3
3	E	146	CYS	3.3
4	F	167	ASP	3.3
3	E	17	SER	3.2
2	B	39	ASP	3.2
2	D	376	ASN	3.2
3	E	205	HIS	3.2
1	A	454	VAL	3.2
3	E	190	THR	3.2
2	B	381	PRO	3.2
2	D	40	LEU	3.2
2	D	45	LEU	3.2
2	B	379	VAL	3.2
3	H	187	VAL	3.2
2	D	7	THR	3.2
3	E	82	GLN	3.1
2	B	67	ARG	3.1
4	F	83	PHE	3.1
3	E	209	SER	3.1
4	F	207	LYS	3.1
2	D	58	VAL	3.1
4	F	15	LEU	3.1
3	E	156	VAL	3.1
2	B	446	HIS	3.1
1	C	337	PRO	3.0
3	E	213	ASP	3.0
3	E	25	SER	3.0
4	F	103	LYS	3.0
3	E	12	VAL	3.0
2	D	39	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	166	SER	3.0
4	F	153	SER	3.0
2	B	452	ASN	3.0
4	F	189	HIS	3.0
4	F	157	ASN	3.0
3	E	66	GLY	3.0
4	F	173	TYR	3.0
4	L	111	ALA	2.9
1	C	338	HIS	2.9
4	F	163	TRP	2.9
3	E	120	ALA	2.9
4	L	128	GLY	2.9
2	D	44	LEU	2.9
2	B	42	GLU	2.9
2	B	38	CYS	2.9
1	C	249	ASN	2.9
1	C	47	GLN	2.9
3	E	203	VAL	2.8
4	F	187	GLU	2.8
4	F	204	PRO	2.8
2	B	29	GLU	2.8
2	D	79	GLN	2.8
3	E	72	ALA	2.8
3	E	122	THR	2.8
2	D	35	SER	2.8
3	H	196	SER	2.7
2	B	6	THR	2.7
3	H	195	PRO	2.7
4	F	160	LEU	2.7
2	D	143	ARG	2.7
4	L	126	THR	2.7
3	H	214	LYS	2.7
1	C	130	CYS	2.7
2	B	378	GLU	2.7
3	H	167	SER	2.7
4	F	199	LYS	2.7
1	C	246	GLY	2.6
2	B	460	CYS	2.6
3	H	218	PRO	2.6
2	B	31	LEU	2.6
4	L	83	PHE	2.6
3	H	129	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	203	SER	2.6
1	C	90	ARG	2.6
3	H	194	TRP	2.6
2	D	34	GLY	2.5
3	E	186	SER	2.5
2	D	258	LEU	2.5
3	H	212	VAL	2.5
2	D	36	PRO	2.5
3	E	88	SER	2.5
4	F	7	SER	2.5
4	F	177	SER	2.5
4	L	106	ILE	2.5
3	H	177	GLN	2.5
2	D	30	ALA	2.5
2	B	52	GLU	2.5
3	H	130	LEU	2.5
4	L	125	LEU	2.5
3	E	175	VAL	2.5
2	B	374	CYS	2.5
3	E	145	GLY	2.5
3	H	219	ARG	2.5
4	L	170	ASP	2.5
4	F	205	ILE	2.4
4	F	77	SER	2.4
2	D	28	ASP	2.4
3	E	181	TYR	2.4
2	D	129[A]	TRP	2.4
3	E	168	GLY	2.4
4	F	16	GLY	2.4
3	E	188	THR	2.4
2	B	181	LYS	2.4
2	B	445	SER	2.4
4	L	206	VAL	2.4
4	F	18	THR	2.4
3	E	176	LEU	2.3
2	B	7	THR	2.3
3	E	124	ALA	2.3
4	F	11	MET	2.3
4	L	205	ILE	2.3
2	D	3	ASN	2.3
3	E	193	THR	2.3
4	F	196	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	451	GLY	2.3
1	A	45	PRO	2.3
2	D	57	PRO	2.3
3	H	147	LEU	2.3
4	F	161	ASN	2.3
2	D	22	MET	2.3
3	H	165	LEU	2.3
3	E	164	SER	2.2
3	H	206	PRO	2.2
4	F	123	GLU	2.2
4	F	168	SER	2.2
2	B	48	ASN	2.2
2	B	26	CYS	2.2
4	L	105	GLU	2.2
2	D	262	LEU	2.2
4	F	211	ARG	2.2
2	B	19	VAL	2.2
4	L	213	GLU	2.2
1	C	171	PHE	2.2
2	D	21	PRO	2.2
2	B	3	ASN	2.2
3	E	182	THR	2.2
1	A	171	PHE	2.1
2	D	56	PHE	2.1
3	H	143	THR	2.1
1	A	47	GLN	2.1
3	E	172	PHE	2.1
2	B	66	ASP	2.1
4	F	143	ASP	2.1
2	B	98	LYS	2.1
3	E	119	SER	2.1
4	F	201	SER	2.1
2	D	468	GLY	2.1
3	E	92	ALA	2.1
2	B	49	CYS	2.1
3	H	17	SER	2.1
1	C	421	LEU	2.1
2	D	257	ALA	2.1
3	H	161	ASN	2.1
1	C	320	ARG	2.1
4	F	155	ARG	2.1
3	H	166	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	107	CYS	2.1
4	F	165	ASP	2.1
3	H	140	SER	2.1
3	H	162	SER	2.1
4	L	127	SER	2.1
3	E	150	GLY	2.0
3	E	71	THR	2.0
3	E	161	ASN	2.0
3	E	81	LEU	2.0
3	H	171	THR	2.0
2	B	62	ARG	2.0
3	E	28	ASN	2.0
1	C	339	ALA	2.0
4	F	139	PHE	2.0
3	E	114	SER	2.0
4	L	140	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
12	NAG	D	3371	14/15	0.88	0.28	3.76	49,69,80,94	0
12	NAG	B	3371	14/15	0.80	0.27	1.36	51,69,76,85	0
13	NAG	D	3320	14/15	0.94	0.10	-0.78	15,30,43,45	0
11	BMA	B	3322	11/12	0.78	0.26	-	62,94,110,118	0
13	BMA	D	3322	11/12	0.73	0.27	-	100,108,112,113	0
11	NAG	B	3320	14/15	0.98	0.08	-	5,18,26,28	0
11	NAG	B	3321	14/15	0.92	0.11	-	29,49,58,65	0
13	NAG	D	3321	14/15	0.88	0.22	-	38,59,76,89	0
11	MAN	B	3324	11/12	0.80	0.30	-	114,116,117,117	0
11	MAN	B	3323	11/12	0.77	0.25	-	45,79,95,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
12	NAG	D	3372	14/15	0.81	0.44	-	93,108,114,117	0
12	NAG	B	3372	14/15	0.90	0.29	-	78,86,91,94	0
13	MAN	D	3323	11/12	0.65	0.21	-	99,105,107,108	0

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SO4	C	460	5/5	0.88	0.24	8.33	42,44,45,63	5
5	SO4	A	459	5/5	0.92	0.18	5.62	34,51,66,77	0
6	GOL	A	461	6/6	0.85	0.19	4.32	38,52,57,64	0
5	SO4	A	458	5/5	0.87	0.15	1.90	86,97,100,104	0
5	SO4	C	458	5/5	0.87	0.19	0.40	63,79,88,91	0
9	MG	D	2001	1/1	0.95	0.10	-0.62	7,7,7,7	1
7	CA	C	2006	1/1	0.99	0.09	-0.81	24,24,24,24	0
7	CA	D	2003	1/1	0.99	0.14	-0.89	13,13,13,13	0
7	CA	C	2007	1/1	0.97	0.09	-1.03	25,25,25,25	0
8	CL	B	473	1/1	0.99	0.10	-1.68	13,13,13,13	0
8	CL	D	473	1/1	0.98	0.08	-1.76	22,22,22,22	0
7	CA	D	2002	1/1	0.98	0.07	-1.82	17,17,17,17	0
7	CA	C	2004	1/1	0.96	0.05	-1.90	34,34,34,34	0
9	MG	B	2001	1/1	0.99	0.09	-1.93	0,0,0,0	1
7	CA	A	2006	1/1	0.99	0.09	-1.97	0,0,0,0	0
7	CA	C	2005	1/1	0.94	0.04	-2.02	29,29,29,29	0
7	CA	A	2004	1/1	0.98	0.04	-2.15	11,11,11,11	0
7	CA	A	2005	1/1	0.99	0.07	-2.40	3,3,3,3	0
7	CA	B	2002	1/1	0.99	0.05	-2.96	14,14,14,14	0
7	CA	B	2003	1/1	1.00	0.13	-3.38	0,0,0,0	0
7	CA	A	2007	1/1	1.00	0.06	-4.10	1,1,1,1	0
8	CL	C	462	1/1	0.89	0.24	-	57,57,57,57	0
5	SO4	A	460	5/5	0.98	0.14	-	40,46,55,60	0
5	SO4	L	215	5/5	0.93	0.21	-	79,80,86,89	0
5	SO4	C	459	5/5	0.90	0.22	-	85,97,101,104	0
10	NAG	D	3099	14/15	0.83	0.34	-	61,76,81,81	0
8	CL	C	461	1/1	0.93	0.08	-	42,42,42,42	0
10	NAG	B	3099	14/15	0.83	0.37	-	75,90,97,102	0

6.5 Other polymers

There are no such residues in this entry.