Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:00 PM GMT

PDB ID	:	4UM8
Title	:	Crystal structure of alpha V beta 6
Authors	:	Dong, X.; Springer, T.A.
Deposited on	:	2014-05-15
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

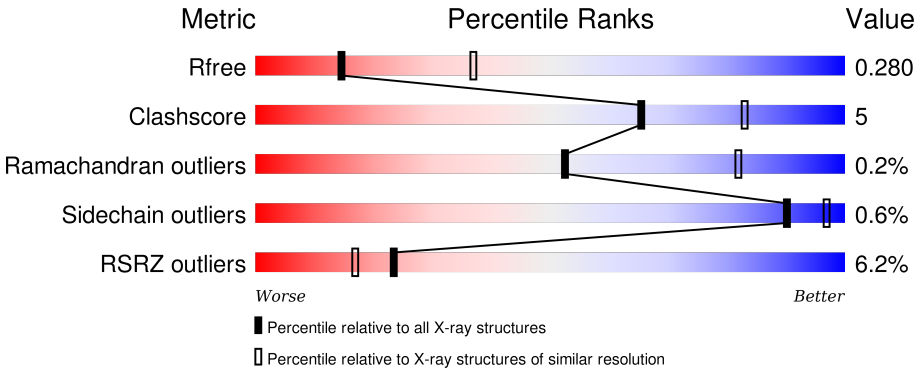
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 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 <=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	681	2% 77% 10% 13%
1	C	681	8% 73% 13% 14%
2	B	788	4% 47% 6% 46%
2	D	788	3% 45% 7% 47%

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
4	SO4	A	1598	-	-	-	X
6	CA	A	2002	-	-	-	X
7	NAG	D	3370	-	-	-	X
7	MAN	D	3373	-	-	-	X
9	NAG	C	3266	X	-	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 16497 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-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	0	0
			4579	2904	776	878	21			
1	C	588	Total	C	N	O	S	0	0	0
			4559	2893	773	872	21			

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	596	THR	-	EXPRESSION TAG	UNP P06756
A	597	GLY	-	EXPRESSION TAG	UNP P06756
A	598	GLY	-	EXPRESSION TAG	UNP P06756
A	599	LEU	-	EXPRESSION TAG	UNP P06756
A	600	GLU	-	EXPRESSION TAG	UNP P06756
A	601	VAL	-	EXPRESSION TAG	UNP P06756
A	602	LEU	-	EXPRESSION TAG	UNP P06756
A	603	PHE	-	EXPRESSION TAG	UNP P06756
A	604	GLN	-	EXPRESSION TAG	UNP P06756
A	605	GLY	-	EXPRESSION TAG	UNP P06756
A	606	PRO	-	EXPRESSION TAG	UNP P06756
A	607	GLY	-	EXPRESSION TAG	UNP P06756
A	608	GLU	-	EXPRESSION TAG	UNP P06756
A	609	ASN	-	EXPRESSION TAG	UNP P06756
A	610	ALA	-	EXPRESSION TAG	UNP P06756
A	611	GLN	-	EXPRESSION TAG	UNP P06756
A	612	LEU	-	EXPRESSION TAG	UNP P06756
A	613	GLU	-	EXPRESSION TAG	UNP P06756
A	614	LYS	-	EXPRESSION TAG	UNP P06756
A	615	GLU	-	EXPRESSION TAG	UNP P06756
A	616	LEU	-	EXPRESSION TAG	UNP P06756
A	617	GLN	-	EXPRESSION TAG	UNP P06756
A	618	ALA	-	EXPRESSION TAG	UNP P06756
A	619	LEU	-	EXPRESSION TAG	UNP P06756
A	620	GLU	-	EXPRESSION TAG	UNP P06756

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Chain	Residue	Modelled	Actual	Comment	Reference
A	621	LYS	-	EXPRESSION TAG	UNP P06756
A	622	GLU	-	EXPRESSION TAG	UNP P06756
A	623	ASN	-	EXPRESSION TAG	UNP P06756
A	624	ALA	-	EXPRESSION TAG	UNP P06756
A	625	GLN	-	EXPRESSION TAG	UNP P06756
A	626	LEU	-	EXPRESSION TAG	UNP P06756
A	627	GLU	-	EXPRESSION TAG	UNP P06756
A	628	TRP	-	EXPRESSION TAG	UNP P06756
A	629	GLU	-	EXPRESSION TAG	UNP P06756
A	630	LEU	-	EXPRESSION TAG	UNP P06756
A	631	GLN	-	EXPRESSION TAG	UNP P06756
A	632	ALA	-	EXPRESSION TAG	UNP P06756
A	633	LEU	-	EXPRESSION TAG	UNP P06756
A	634	GLU	-	EXPRESSION TAG	UNP P06756
A	635	LYS	-	EXPRESSION TAG	UNP P06756
A	636	GLU	-	EXPRESSION TAG	UNP P06756
A	637	LEU	-	EXPRESSION TAG	UNP P06756
A	638	ALA	-	EXPRESSION TAG	UNP P06756
A	639	GLN	-	EXPRESSION TAG	UNP P06756
A	640	THR	-	EXPRESSION TAG	UNP P06756
A	641	THR	-	EXPRESSION TAG	UNP P06756
A	642	GLY	-	EXPRESSION TAG	UNP P06756
A	643	TRP	-	EXPRESSION TAG	UNP P06756
A	644	ARG	-	EXPRESSION TAG	UNP P06756
A	645	GLY	-	EXPRESSION TAG	UNP P06756
A	646	GLY	-	EXPRESSION TAG	UNP P06756
A	647	HIS	-	EXPRESSION TAG	UNP P06756
A	648	VAL	-	EXPRESSION TAG	UNP P06756
A	649	VAL	-	EXPRESSION TAG	UNP P06756
A	650	GLU	-	EXPRESSION TAG	UNP P06756
A	651	GLY	-	EXPRESSION TAG	UNP P06756
A	652	LEU	-	EXPRESSION TAG	UNP P06756
A	653	ALA	-	EXPRESSION TAG	UNP P06756
A	654	GLY	-	EXPRESSION TAG	UNP P06756
A	655	GLU	-	EXPRESSION TAG	UNP P06756
A	656	LEU	-	EXPRESSION TAG	UNP P06756
A	657	GLU	-	EXPRESSION TAG	UNP P06756
A	658	GLN	-	EXPRESSION TAG	UNP P06756
A	659	LEU	-	EXPRESSION TAG	UNP P06756
A	660	ARG	-	EXPRESSION TAG	UNP P06756
A	661	ALA	-	EXPRESSION TAG	UNP P06756
A	662	ARG	-	EXPRESSION TAG	UNP P06756

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Chain	Residue	Modelled	Actual	Comment	Reference
A	663	LEU	-	EXPRESSION TAG	UNP P06756
A	664	GLU	-	EXPRESSION TAG	UNP P06756
A	665	HIS	-	EXPRESSION TAG	UNP P06756
A	666	HIS	-	EXPRESSION TAG	UNP P06756
A	667	PRO	-	EXPRESSION TAG	UNP P06756
A	668	GLN	-	EXPRESSION TAG	UNP P06756
A	669	GLY	-	EXPRESSION TAG	UNP P06756
A	670	GLN	-	EXPRESSION TAG	UNP P06756
A	671	ARG	-	EXPRESSION TAG	UNP P06756
A	672	GLU	-	EXPRESSION TAG	UNP P06756
A	673	PRO	-	EXPRESSION TAG	UNP P06756
A	674	ALA	-	EXPRESSION TAG	UNP P06756
A	675	GLY	-	EXPRESSION TAG	UNP P06756
A	676	HIS	-	EXPRESSION TAG	UNP P06756
A	677	HIS	-	EXPRESSION TAG	UNP P06756
A	678	HIS	-	EXPRESSION TAG	UNP P06756
A	679	HIS	-	EXPRESSION TAG	UNP P06756
A	680	HIS	-	EXPRESSION TAG	UNP P06756
A	681	HIS	-	EXPRESSION TAG	UNP P06756
A	400	CYS	MET	ENGINEERED MUTATION	UNP P06756
C	596	THR	-	EXPRESSION TAG	UNP P06756
C	597	GLY	-	EXPRESSION TAG	UNP P06756
C	598	GLY	-	EXPRESSION TAG	UNP P06756
C	599	LEU	-	EXPRESSION TAG	UNP P06756
C	600	GLU	-	EXPRESSION TAG	UNP P06756
C	601	VAL	-	EXPRESSION TAG	UNP P06756
C	602	LEU	-	EXPRESSION TAG	UNP P06756
C	603	PHE	-	EXPRESSION TAG	UNP P06756
C	604	GLN	-	EXPRESSION TAG	UNP P06756
C	605	GLY	-	EXPRESSION TAG	UNP P06756
C	606	PRO	-	EXPRESSION TAG	UNP P06756
C	607	GLY	-	EXPRESSION TAG	UNP P06756
C	608	GLU	-	EXPRESSION TAG	UNP P06756
C	609	ASN	-	EXPRESSION TAG	UNP P06756
C	610	ALA	-	EXPRESSION TAG	UNP P06756
C	611	GLN	-	EXPRESSION TAG	UNP P06756
C	612	LEU	-	EXPRESSION TAG	UNP P06756
C	613	GLU	-	EXPRESSION TAG	UNP P06756
C	614	LYS	-	EXPRESSION TAG	UNP P06756
C	615	GLU	-	EXPRESSION TAG	UNP P06756
C	616	LEU	-	EXPRESSION TAG	UNP P06756
C	617	GLN	-	EXPRESSION TAG	UNP P06756

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Chain	Residue	Modelled	Actual	Comment	Reference
C	618	ALA	-	EXPRESSION TAG	UNP P06756
C	619	LEU	-	EXPRESSION TAG	UNP P06756
C	620	GLU	-	EXPRESSION TAG	UNP P06756
C	621	LYS	-	EXPRESSION TAG	UNP P06756
C	622	GLU	-	EXPRESSION TAG	UNP P06756
C	623	ASN	-	EXPRESSION TAG	UNP P06756
C	624	ALA	-	EXPRESSION TAG	UNP P06756
C	625	GLN	-	EXPRESSION TAG	UNP P06756
C	626	LEU	-	EXPRESSION TAG	UNP P06756
C	627	GLU	-	EXPRESSION TAG	UNP P06756
C	628	TRP	-	EXPRESSION TAG	UNP P06756
C	629	GLU	-	EXPRESSION TAG	UNP P06756
C	630	LEU	-	EXPRESSION TAG	UNP P06756
C	631	GLN	-	EXPRESSION TAG	UNP P06756
C	632	ALA	-	EXPRESSION TAG	UNP P06756
C	633	LEU	-	EXPRESSION TAG	UNP P06756
C	634	GLU	-	EXPRESSION TAG	UNP P06756
C	635	LYS	-	EXPRESSION TAG	UNP P06756
C	636	GLU	-	EXPRESSION TAG	UNP P06756
C	637	LEU	-	EXPRESSION TAG	UNP P06756
C	638	ALA	-	EXPRESSION TAG	UNP P06756
C	639	GLN	-	EXPRESSION TAG	UNP P06756
C	640	THR	-	EXPRESSION TAG	UNP P06756
C	641	THR	-	EXPRESSION TAG	UNP P06756
C	642	GLY	-	EXPRESSION TAG	UNP P06756
C	643	TRP	-	EXPRESSION TAG	UNP P06756
C	644	ARG	-	EXPRESSION TAG	UNP P06756
C	645	GLY	-	EXPRESSION TAG	UNP P06756
C	646	GLY	-	EXPRESSION TAG	UNP P06756
C	647	HIS	-	EXPRESSION TAG	UNP P06756
C	648	VAL	-	EXPRESSION TAG	UNP P06756
C	649	VAL	-	EXPRESSION TAG	UNP P06756
C	650	GLU	-	EXPRESSION TAG	UNP P06756
C	651	GLY	-	EXPRESSION TAG	UNP P06756
C	652	LEU	-	EXPRESSION TAG	UNP P06756
C	653	ALA	-	EXPRESSION TAG	UNP P06756
C	654	GLY	-	EXPRESSION TAG	UNP P06756
C	655	GLU	-	EXPRESSION TAG	UNP P06756
C	656	LEU	-	EXPRESSION TAG	UNP P06756
C	657	GLU	-	EXPRESSION TAG	UNP P06756
C	658	GLN	-	EXPRESSION TAG	UNP P06756
C	659	LEU	-	EXPRESSION TAG	UNP P06756

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Chain	Residue	Modelled	Actual	Comment	Reference
C	660	ARG	-	EXPRESSION TAG	UNP P06756
C	661	ALA	-	EXPRESSION TAG	UNP P06756
C	662	ARG	-	EXPRESSION TAG	UNP P06756
C	663	LEU	-	EXPRESSION TAG	UNP P06756
C	664	GLU	-	EXPRESSION TAG	UNP P06756
C	665	HIS	-	EXPRESSION TAG	UNP P06756
C	666	HIS	-	EXPRESSION TAG	UNP P06756
C	667	PRO	-	EXPRESSION TAG	UNP P06756
C	668	GLN	-	EXPRESSION TAG	UNP P06756
C	669	GLY	-	EXPRESSION TAG	UNP P06756
C	670	GLN	-	EXPRESSION TAG	UNP P06756
C	671	ARG	-	EXPRESSION TAG	UNP P06756
C	672	GLU	-	EXPRESSION TAG	UNP P06756
C	673	PRO	-	EXPRESSION TAG	UNP P06756
C	674	ALA	-	EXPRESSION TAG	UNP P06756
C	675	GLY	-	EXPRESSION TAG	UNP P06756
C	676	HIS	-	EXPRESSION TAG	UNP P06756
C	677	HIS	-	EXPRESSION TAG	UNP P06756
C	678	HIS	-	EXPRESSION TAG	UNP P06756
C	679	HIS	-	EXPRESSION TAG	UNP P06756
C	680	HIS	-	EXPRESSION TAG	UNP P06756
C	681	HIS	-	EXPRESSION TAG	UNP P06756
C	400	CYS	MET	ENGINEERED MUTATION	UNP P06756

- Molecule 2 is a protein called INTEGRIN BETA-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3252	2051	548	628	25			
2	D	414	Total	C	N	O	S	0	0	0
			3202	2020	539	618	25			

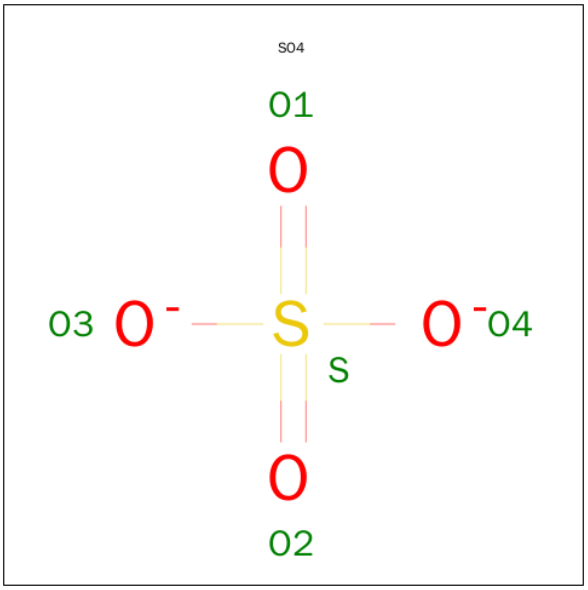
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	270	CYS	ILE	ENGINEERED MUTATION	UNP P18564
D	270	CYS	ILE	ENGINEERED MUTATION	UNP P18564

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	C	2	Total Cl 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ni 1 1	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total Ca 4 4	0	0
6	D	1	Total Ca 1 1	0	0
6	C	4	Total Ca 4 4	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 8 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 9 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	6	Total C N O 72 40 2 30	0	0
9	C	6	Total C N O 72 40 2 30	0	0

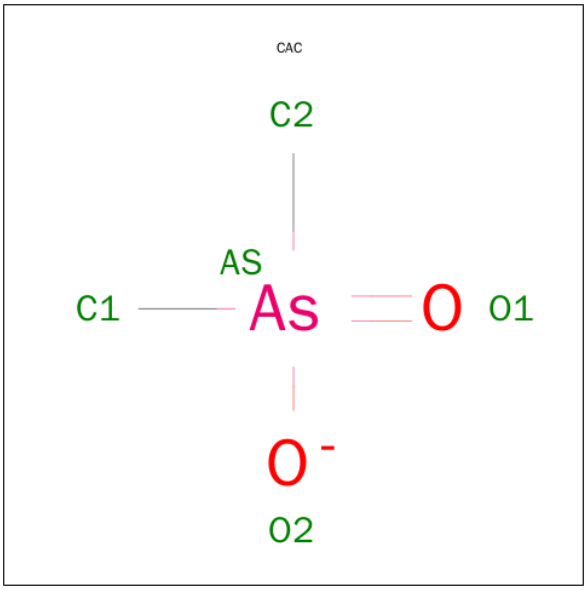
- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	3	Total C N O 39 22 2 15	0	0
10	C	3	Total C N O 39 22 2 15	0	0

- Molecule 11 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	2	Total C N O 28 16 2 10	0	0
11	C	2	Total C N O 28 16 2 10	0	0
11	C	2	Total C N O 28 16 2 10	0	0

- Molecule 12 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).

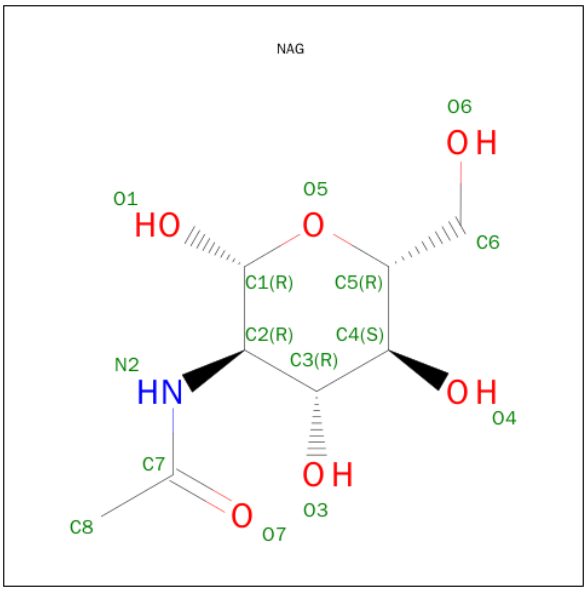


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total As C O 5 1 2 2	0	0
12	D	1	Total As C O 5 1 2 2	0	0

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 14 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 15 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	7	Total C N O 83 46 2 35	0	0

- Molecule 16 is water.

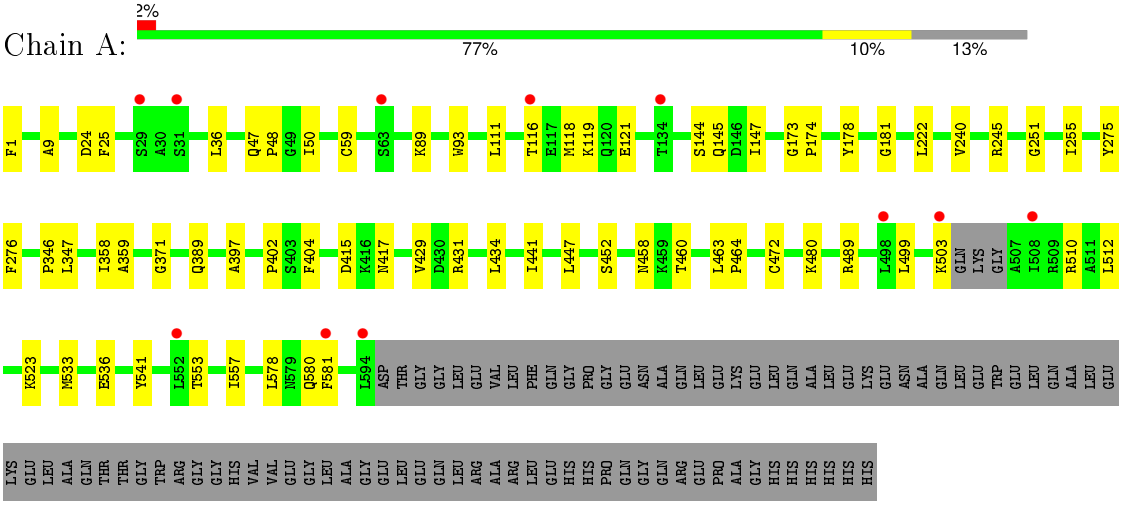
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	65	Total O 65 65	0	0
16	B	32	Total O 32 32	0	0
16	C	38	Total O 38 38	0	0
16	D	26	Total O 26 26	0	0

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.

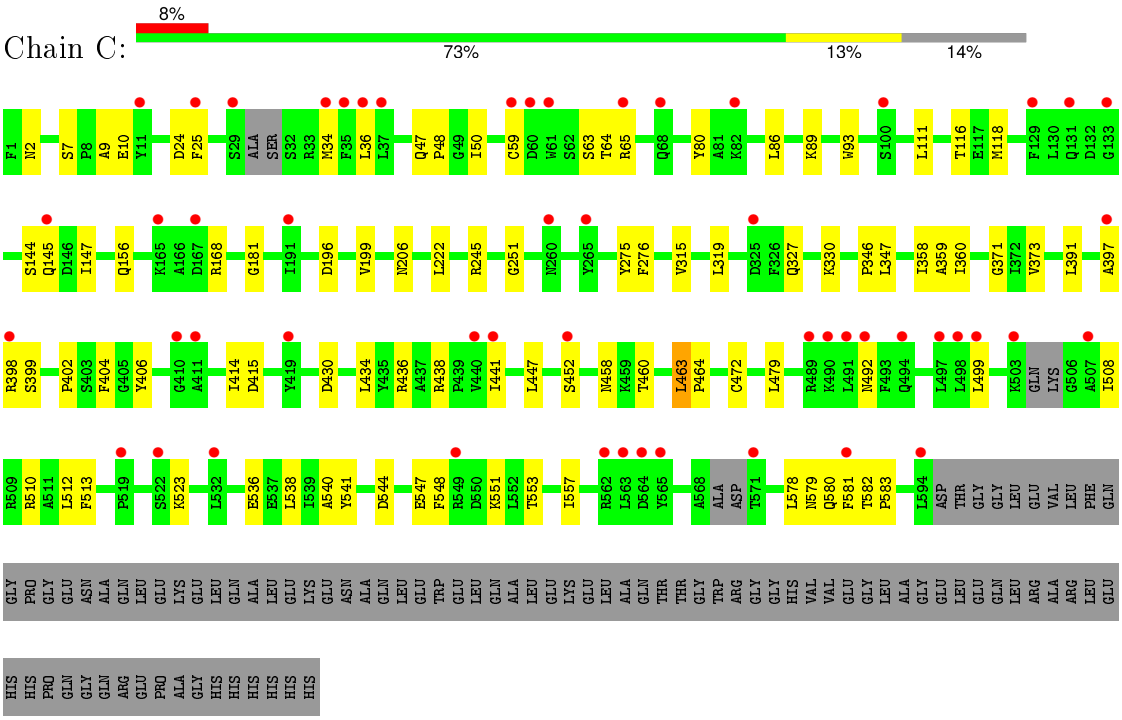
- Molecule 1: INTEGRIN ALPHA-V

Chain A:



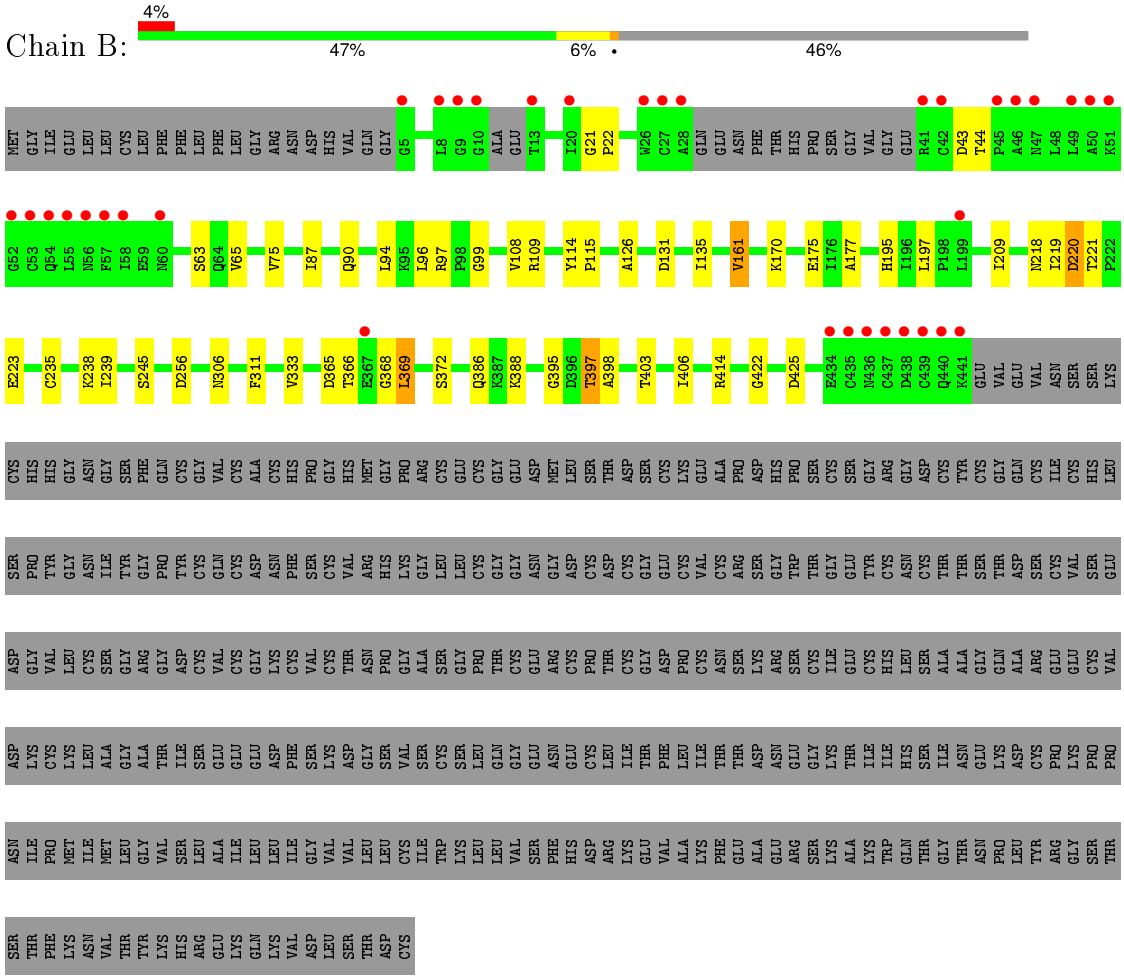
- Molecule 1: INTEGRIN ALPHA-V

Chain C:



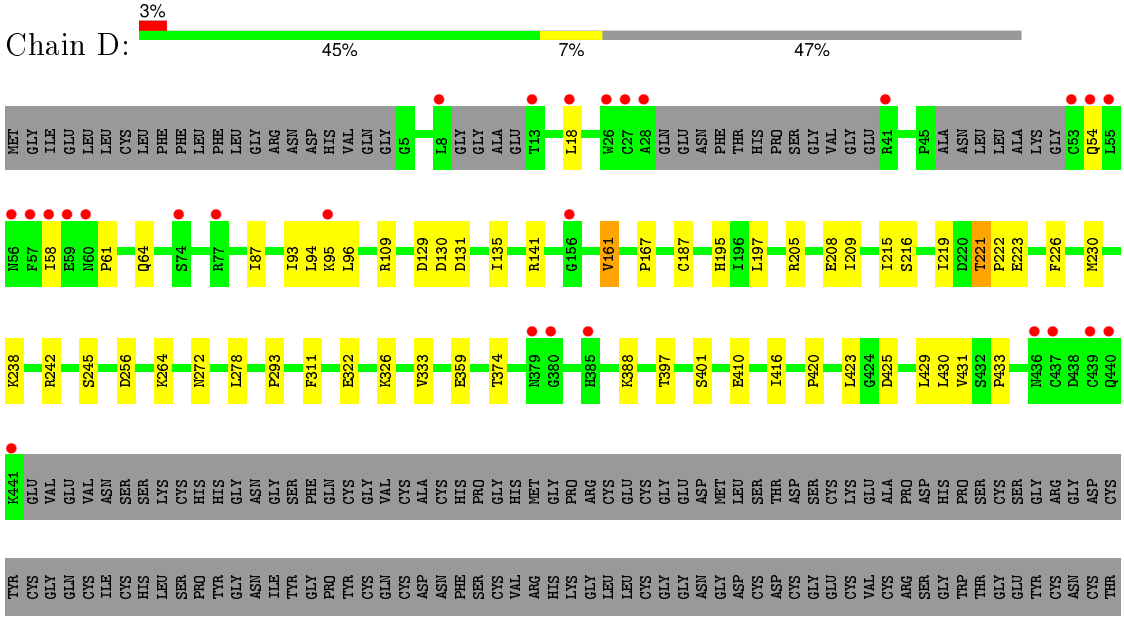
• Molecule 2: INTEGRIN BETA-6

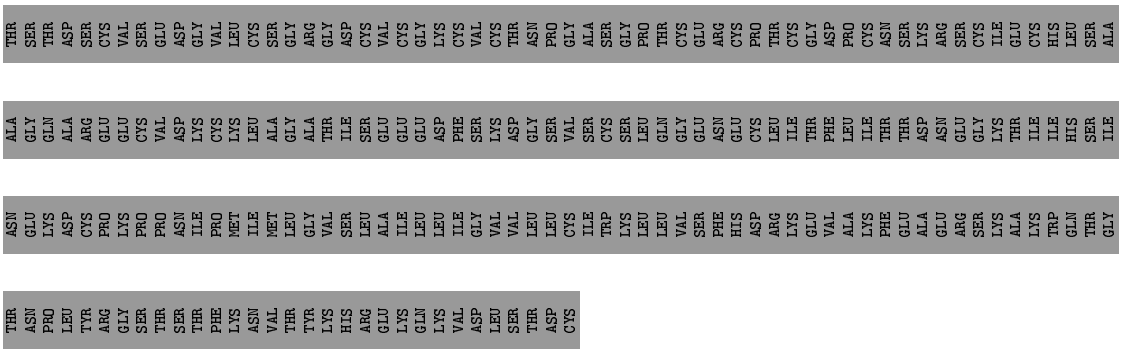
Chain B:



• Molecule 2: INTEGRIN BETA-6

Chain D:




THR SER THR ASP SER CYS VAL SER GLU ASP GLY VAL LEU CYS SER GLY ARG GLY ASP CYS VAL CYS GLY LYS CYS VAL CYS THR ASN PRO GLY ALA SER GLY PRO THR CYS GLU ARG CYS PRO THR CYS GLY ASP PRO CYS ASN SER LYS ARG SER CYS ILE GLU CYS HIS LEU SER ALA
ALA GLY GLN ALA ARG GLU GLU CYS VAL ASP LYS CYS LYS LEU ALA GLY ALA THR ILE SER GLU GLU GLU ASP PHE SER LYS ASP GLY SER VAL SER CYS SER LEU GLN GLY GLU ASN GLU CYS LEU ILE THR PHE LEU ILE THR THR ASP ASN GLU GLY LYS THR ILE ILE HIS SER ILE
ASN GLU LYS ASP CYS PRO LYS PRO PRO ASN ILE PRO MET ILE MET LEU GLY VAL SER LEU ALA ILE LEU LEU ILE GLY VAL VAL LEU LEU CYS ILE TRP LYS LEU LEU VAL SER PHE HIS ASP ARG LYS GLU VAL ALA LYS PHE GLU ALA GLU ARG SER LYS ALA LYS TRP GLN THR GLY
THR ASN PRO LEU TYR ARG GLY SER THR SER THR PHE LYS ASN VAL THR TYR LYS HIS ARG GLU LYS GLN LYS VAL ASP LEU SER THR ASP CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	184.45Å 170.01Å 102.39Å 90.00° 98.68° 90.00°	Depositor
Resolution (Å)	48.66 – 2.85 48.66 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.4 (48.66-2.85) 96.4 (48.66-2.85)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.86Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.238 , 0.281 0.238 , 0.280	Depositor DCC
R_{free} test set	1796 reflections (2.57%)	DCC
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 75.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 69928 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	16497	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, MG, BMA, NAG, CL, CA, SO4, CAC, 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	0.21	0/4682	0.39	0/6339
1	C	0.21	0/4660	0.37	0/6305
2	B	0.21	0/3308	0.40	0/4481
2	D	0.21	0/3258	0.39	0/4413
All	All	0.21	0/15908	0.39	0/21538

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
9	C	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	C	3266	NAG	C1

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	4579	0	4426	34	1
1	C	4559	0	4408	51	1
2	B	3252	0	3234	35	0
2	D	3202	0	3176	36	0
3	A	1	0	0	0	0
3	C	2	0	0	0	0
4	A	15	0	0	1	0
5	A	1	0	0	0	0
6	A	4	0	0	0	0
6	B	1	0	0	0	0
6	C	4	0	0	0	0
6	D	1	0	0	0	0
7	A	50	0	43	1	0
7	C	50	0	43	1	0
7	D	50	0	43	2	0
8	A	122	0	104	1	0
9	A	72	0	61	1	0
9	C	72	0	61	1	0
10	A	39	0	34	1	0
10	C	39	0	34	0	0
11	A	28	0	25	0	0
11	C	56	0	50	0	0
12	B	5	0	0	0	0
12	D	5	0	0	0	0
13	B	1	0	0	0	0
13	D	1	0	0	0	0
14	B	14	0	13	0	0
14	D	28	0	26	0	0
15	C	83	0	70	2	0
16	A	65	0	0	0	0
16	B	32	0	0	0	0
16	C	38	0	0	0	0
16	D	26	0	0	1	0
All	All	16497	0	15851	160	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 5.

All (160) 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:B:109:ARG:NH2	2:B:397:THR:OG1	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:ASP:N	2:B:220:ASP:OD1	2.24	0.70
1:C:116:THR:HG22	1:C:118:MET:H	1.55	0.70
1:A:480:LYS:HB2	1:A:533:MET:HB3	1.74	0.70
1:A:116:THR:HG22	1:A:118:MET:H	1.57	0.70
1:C:245:ARG:NH2	2:D:256:ASP:OD2	2.26	0.69
1:C:406:TYR:OH	2:D:264:LYS:NZ	2.25	0.69
2:D:230:MET:HG2	2:D:272:ASN:HD21	1.58	0.67
1:C:548:PHE:O	1:C:551:LYS:NZ	2.29	0.65
2:D:420:PRO:HG2	2:D:423:LEU:HB2	1.77	0.64
1:C:371:GLY:HA3	1:C:404:PHE:HB3	1.78	0.64
2:B:366:THR:HG22	2:B:368:GLY:H	1.63	0.63
1:A:24:ASP:OD1	1:A:25:PHE:N	2.33	0.61
1:A:245:ARG:NH2	2:B:256:ASP:OD2	2.33	0.61
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.82	0.60
1:C:24:ASP:OD1	1:C:25:PHE:N	2.34	0.60
2:B:369:LEU:HD11	2:B:406:ILE:HG12	1.84	0.60
2:B:170:LYS:HB2	2:B:175:GLU:HG2	1.84	0.60
1:C:347:LEU:HD11	1:C:359:ALA:HB2	1.83	0.59
1:C:510:ARG:NH1	1:C:553:THR:O	2.33	0.59
1:C:398:ARG:NH1	1:C:430:ASP:OD2	2.36	0.59
15:C:3524:NAG:O3	15:C:3525:NAG:N2	2.37	0.58
2:D:187:CYS:HB3	2:D:216:SER:O	2.04	0.58
1:C:319:LEU:HB2	1:C:327:GLN:HB3	1.85	0.57
1:A:489:ARG:NH1	4:A:1596:SO4:O2	2.37	0.57
2:D:359:GLU:HB2	2:D:388:LYS:HD3	1.85	0.57
1:A:50:ILE:HD13	1:A:89:LYS:HB2	1.86	0.57
2:D:221:THR:HG22	2:D:222:PRO:HD2	1.86	0.56
2:D:322:GLU:HG3	2:D:333:VAL:HG21	1.86	0.56
2:D:141:ARG:NH1	16:D:4005:HOH:O	2.39	0.55
1:A:415:ASP:OD2	1:A:417:ASN:ND2	2.39	0.55
1:A:181:GLY:HA3	1:A:222:LEU:HB3	1.88	0.55
2:D:18:LEU:HD13	2:D:61:PRO:HG3	1.88	0.55
1:C:34:MET:HE2	1:C:414:ILE:HA	1.89	0.55
1:C:93:TRP:CD1	1:C:111:LEU:HD12	2.42	0.55
1:A:503:LYS:HD3	1:A:553:THR:HG21	1.88	0.54
2:B:115:PRO:HB2	2:B:245:SER:HB3	1.90	0.54
1:C:346:PRO:HA	1:C:358:ILE:HG13	1.89	0.54
1:A:371:GLY:HA3	1:A:404:PHE:HB3	1.88	0.54
2:B:366:THR:HB	2:B:369:LEU:H	1.72	0.54
1:C:330:LYS:O	7:D:3373:MAN:O3	2.25	0.53
1:A:251:GLY:HA3	1:A:276:PHE:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:CYS:HA	1:A:541:TYR:HA	1.90	0.53
2:B:366:THR:HB	2:B:369:LEU:HB2	1.90	0.53
1:A:347:LEU:HD11	1:A:359:ALA:HB2	1.91	0.53
2:B:87:ILE:HG22	2:B:425:ASP:HB3	1.91	0.53
1:C:116:THR:HG23	1:C:147:ILE:HG21	1.90	0.52
1:C:7:SER:O	1:C:436:ARG:NH2	2.41	0.52
2:B:22:PRO:HG3	2:B:99:GLY:HA3	1.91	0.52
2:B:75:VAL:HG21	2:B:109:ARG:HH11	1.75	0.51
2:D:226:PHE:HB3	2:D:293:PRO:HG2	1.91	0.51
1:C:544:ASP:HB3	1:C:547:GLU:HG3	1.93	0.51
2:D:129:ASP:HA	2:D:215:ILE:HD11	1.93	0.51
2:B:126:ALA:HB3	2:B:218:ASN:HB3	1.93	0.51
1:C:397:ALA:HB2	1:C:402:PRO:HD3	1.92	0.51
1:A:144:SER:OG	1:A:145:GLN:N	2.44	0.51
1:A:36:LEU:HB2	1:A:59:CYS:HB2	1.93	0.51
1:C:315:VAL:HG21	1:C:360:ILE:HD13	1.93	0.50
1:C:508:ILE:HD13	1:C:548:PHE:HB3	1.93	0.50
1:A:441:ILE:HB	1:A:578:LEU:HD23	1.92	0.50
1:C:2:ASN:O	1:C:438:ARG:N	2.37	0.49
2:B:87:ILE:O	2:B:90:GLN:NE2	2.43	0.49
2:B:311:PHE:HB2	2:B:333:VAL:HG12	1.94	0.49
1:A:397:ALA:HB2	1:A:402:PRO:HD3	1.95	0.49
2:D:410:GLU:HB2	2:D:433:PRO:HG3	1.94	0.49
1:C:499:LEU:HD12	1:C:512:LEU:HA	1.95	0.48
1:C:50:ILE:HD13	1:C:89:LYS:HB2	1.94	0.48
2:D:238:LYS:NZ	2:D:278:LEU:O	2.46	0.48
1:C:513:PHE:HA	1:C:540:ALA:HA	1.95	0.48
1:C:373:VAL:HB	1:C:391:LEU:HB2	1.95	0.48
1:A:499:LEU:HD12	1:A:512:LEU:HA	1.95	0.48
2:D:93:ILE:HG12	2:D:430:LEU:HB3	1.95	0.47
1:C:36:LEU:HB2	1:C:59:CYS:HB2	1.94	0.47
2:D:131:ASP:O	2:D:135:ILE:HG13	2.14	0.47
2:D:195:HIS:NE2	2:D:238:LYS:O	2.35	0.47
2:B:195:HIS:NE2	2:B:238:LYS:O	2.43	0.47
1:A:523:LYS:HG2	1:A:536:GLU:OE1	2.14	0.47
1:C:441:ILE:HB	1:C:578:LEU:HD23	1.96	0.47
1:C:181:GLY:HA3	1:C:222:LEU:HB3	1.96	0.47
2:D:311:PHE:HB2	2:D:333:VAL:HG12	1.96	0.47
2:D:242:ARG:HB2	2:D:245:SER:OG	2.14	0.47
1:C:523:LYS:HG2	1:C:536:GLU:OE1	2.15	0.47
1:A:116:THR:HG23	1:A:147:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:SER:OG	1:C:64:THR:N	2.47	0.47
1:C:10:GLU:H	1:C:65:ARG:NH1	2.12	0.47
7:A:3046:BMA:H62	7:A:3047:MAN:H2	1.59	0.47
1:A:346:PRO:HA	1:A:358:ILE:HG13	1.97	0.47
1:A:93:TRP:CD1	1:A:111:LEU:HD12	2.50	0.46
1:C:472:CYS:HA	1:C:541:TYR:HA	1.97	0.46
1:A:458:ASN:OD1	1:A:460:THR:OG1	2.18	0.46
2:D:109:ARG:HH21	2:D:397:THR:HB	1.80	0.46
2:B:108:VAL:HG23	2:B:398:ALA:HB3	1.98	0.46
2:D:94:LEU:HD21	2:D:96:LEU:HD12	1.98	0.46
2:B:386:GLN:NE2	2:B:388:LYS:O	2.46	0.46
7:D:3372:BMA:H61	7:D:3373:MAN:H2	1.55	0.45
15:C:3526:BMA:H61	15:C:3527:MAN:H2	1.30	0.45
2:D:64:GLN:HG2	2:D:95:LYS:HD2	1.99	0.45
2:B:43:ASP:OD1	2:B:44:THR:N	2.47	0.45
2:B:22:PRO:HA	2:B:97:ARG:NH1	2.32	0.45
1:C:251:GLY:HA3	1:C:276:PHE:HB3	1.98	0.45
2:B:372:SER:HG	2:B:403:THR:HG1	1.50	0.44
2:D:205:ARG:NH1	2:D:208:GLU:OE1	2.49	0.44
2:B:75:VAL:HG21	2:B:109:ARG:NH1	2.33	0.44
1:C:144:SER:OG	1:C:145:GLN:N	2.48	0.44
2:B:21:GLY:HA2	2:B:22:PRO:HD3	1.86	0.44
2:D:109:ARG:NH2	2:D:397:THR:HB	2.33	0.44
2:B:235:CYS:HB2	2:B:239:ILE:HD13	2.00	0.44
2:B:109:ARG:NE	2:B:395:GLY:O	2.51	0.44
2:B:22:PRO:HA	2:B:97:ARG:HH11	1.83	0.43
1:C:582:THR:HA	1:C:583:PRO:HD3	1.88	0.43
1:C:463:LEU:HD23	1:C:464:PRO:HD2	2.00	0.43
1:C:580:GLN:HG3	1:C:581:PHE:H	1.84	0.43
1:A:9:ALA:HB3	1:A:434:LEU:HB3	2.01	0.43
1:C:80:TYR:HB2	1:C:86:LEU:HD13	2.01	0.43
10:A:3459:NAG:H4	10:A:3460:BMA:O2	2.14	0.43
2:D:416:ILE:HB	2:D:429:LEU:HB2	2.00	0.43
1:A:47:GLN:HA	1:A:48:PRO:HD3	1.90	0.43
2:B:114:TYR:HA	2:B:115:PRO:HD3	1.91	0.42
1:C:579:ASN:OD1	1:C:580:GLN:N	2.52	0.42
2:B:197:LEU:HD22	2:B:209:ILE:HD12	2.01	0.42
9:C:3268:BMA:H62	9:C:3270:MAN:H2	1.76	0.42
1:A:429:VAL:HG23	1:A:431:ARG:HG2	2.01	0.42
1:A:463:LEU:HD23	1:A:464:PRO:HD2	2.02	0.42
9:A:3268:BMA:H62	9:A:3270:MAN:H2	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:LEU:HA	1:C:479:LEU:HD23	1.91	0.42
2:D:94:LEU:HD22	2:D:431:VAL:HG22	2.00	0.42
2:D:374:THR:OG1	2:D:401:SER:HB2	2.20	0.42
2:D:161:VAL:O	2:D:223:GLU:HB3	2.20	0.42
1:C:398:ARG:HG3	1:C:399:SER:H	1.84	0.42
1:A:510:ARG:NH1	1:A:553:THR:O	2.52	0.42
2:B:161:VAL:O	2:B:223:GLU:HB3	2.20	0.42
2:B:131:ASP:O	2:B:135:ILE:HG13	2.20	0.42
1:A:119:LYS:HG3	1:A:121:GLU:HG2	2.02	0.42
1:A:580:GLN:HG3	1:A:581:PHE:H	1.85	0.42
2:D:87:ILE:HG22	2:D:425:ASP:HB3	2.02	0.42
1:A:447:LEU:HD21	1:A:557:ILE:HG22	2.02	0.42
1:C:492:ASN:N	1:C:492:ASN:OD1	2.47	0.41
2:B:219:ILE:HG22	2:B:221:THR:H	1.85	0.41
2:D:130:ASP:N	2:D:130:ASP:OD1	2.53	0.41
1:A:240:VAL:HG22	1:A:255:ILE:HG12	2.01	0.41
1:C:47:GLN:HA	1:C:48:PRO:HD3	1.89	0.41
1:C:147:ILE:HG13	1:C:147:ILE:H	1.67	0.41
1:C:9:ALA:HB3	1:C:434:LEU:HB3	2.03	0.41
2:D:322:GLU:O	2:D:326:LYS:HG3	2.20	0.41
2:D:197:LEU:HD22	2:D:209:ILE:HD12	2.01	0.41
2:B:63:SER:HB3	2:B:96:LEU:HD23	2.02	0.41
1:C:196:ASP:HB3	1:C:199:VAL:HB	2.03	0.41
2:D:219:ILE:HG22	2:D:221:THR:H	1.84	0.41
2:D:54:GLN:O	2:D:58:ILE:HG13	2.21	0.41
7:C:3459:NAG:H61	7:C:3460:BMA:O2	2.21	0.41
1:A:173:GLY:HA2	1:A:174:PRO:HD3	1.90	0.41
1:C:458:ASN:OD1	1:C:460:THR:OG1	2.33	0.41
2:B:65:VAL:HG12	2:B:94:LEU:HD13	2.02	0.41
1:C:156:GLN:OE1	2:D:167:PRO:HG3	2.21	0.41
2:B:306:ASN:HD21	2:B:422:GLY:C	2.24	0.40
2:B:177:ALA:HA	2:D:374:THR:HG21	2.03	0.40
1:C:415:ASP:OD1	1:C:415:ASP:N	2.51	0.40
1:C:447:LEU:HD21	1:C:557:ILE:HG22	2.03	0.40
1:C:168:ARG:NH2	1:C:206:ASN:O	2.54	0.40
8:A:3526:BMA:H61	8:A:3527:MAN:H2	1.85	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)
1:A:452:SER:OG	1:C:452:SER:OG[4_555]	2.19	0.01

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	587/681 (86%)	562 (96%)	25 (4%)	0	100 100
1	C	580/681 (85%)	557 (96%)	23 (4%)	0	100 100
2	B	417/788 (53%)	397 (95%)	18 (4%)	2 (0%)	34 67
2	D	406/788 (52%)	389 (96%)	16 (4%)	1 (0%)	52 82
All	All	1990/2938 (68%)	1905 (96%)	82 (4%)	3 (0%)	52 82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	365	ASP
2	B	161	VAL
2	D	161	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	485/555 (87%)	483 (100%)	2 (0%)	93 98
1	C	483/555 (87%)	480 (99%)	3 (1%)	90 97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	371/685 (54%)	367 (99%)	4 (1%)	80 94
2	D	368/685 (54%)	367 (100%)	1 (0%)	94 98
All	All	1707/2480 (69%)	1697 (99%)	10 (1%)	90 97

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	TYR
1	A	275	TYR
2	B	220	ASP
2	B	369	LEU
2	B	397	THR
2	B	414	ARG
1	C	275	TYR
1	C	463	LEU
1	C	538	LEU
2	D	221	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	GLN
1	A	474	ASN
1	C	152	GLN
1	C	207	GLN
2	D	304	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)

53 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	$\#\|Z\| > 2$
7	NAG	A	3044	1,7	14,14,15	0.30	0	15,19,21	0.42	0
7	NAG	A	3045	7	14,14,15	0.32	0	15,19,21	0.55	0
7	BMA	A	3046	7	11,11,12	0.59	0	14,15,17	0.84	0
7	MAN	A	3047	7	11,11,12	0.74	0	14,15,17	1.03	2 (14%)
8	NAG	A	3260	1,8	14,14,15	0.18	0	15,19,21	0.25	0
8	NAG	A	3261	8	14,14,15	0.21	0	15,19,21	0.26	0
8	BMA	A	3262	8	11,11,12	0.79	0	14,15,17	0.83	0
8	MAN	A	3263	8	11,11,12	0.86	0	14,15,17	1.09	1 (7%)
8	MAN	A	3264	8	11,11,12	0.70	0	14,15,17	0.99	2 (14%)
9	NAG	A	3266	1,9	14,14,15	1.14	1 (7%)	15,19,21	0.97	1 (6%)
9	NAG	A	3267	9	14,14,15	0.46	0	15,19,21	0.23	0
9	BMA	A	3268	9	11,11,12	0.79	1 (9%)	14,15,17	0.81	0
9	MAN	A	3269	9	11,11,12	0.74	1 (9%)	14,15,17	0.93	1 (7%)
9	MAN	A	3270	9	11,11,12	0.77	1 (9%)	14,15,17	0.94	1 (7%)
9	MAN	A	3271	9	11,11,12	0.76	1 (9%)	14,15,17	0.97	2 (14%)
10	NAG	A	3458	1,10	14,14,15	0.30	0	15,19,21	0.45	0
10	NAG	A	3459	10	14,14,15	0.29	0	15,19,21	0.51	0
10	BMA	A	3460	10	11,11,12	0.82	0	14,15,17	1.10	2 (14%)
8	NAG	A	3524	1,8	14,14,15	0.36	0	15,19,21	0.49	0
8	NAG	A	3525	8	14,14,15	0.28	0	15,19,21	0.36	0
8	BMA	A	3526	8	11,11,12	0.61	0	14,15,17	1.08	2 (14%)
8	MAN	A	3527	8	11,11,12	0.72	0	14,15,17	1.30	2 (14%)
8	MAN	A	3528	8	11,11,12	0.61	0	14,15,17	1.14	2 (14%)
11	NAG	A	3585	1,11	14,14,15	0.33	0	15,19,21	0.36	0
11	NAG	A	3586	11	14,14,15	0.29	0	15,19,21	0.39	0
10	NAG	C	3044	1,10	14,14,15	0.51	0	15,19,21	0.49	0
10	NAG	C	3045	10	14,14,15	0.41	0	15,19,21	0.71	1 (6%)
10	BMA	C	3046	10	11,11,12	0.54	0	14,15,17	1.03	1 (7%)
11	NAG	C	3260	1,11	14,14,15	0.26	0	15,19,21	0.31	0
11	NAG	C	3261	11	14,14,15	0.22	0	15,19,21	0.35	0
9	NAG	C	3266	1,9	14,14,15	1.71	2 (14%)	15,19,21	1.34	2 (13%)
9	NAG	C	3267	9	14,14,15	0.41	0	15,19,21	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BMA	C	3268	9	11,11,12	0.71	0	14,15,17	0.78	0
9	MAN	C	3269	9	11,11,12	0.77	1 (9%)	14,15,17	0.90	1 (7%)
9	MAN	C	3270	9	11,11,12	0.69	0	14,15,17	1.05	2 (14%)
9	MAN	C	3271	9	11,11,12	0.67	0	14,15,17	1.01	2 (14%)
7	NAG	C	3458	1,7	14,14,15	0.33	0	15,19,21	0.59	0
7	NAG	C	3459	7	14,14,15	0.36	0	15,19,21	0.45	0
7	BMA	C	3460	7	11,11,12	1.01	1 (9%)	14,15,17	1.32	2 (14%)
7	MAN	C	3461	7	11,11,12	1.12	2 (18%)	14,15,17	1.24	3 (21%)
15	NAG	C	3524	1,15	14,14,15	1.03	2 (14%)	15,19,21	0.83	1 (6%)
15	NAG	C	3525	15	14,14,15	0.58	1 (7%)	15,19,21	0.71	1 (6%)
15	BMA	C	3526	15	11,11,12	1.02	1 (9%)	14,15,17	1.61	4 (28%)
15	MAN	C	3527	15	11,11,12	0.79	0	14,15,17	1.47	2 (14%)
15	MAN	C	3528	15	11,11,12	0.98	1 (9%)	14,15,17	0.87	1 (7%)
15	MAN	C	3529	15	11,11,12	0.72	0	14,15,17	0.97	2 (14%)
15	MAN	C	3530	15	11,11,12	0.58	0	14,15,17	1.13	2 (14%)
11	NAG	C	3585	1,11	14,14,15	0.38	0	15,19,21	0.22	0
11	NAG	C	3586	11	14,14,15	0.28	0	15,19,21	0.35	0
7	NAG	D	3370	2,7	14,14,15	0.60	1 (7%)	15,19,21	0.41	0
7	NAG	D	3371	7	14,14,15	0.33	0	15,19,21	0.65	0
7	BMA	D	3372	7	11,11,12	0.57	0	14,15,17	1.17	1 (7%)
7	MAN	D	3373	7	11,11,12	0.73	0	14,15,17	1.02	2 (14%)

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
7	NAG	A	3044	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	3045	7	-	0/6/23/26	0/1/1/1
7	BMA	A	3046	7	-	0/2/19/22	0/1/1/1
7	MAN	A	3047	7	-	0/2/19/22	0/1/1/1
8	NAG	A	3260	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	3261	8	-	0/6/23/26	0/1/1/1
8	BMA	A	3262	8	-	0/2/19/22	0/1/1/1
8	MAN	A	3263	8	-	0/2/19/22	0/1/1/1
8	MAN	A	3264	8	-	0/2/19/22	0/1/1/1
9	NAG	A	3266	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	3267	9	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	A	3268	9	-	0/2/19/22	0/1/1/1
9	MAN	A	3269	9	-	0/2/19/22	0/1/1/1
9	MAN	A	3270	9	-	0/2/19/22	0/1/1/1
9	MAN	A	3271	9	-	0/2/19/22	0/1/1/1
10	NAG	A	3458	1,10	-	0/6/23/26	0/1/1/1
10	NAG	A	3459	10	-	0/6/23/26	0/1/1/1
10	BMA	A	3460	10	-	0/2/19/22	0/1/1/1
8	NAG	A	3524	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	3525	8	-	0/6/23/26	0/1/1/1
8	BMA	A	3526	8	-	0/2/19/22	0/1/1/1
8	MAN	A	3527	8	-	0/2/19/22	1/1/1/1
8	MAN	A	3528	8	-	0/2/19/22	0/1/1/1
11	NAG	A	3585	1,11	-	0/6/23/26	0/1/1/1
11	NAG	A	3586	11	-	0/6/23/26	0/1/1/1
10	NAG	C	3044	1,10	-	0/6/23/26	0/1/1/1
10	NAG	C	3045	10	-	0/6/23/26	0/1/1/1
10	BMA	C	3046	10	-	0/2/19/22	0/1/1/1
11	NAG	C	3260	1,11	-	0/6/23/26	0/1/1/1
11	NAG	C	3261	11	-	0/6/23/26	0/1/1/1
9	NAG	C	3266	1,9	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	C	3267	9	-	0/6/23/26	0/1/1/1
9	BMA	C	3268	9	-	0/2/19/22	0/1/1/1
9	MAN	C	3269	9	-	0/2/19/22	0/1/1/1
9	MAN	C	3270	9	-	0/2/19/22	0/1/1/1
9	MAN	C	3271	9	-	0/2/19/22	0/1/1/1
7	NAG	C	3458	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	3459	7	-	0/6/23/26	0/1/1/1
7	BMA	C	3460	7	-	0/2/19/22	0/1/1/1
7	MAN	C	3461	7	-	0/2/19/22	0/1/1/1
15	NAG	C	3524	1,15	-	0/6/23/26	0/1/1/1
15	NAG	C	3525	15	-	0/6/23/26	0/1/1/1
15	BMA	C	3526	15	-	0/2/19/22	0/1/1/1
15	MAN	C	3527	15	-	0/2/19/22	0/1/1/1
15	MAN	C	3528	15	-	0/2/19/22	0/1/1/1
15	MAN	C	3529	15	-	0/2/19/22	0/1/1/1
15	MAN	C	3530	15	-	0/2/19/22	0/1/1/1
11	NAG	C	3585	1,11	-	0/6/23/26	0/1/1/1
11	NAG	C	3586	11	-	0/6/23/26	0/1/1/1
7	NAG	D	3370	2,7	-	0/6/23/26	0/1/1/1
7	NAG	D	3371	7	-	0/6/23/26	0/1/1/1
7	BMA	D	3372	7	-	0/2/19/22	0/1/1/1
7	MAN	D	3373	7	-	0/2/19/22	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	3266	NAG	O5-C1	-5.89	1.33	1.43
9	A	3266	NAG	O5-C1	-4.10	1.36	1.43
15	C	3524	NAG	O5-C1	-3.08	1.38	1.43
15	C	3528	MAN	O5-C1	-2.56	1.39	1.43
9	C	3266	NAG	C1-C2	-2.29	1.49	1.52
7	C	3461	MAN	O5-C1	-2.24	1.40	1.43
9	A	3268	BMA	O5-C1	-2.23	1.40	1.43
15	C	3524	NAG	C1-C2	-2.11	1.49	1.52
9	C	3269	MAN	O5-C1	-2.11	1.40	1.43
9	A	3270	MAN	O5-C1	-2.09	1.40	1.43
7	D	3370	NAG	O5-C1	-2.05	1.40	1.43
9	A	3269	MAN	O5-C1	-2.03	1.40	1.43
9	A	3271	MAN	O5-C1	-2.00	1.40	1.43
7	C	3461	MAN	C4-C5	2.04	1.57	1.53
15	C	3525	NAG	C1-C2	2.10	1.55	1.52
15	C	3526	BMA	O3-C3	2.21	1.48	1.43
7	C	3460	BMA	C2-C3	2.28	1.55	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	3266	NAG	C1-O5-C5	-3.12	108.29	112.25
10	A	3460	BMA	O2-C2-C3	-2.82	104.45	110.12
15	C	3526	BMA	C1-C2-C3	-2.41	106.69	109.54
15	C	3526	BMA	C3-C4-C5	-2.40	106.02	110.20
9	C	3271	MAN	O2-C2-C3	-2.29	105.52	110.12
8	A	3526	BMA	O2-C2-C3	-2.27	105.56	110.12
7	A	3047	MAN	O2-C2-C3	-2.27	105.56	110.12
9	A	3271	MAN	O2-C2-C3	-2.26	105.58	110.12
7	D	3373	MAN	O2-C2-C3	-2.25	105.59	110.12
8	A	3263	MAN	O2-C2-C3	-2.23	105.63	110.12
8	A	3264	MAN	O2-C2-C3	-2.23	105.64	110.12
9	C	3270	MAN	O2-C2-C3	-2.22	105.66	110.12
15	C	3530	MAN	O2-C2-C3	-2.21	105.68	110.12
9	A	3270	MAN	O2-C2-C3	-2.20	105.70	110.12
8	A	3527	MAN	O2-C2-C3	-2.18	105.74	110.12
9	C	3269	MAN	O2-C2-C3	-2.17	105.76	110.12
15	C	3529	MAN	O2-C2-C3	-2.16	105.78	110.12
9	A	3269	MAN	O2-C2-C3	-2.16	105.78	110.12
10	A	3460	BMA	C1-C2-C3	-2.15	107.00	109.54
15	C	3527	MAN	O2-C2-C3	-2.15	105.80	110.12
8	A	3528	MAN	O2-C2-C3	-2.14	105.81	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	3461	MAN	O2-C2-C3	-2.09	105.91	110.12
15	C	3528	MAN	O2-C2-C3	-2.05	106.00	110.12
15	C	3529	MAN	C1-O5-C5	2.04	114.84	112.25
7	A	3047	MAN	C1-O5-C5	2.05	114.85	112.25
9	A	3271	MAN	C1-O5-C5	2.08	114.88	112.25
7	D	3373	MAN	C1-O5-C5	2.09	114.90	112.25
10	C	3045	NAG	C1-O5-C5	2.11	114.92	112.25
8	A	3526	BMA	C1-O5-C5	2.17	115.00	112.25
7	C	3461	MAN	C3-C4-C5	2.20	114.04	110.20
8	A	3264	MAN	C1-O5-C5	2.28	115.15	112.25
15	C	3526	BMA	O3-C3-C4	2.30	115.52	110.34
9	C	3271	MAN	C1-O5-C5	2.34	115.22	112.25
9	C	3270	MAN	C1-O5-C5	2.34	115.22	112.25
15	C	3524	NAG	C3-C4-C5	2.36	114.32	110.20
15	C	3525	NAG	C1-O5-C5	2.39	115.28	112.25
15	C	3530	MAN	C1-O5-C5	2.51	115.43	112.25
7	C	3460	BMA	O5-C1-C2	2.56	115.01	110.86
9	A	3266	NAG	C3-C4-C5	2.57	114.68	110.20
7	C	3461	MAN	C1-O5-C5	2.70	115.67	112.25
10	C	3046	BMA	C1-O5-C5	2.83	115.84	112.25
7	C	3460	BMA	C1-C2-C3	2.86	112.92	109.54
8	A	3528	MAN	C1-O5-C5	3.04	116.11	112.25
9	C	3266	NAG	C3-C4-C5	3.33	116.00	110.20
7	D	3372	BMA	C1-O5-C5	3.41	116.58	112.25
8	A	3527	MAN	C1-O5-C5	3.62	116.84	112.25
15	C	3527	MAN	C1-O5-C5	3.87	117.15	112.25
15	C	3526	BMA	O3-C3-C2	3.90	117.05	110.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	C	3266	NAG	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	3527	MAN	C1-C2-C3-C4-C5-O5

18 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	3046	BMA	1	0
7	A	3047	MAN	1	0
9	A	3268	BMA	1	0
9	A	3270	MAN	1	0
10	A	3459	NAG	1	0
10	A	3460	BMA	1	0
8	A	3526	BMA	1	0
8	A	3527	MAN	1	0
9	C	3268	BMA	1	0
9	C	3270	MAN	1	0
7	C	3459	NAG	1	0
7	C	3460	BMA	1	0
15	C	3524	NAG	1	0
15	C	3525	NAG	1	0
15	C	3526	BMA	1	0
15	C	3527	MAN	1	0
7	D	3372	BMA	1	0
7	D	3373	MAN	2	0

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	SO4	A	1596	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	A	1597	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	A	1598	-	4,4,4	0.24	0	6,6,6	0.08	0
12	CAC	B	1442	-	0,4,4	0.00	-	0,6,6	0.00	-
14	NAG	B	3243	2	14,14,15	0.30	0	15,19,21	0.27	0
12	CAC	D	1442	-	0,4,4	0.00	-	0,6,6	0.00	-
14	NAG	D	3080	2	14,14,15	0.39	0	15,19,21	0.55	0
14	NAG	D	3243	2	14,14,15	0.30	0	15,19,21	0.28	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
4	SO4	A	1596	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1597	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1598	-	-	0/0/0/0	0/0/0/0
12	CAC	B	1442	-	-	0/0/0/0	0/0/0/0
14	NAG	B	3243	2	-	0/6/23/26	0/1/1/1
12	CAC	D	1442	-	-	0/0/0/0	0/0/0/0
14	NAG	D	3080	2	-	0/6/23/26	0/1/1/1
14	NAG	D	3243	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1596	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	591/681 (86%)	-0.00	11 (1%)	70	66	34, 64, 109, 185	0
1	C	588/681 (86%)	0.57	53 (9%)	12	7	52, 100, 155, 201	0
2	B	423/788 (53%)	0.41	35 (8%)	14	9	25, 70, 166, 245	0
2	D	414/788 (52%)	0.33	27 (6%)	22	16	33, 77, 150, 205	0
All	All	2016/2938 (68%)	0.32	126 (6%)	23	17	25, 78, 150, 245	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	8	LEU	7.6
2	B	58	ILE	7.4
2	B	55	LEU	7.2
1	C	129	PHE	7.1
2	B	50	ALA	6.8
2	B	53	CYS	6.6
1	C	532	LEU	5.9
2	B	56	ASN	5.6
1	C	60	ASP	5.5
2	B	49	LEU	5.4
1	C	265	TYR	5.4
2	B	54	GLN	5.3
2	B	57	PHE	5.2
2	D	58	ILE	5.1
2	D	55	LEU	5.1
2	D	27	CYS	5.0
1	C	61	TRP	4.8
2	B	52	GLY	4.8
2	B	26	TRP	4.6
2	B	8	LEU	4.5
2	B	46	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	41	ARG	4.3
2	D	60	ASN	4.3
1	C	82	LYS	4.2
2	B	51	LYS	4.2
2	B	436	ASN	4.2
2	B	439	CYS	4.2
2	B	27	CYS	4.1
1	C	562	ARG	4.1
2	D	28	ALA	4.0
2	B	10	GLY	4.0
2	D	26	TRP	4.0
1	C	503	LYS	4.0
2	B	367	GLU	4.0
2	B	435	CYS	3.9
2	B	28	ALA	3.9
1	C	167	ASP	3.7
2	D	379	ASN	3.6
1	C	133	GLY	3.6
2	D	59	GLU	3.6
1	C	11	TYR	3.6
1	C	494	GLN	3.5
2	D	57	PHE	3.5
1	C	563	LEU	3.5
2	B	441	LYS	3.4
1	C	100	SER	3.4
1	C	131	GLN	3.3
1	C	325	ASP	3.3
2	D	440	GLN	3.2
1	A	552	LEU	3.2
1	A	594	LEU	3.2
2	B	45	PRO	3.2
1	C	36	LEU	3.2
2	D	18	LEU	3.2
1	C	497	LEU	3.1
2	B	47	ASN	3.1
1	C	594	LEU	3.1
1	C	490	LYS	3.1
1	C	165	LYS	3.1
2	D	439	CYS	3.0
1	C	507	ALA	3.0
2	B	440	GLN	3.0
2	D	441	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	498	LEU	2.8
1	C	519	PRO	2.8
1	C	35	PHE	2.8
1	C	37	LEU	2.8
1	C	29	SER	2.8
1	C	260	ASN	2.8
1	C	59	CYS	2.7
2	D	95	LYS	2.7
2	D	53	CYS	2.7
2	D	380	GLY	2.7
2	B	60	ASN	2.6
2	B	20	ILE	2.6
2	B	434	GLU	2.6
1	A	134	THR	2.6
1	C	489	ARG	2.6
2	B	437	CYS	2.5
1	A	29	SER	2.5
1	C	34	MET	2.5
1	C	25	PHE	2.5
2	B	9	GLY	2.5
1	C	397	ALA	2.5
2	D	54	GLN	2.5
2	B	42	CYS	2.5
1	C	191	ILE	2.4
2	D	13	THR	2.4
1	A	498	LEU	2.4
1	C	419	TYR	2.3
2	D	77	ARG	2.3
1	C	565	TYR	2.3
1	C	65	ARG	2.3
1	C	440	VAL	2.3
2	D	56	ASN	2.3
1	C	441	ILE	2.3
2	B	438	ASP	2.3
2	D	41	ARG	2.3
1	C	499	LEU	2.3
1	C	571	THR	2.3
1	C	549	ARG	2.2
2	B	199	LEU	2.2
1	C	492	ASN	2.2
2	B	13	THR	2.2
1	A	63	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	74	SER	2.2
1	C	491	LEU	2.1
1	A	31	SER	2.1
1	A	508	ILE	2.1
1	C	564	ASP	2.1
2	D	156	GLY	2.1
1	A	503	LYS	2.1
1	C	68	GLN	2.1
1	C	411	ALA	2.1
2	D	436	ASN	2.1
1	C	522	SER	2.1
1	C	452	SER	2.0
1	C	410	GLY	2.0
1	C	398	ARG	2.0
2	D	437	CYS	2.0
1	C	581	PHE	2.0
1	A	116	THR	2.0
2	D	385	HIS	2.0
1	C	145	GLN	2.0
2	B	5	GLY	2.0
1	A	581	PHE	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	NAG	D	3370	14/15	0.64	0.44	5.25	120,139,148,162	0
7	MAN	D	3373	11/12	0.70	0.37	3.40	153,162,169,169	0
15	MAN	C	3528	11/12	0.73	0.33	1.86	131,142,151,152	0
15	MAN	C	3530	11/12	0.71	0.27	1.75	128,136,161,170	0
10	NAG	A	3459	14/15	0.74	0.24	1.17	132,155,172,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	NAG	A	3458	14/15	0.82	0.24	1.06	105,125,137,138	0
7	NAG	C	3459	14/15	0.73	0.22	0.58	117,137,149,149	0
10	NAG	C	3044	14/15	0.86	0.21	0.39	88,102,119,139	0
7	NAG	C	3458	14/15	0.92	0.20	-0.03	81,104,118,130	0
7	NAG	A	3044	14/15	0.93	0.16	-0.14	40,72,97,108	0
9	NAG	A	3266	14/15	0.96	0.17	-0.48	50,64,81,97	0
8	NAG	A	3260	14/15	0.95	0.13	-0.49	60,82,102,102	0
11	NAG	A	3585	14/15	0.94	0.18	-1.10	89,112,120,132	0
9	NAG	C	3266	14/15	0.87	0.18	-1.12	73,84,104,108	0
11	NAG	C	3260	14/15	0.88	0.23	-	83,105,113,120	0
10	NAG	C	3045	14/15	0.88	0.31	-	119,136,147,154	0
9	MAN	A	3269	11/12	0.82	0.27	-	104,115,137,152	0
9	MAN	A	3271	11/12	0.90	0.19	-	110,121,130,130	0
7	MAN	A	3047	11/12	0.64	0.22	-	138,152,165,166	0
7	BMA	C	3460	11/12	0.66	0.30	-	149,163,235,236	0
8	NAG	A	3524	14/15	0.89	0.17	-	78,105,117,118	0
10	BMA	A	3460	11/12	0.68	0.42	-	175,182,191,192	0
9	BMA	C	3268	11/12	0.87	0.19	-	112,117,158,163	0
8	BMA	A	3526	11/12	0.79	0.29	-	135,141,150,154	0
8	NAG	A	3261	14/15	0.87	0.23	-	99,123,133,148	0
9	MAN	C	3270	11/12	0.80	0.38	-	166,172,177,180	0
7	BMA	A	3046	11/12	0.67	0.25	-	137,148,165,170	0
9	MAN	C	3269	11/12	0.89	0.28	-	103,111,115,117	0
8	MAN	A	3528	11/12	0.75	0.42	-	152,163,169,172	0
8	NAG	A	3525	14/15	0.87	0.23	-	100,119,131,142	0
9	BMA	A	3268	11/12	0.82	0.16	-	93,117,134,137	0
7	MAN	C	3461	11/12	0.80	0.25	-	95,155,172,173	0
11	NAG	C	3586	14/15	0.65	0.38	-	149,155,163,168	0
15	MAN	C	3527	11/12	0.80	0.28	-	130,139,148,152	0
15	NAG	C	3525	14/15	0.58	0.41	-	134,143,150,152	0
15	BMA	C	3526	11/12	0.81	0.21	-	120,130,140,143	0
7	NAG	D	3371	14/15	0.80	0.23	-	153,165,173,182	0
8	MAN	A	3263	11/12	0.68	0.28	-	161,170,185,192	0
11	NAG	C	3585	14/15	0.91	0.19	-	89,106,134,139	0
8	MAN	A	3527	11/12	0.51	0.34	-	144,157,163,168	0
11	NAG	A	3586	14/15	0.79	0.37	-	124,147,157,161	0
9	MAN	A	3270	11/12	0.87	0.20	-	119,137,139,139	0
15	MAN	C	3529	11/12	0.71	0.29	-	118,135,150,152	0
7	NAG	A	3045	14/15	0.79	0.23	-	103,130,141,149	0
7	BMA	D	3372	11/12	0.68	0.48	-	168,186,195,202	0
15	NAG	C	3524	14/15	0.86	0.30	-	103,121,128,139	0
8	BMA	A	3262	11/12	0.69	0.27	-	149,158,166,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	MAN	C	3271	11/12	0.81	0.47	-	178,185,187,188	0
10	BMA	C	3046	11/12	0.61	0.18	-	125,146,155,161	0
11	NAG	C	3261	14/15	0.78	0.32	-	111,124,129,133	0
8	MAN	A	3264	11/12	0.62	0.56	-	169,187,191,194	0
9	NAG	A	3267	14/15	0.94	0.17	-	59,69,92,107	0
9	NAG	C	3267	14/15	0.92	0.21	-	69,88,101,105	0

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	CA	A	2002	1/1	0.46	0.52	16.22	219,219,219,219	0
4	SO4	A	1598	5/5	0.82	0.46	6.28	155,156,156,157	5
4	SO4	A	1597	5/5	0.94	0.25	1.66	133,133,136,140	0
6	CA	A	2003	1/1	0.95	0.19	1.46	71,71,71,71	0
12	CAC	D	1442	5/5	0.91	0.26	0.89	28,51,133,223	0
6	CA	D	2003	1/1	0.98	0.19	0.79	90,90,90,90	0
6	CA	A	2001	1/1	0.99	0.14	-0.58	76,76,76,76	0
6	CA	A	2004	1/1	0.95	0.13	-0.74	58,58,58,58	0
6	CA	C	2002	1/1	0.81	0.11	-1.06	106,106,106,106	0
12	CAC	B	1442	5/5	0.96	0.16	-1.06	37,68,85,295	0
6	CA	B	2003	1/1	0.98	0.10	-1.40	64,64,64,64	0
13	MG	B	2001	1/1	0.88	0.13	-1.79	63,63,63,63	0
6	CA	C	2004	1/1	0.70	0.07	-1.94	151,151,151,151	0
6	CA	C	2001	1/1	0.78	0.07	-1.98	104,104,104,104	0
13	MG	D	2001	1/1	0.90	0.15	-2.75	117,117,117,117	0
6	CA	C	2003	1/1	0.79	0.04	-3.16	115,115,115,115	0
5	NI	A	1599	1/1	0.97	0.04	-	97,97,97,97	0
4	SO4	A	1596	5/5	0.99	0.11	-	64,65,71,72	5
14	NAG	D	3080	14/15	0.79	0.31	-	94,127,134,139	0
14	NAG	D	3243	14/15	0.90	0.36	-	104,128,144,152	0
3	CL	A	1595	1/1	0.88	0.10	-	75,75,75,75	0
14	NAG	B	3243	14/15	0.88	0.29	-	100,112,118,118	0
3	CL	C	1596	1/1	0.90	0.14	-	96,96,96,96	0
3	CL	C	1595	1/1	0.77	0.11	-	111,111,111,111	1

6.5 Other polymers (i)

There are no such residues in this entry.