Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:44 PM GMT

PDB ID	:	4MIV
Title	:	Crystal Structure of Sulfamidase, Crystal Form L
Authors	:	Sidhu, N.S.; Uson, I.; Schreiber, K.; Proepper, K.; Becker, S.; Sheldrick, G.M.; Gaertner, J.; Kraetzner, R.; Steinfeld, R.
Deposited on	:	2013-09-02
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

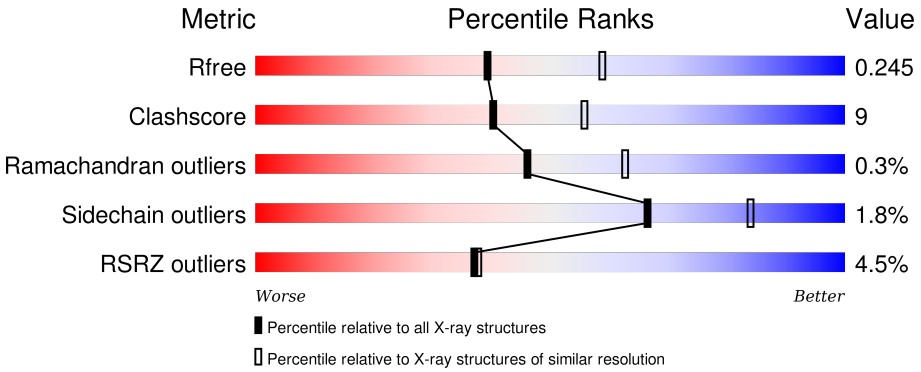
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	510	80% 13% • 5%
1	B	510	80% 13% • 6%
1	C	510	% 81% 13% • 5%
1	D	510	81% 11% • 6%
1	E	510	8% 81% 13% • 5%

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Mol	Chain	Length	Quality of chain
1	F	510	5% 80% 13% • 6%
1	G	510	8% 81% 11% • 6%
1	H	510	12% 80% 13% • 5%

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
3	NAG	D	602	-	-	-	X
6	PEG	D	609	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 31167 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 N-sulphoglucosamine sulphohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	P	S	0	2	0
			3869	2478	670	708	1	12			
1	B	481	Total	C	N	O	P	S	0	2	0
			3860	2467	676	705	1	11			
1	C	484	Total	C	N	O	P	S	0	0	0
			3854	2467	670	705	1	11			
1	D	480	Total	C	N	O	P	S	0	1	0
			3835	2454	671	698	1	11			
1	E	483	Total	C	N	O	P	S	0	1	0
			3607	2308	617	670	1	11			
1	F	478	Total	C	N	O	P	S	0	0	0
			3703	2373	636	682	1	11			
1	G	479	Total	C	N	O	S		0	1	0
			3685	2362	641	671	11				
1	H	482	Total	C	N	O	S		0	0	0
			3617	2317	627	663	10				

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	FGP	CYS	MODIFIED RESIDUE	UNP P51688
A	503	ARG	-	EXPRESSION TAG	UNP P51688
A	504	SER	-	EXPRESSION TAG	UNP P51688
A	505	HIS	-	EXPRESSION TAG	UNP P51688
A	506	HIS	-	EXPRESSION TAG	UNP P51688
A	507	HIS	-	EXPRESSION TAG	UNP P51688
A	508	HIS	-	EXPRESSION TAG	UNP P51688
A	509	HIS	-	EXPRESSION TAG	UNP P51688
A	510	HIS	-	EXPRESSION TAG	UNP P51688
B	70	FGP	CYS	MODIFIED RESIDUE	UNP P51688
B	503	ARG	-	EXPRESSION TAG	UNP P51688
B	504	SER	-	EXPRESSION TAG	UNP P51688
B	505	HIS	-	EXPRESSION TAG	UNP P51688

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Chain	Residue	Modelled	Actual	Comment	Reference
B	506	HIS	-	EXPRESSION TAG	UNP P51688
B	507	HIS	-	EXPRESSION TAG	UNP P51688
B	508	HIS	-	EXPRESSION TAG	UNP P51688
B	509	HIS	-	EXPRESSION TAG	UNP P51688
B	510	HIS	-	EXPRESSION TAG	UNP P51688
C	70	FGP	CYS	MODIFIED RESIDUE	UNP P51688
C	503	ARG	-	EXPRESSION TAG	UNP P51688
C	504	SER	-	EXPRESSION TAG	UNP P51688
C	505	HIS	-	EXPRESSION TAG	UNP P51688
C	506	HIS	-	EXPRESSION TAG	UNP P51688
C	507	HIS	-	EXPRESSION TAG	UNP P51688
C	508	HIS	-	EXPRESSION TAG	UNP P51688
C	509	HIS	-	EXPRESSION TAG	UNP P51688
C	510	HIS	-	EXPRESSION TAG	UNP P51688
D	70	FGP	CYS	MODIFIED RESIDUE	UNP P51688
D	503	ARG	-	EXPRESSION TAG	UNP P51688
D	504	SER	-	EXPRESSION TAG	UNP P51688
D	505	HIS	-	EXPRESSION TAG	UNP P51688
D	506	HIS	-	EXPRESSION TAG	UNP P51688
D	507	HIS	-	EXPRESSION TAG	UNP P51688
D	508	HIS	-	EXPRESSION TAG	UNP P51688
D	509	HIS	-	EXPRESSION TAG	UNP P51688
D	510	HIS	-	EXPRESSION TAG	UNP P51688
E	70	FGP	CYS	MODIFIED RESIDUE	UNP P51688
E	503	ARG	-	EXPRESSION TAG	UNP P51688
E	504	SER	-	EXPRESSION TAG	UNP P51688
E	505	HIS	-	EXPRESSION TAG	UNP P51688
E	506	HIS	-	EXPRESSION TAG	UNP P51688
E	507	HIS	-	EXPRESSION TAG	UNP P51688
E	508	HIS	-	EXPRESSION TAG	UNP P51688
E	509	HIS	-	EXPRESSION TAG	UNP P51688
E	510	HIS	-	EXPRESSION TAG	UNP P51688
F	70	FGP	CYS	MODIFIED RESIDUE	UNP P51688
F	503	ARG	-	EXPRESSION TAG	UNP P51688
F	504	SER	-	EXPRESSION TAG	UNP P51688
F	505	HIS	-	EXPRESSION TAG	UNP P51688
F	506	HIS	-	EXPRESSION TAG	UNP P51688
F	507	HIS	-	EXPRESSION TAG	UNP P51688
F	508	HIS	-	EXPRESSION TAG	UNP P51688
F	509	HIS	-	EXPRESSION TAG	UNP P51688
F	510	HIS	-	EXPRESSION TAG	UNP P51688
G	70	FGP	CYS	MODIFIED RESIDUE	UNP P51688

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Chain	Residue	Modelled	Actual	Comment	Reference
G	503	ARG	-	EXPRESSION TAG	UNP P51688
G	504	SER	-	EXPRESSION TAG	UNP P51688
G	505	HIS	-	EXPRESSION TAG	UNP P51688
G	506	HIS	-	EXPRESSION TAG	UNP P51688
G	507	HIS	-	EXPRESSION TAG	UNP P51688
G	508	HIS	-	EXPRESSION TAG	UNP P51688
G	509	HIS	-	EXPRESSION TAG	UNP P51688
G	510	HIS	-	EXPRESSION TAG	UNP P51688
H	70	FGP	CYS	MODIFIED RESIDUE	UNP P51688
H	503	ARG	-	EXPRESSION TAG	UNP P51688
H	504	SER	-	EXPRESSION TAG	UNP P51688
H	505	HIS	-	EXPRESSION TAG	UNP P51688
H	506	HIS	-	EXPRESSION TAG	UNP P51688
H	507	HIS	-	EXPRESSION TAG	UNP P51688
H	508	HIS	-	EXPRESSION TAG	UNP P51688
H	509	HIS	-	EXPRESSION TAG	UNP P51688
H	510	HIS	-	EXPRESSION TAG	UNP P51688

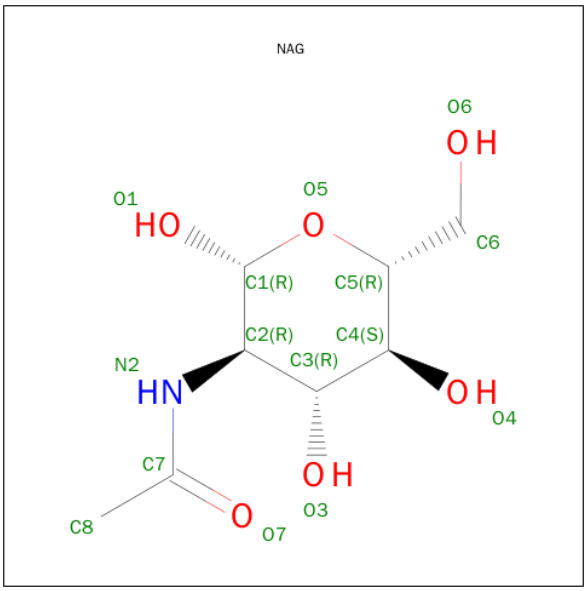
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			27	16	2	9		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			27	16	2	9		
3	C	2	Total	C	N	O	0	0
			27	16	2	9		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			25	14	2	9		
3	H	2	Total	C	N	O	0	0
			27	16	2	9		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

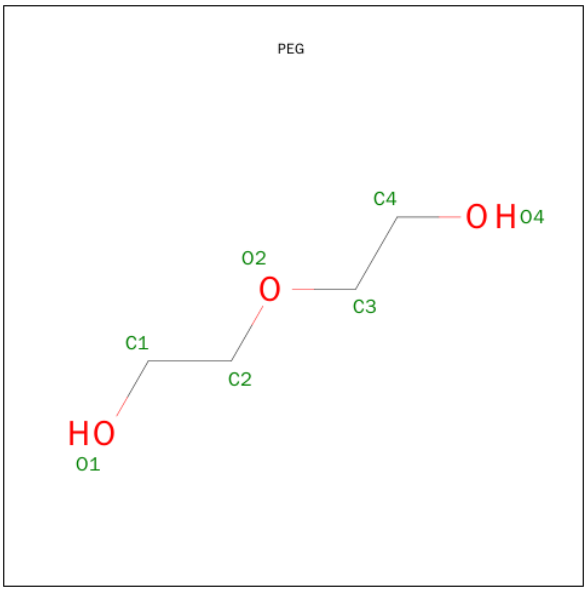


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 10 6 1 3	0	0
4	H	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 5 4 1	0	0

- Molecule 7 is water.

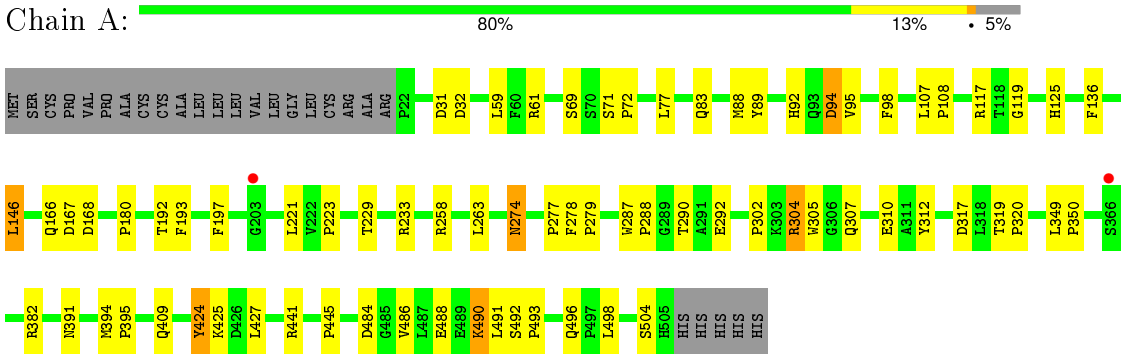
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	97	Total O 97 97	0	0
7	B	112	Total O 112 112	0	0
7	C	87	Total O 87 87	0	0
7	D	107	Total O 107 107	0	0
7	E	8	Total O 8 8	0	0
7	F	26	Total O 26 26	0	0
7	G	29	Total O 29 29	0	0
7	H	9	Total O 9 9	0	0

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.

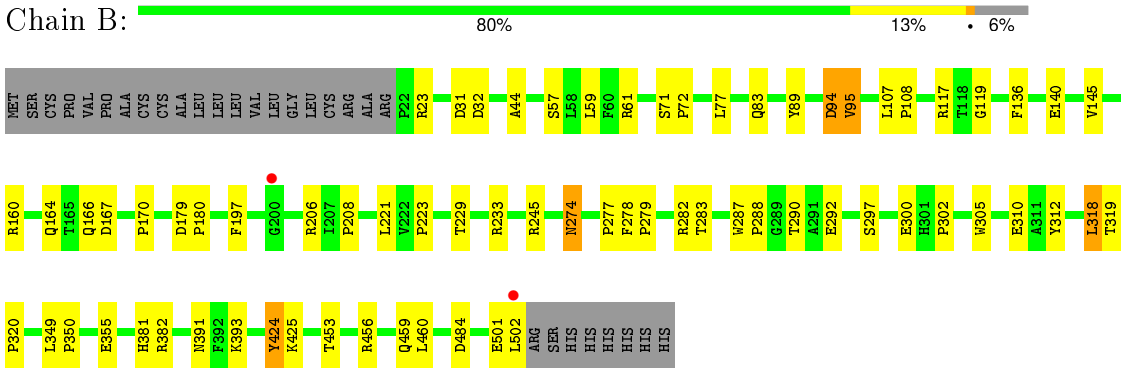
- Molecule 1: N-sulphoglucosamine sulphohydrolase

Chain A:



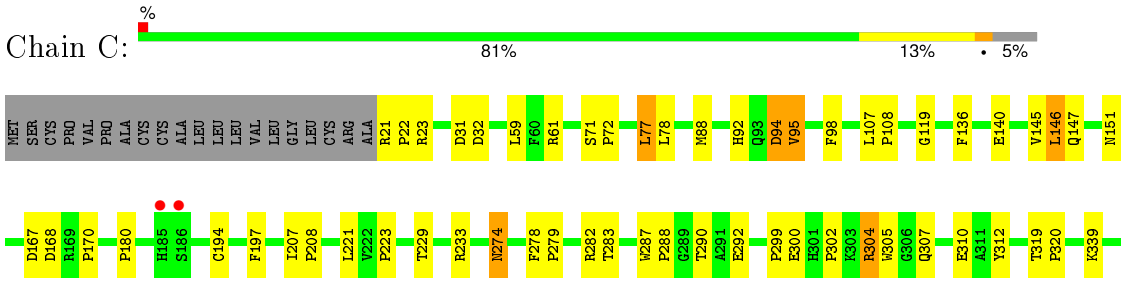
- Molecule 1: N-sulphoglucosamine sulphohydrolase

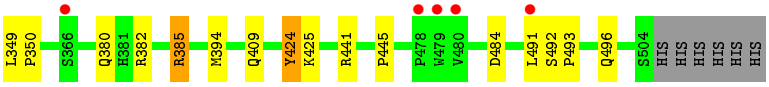
Chain B:



- Molecule 1: N-sulphoglucosamine sulphohydrolase

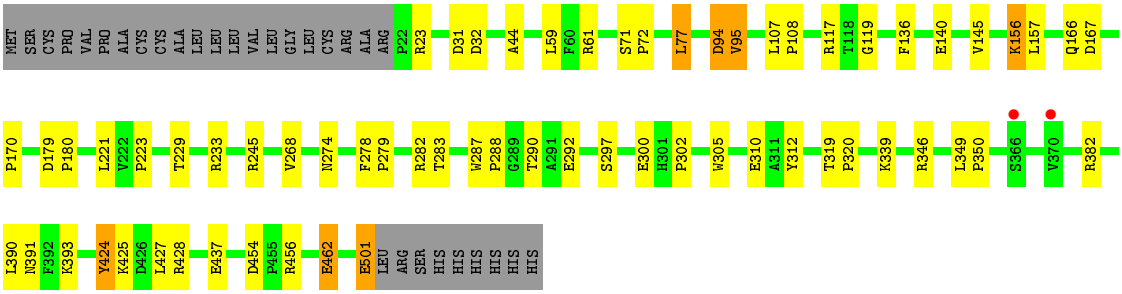
Chain C:





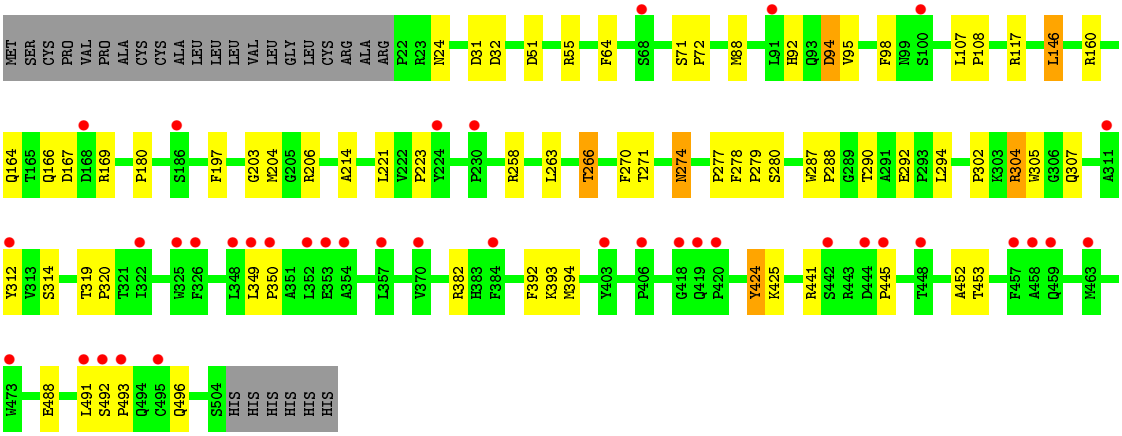
• Molecule 1: N-sulphoglucosamine sulphohydrolase

Chain D:



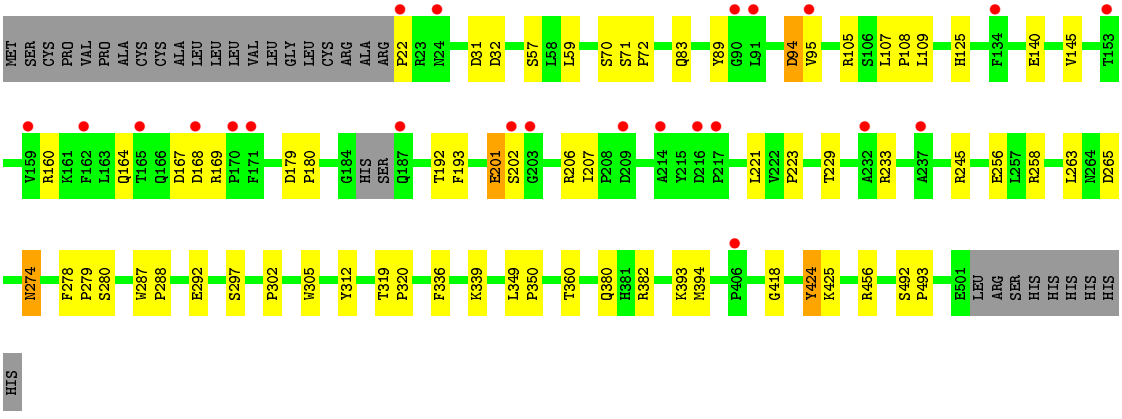
• Molecule 1: N-sulphoglucosamine sulphohydrolase

Chain E:



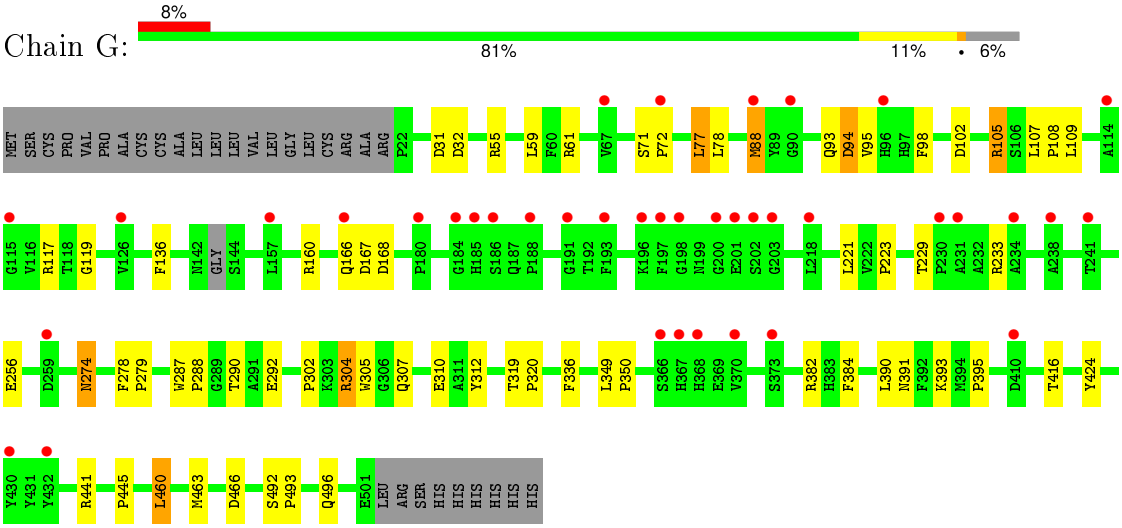
• Molecule 1: N-sulphoglucosamine sulphohydrolase

Chain F:



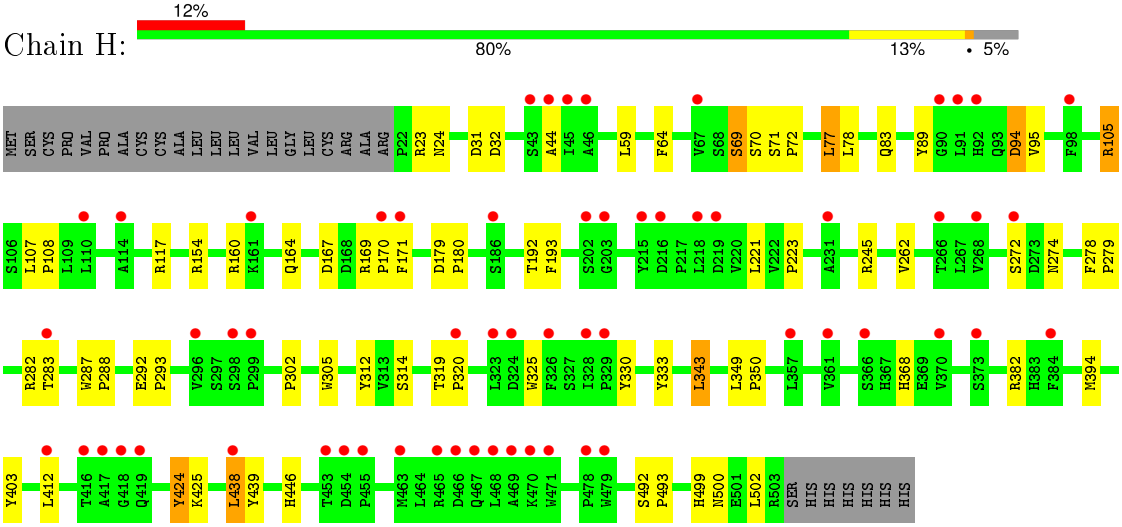
• Molecule 1: N-sulphoglucosamine sulphohydrolase

Chain G:



• Molecule 1: N-sulphoglucosamine sulphohydrolase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.93Å 211.45Å 108.35Å 90.00° 102.69° 90.00°	Depositor
Resolution (Å)	48.85 – 2.40 48.85 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.85-2.40) 99.3 (48.85-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.216 , 0.245 0.217 , 0.245	Depositor DCC
R_{free} test set	8462 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 37.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 174736 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31167	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.73 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.6261e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CA, PEG, FGP, NAG, CL

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	0.24	0/3986	0.41	0/5443
1	B	0.25	0/3977	0.41	0/5429
1	C	0.25	0/3964	0.42	0/5415
1	D	0.25	0/3946	0.41	0/5387
1	E	0.23	0/3710	0.39	0/5081
1	F	0.23	0/3809	0.39	0/5202
1	G	0.23	0/3794	0.39	0/5187
1	H	0.22	0/3725	0.39	0/5100
All	All	0.24	0/30911	0.40	0/42244

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
1	A	0	1
1	H	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	69	SER	Mainchain
1	H	69	SER	Mainchain
1	H	70	FGP	Mainchain

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	3869	0	3671	61	0
1	B	3860	0	3696	70	0
1	C	3854	0	3663	64	0
1	D	3835	0	3648	55	0
1	E	3607	0	3129	65	0
1	F	3703	0	3368	58	0
1	G	3685	0	3350	80	0
1	H	3617	0	3180	76	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	84	0	75	0	0
3	B	83	0	72	6	0
3	C	82	0	69	2	0
3	D	84	0	75	0	0
3	E	56	0	50	0	0
3	F	56	0	50	3	0
3	G	25	0	21	1	0
3	H	55	0	47	7	0
4	A	14	0	13	2	0
4	B	14	0	13	0	0
4	C	14	0	13	2	0
4	D	14	0	13	0	0
4	F	28	0	26	0	0
4	G	24	0	19	0	0
4	H	14	0	13	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	D	5	0	4	1	0
7	A	97	0	0	4	0
7	B	112	0	0	1	0
7	C	87	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	107	0	0	2	0
7	E	8	0	0	2	0
7	F	26	0	0	2	0
7	G	29	0	0	2	0
7	H	9	0	0	0	0
All	All	31167	0	28278	512	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 9.

All (512) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:MET:CE	1:G:98:PHE:HB3	1.79	1.11
1:G:88:MET:HE1	1:G:98:PHE:CB	1.80	1.09
1:E:24:ASN:HB2	1:E:266:THR:HG22	1.30	1.08
1:A:394[A]:MET:HG3	1:B:391[A]:ASN:OD1	1.53	1.06
1:E:24:ASN:HB2	1:E:266:THR:CG2	1.88	1.04
1:B:453:THR:HG22	7:B:800:HOH:O	1.59	1.03
1:E:271:THR:CG2	1:E:294:LEU:HD13	1.89	1.02
1:B:61:ARG:HD2	1:B:310:GLU:OE2	1.63	0.97
1:E:271:THR:HG21	1:E:294:LEU:HD13	1.48	0.95
1:D:268:VAL:HG13	1:D:297:SER:HB3	1.47	0.94
1:G:391:ASN:OD1	1:H:394:MET:HG3	1.67	0.94
1:C:140:GLU:HB3	1:C:145:VAL:HG22	1.51	0.92
1:G:88:MET:CE	1:G:98:PHE:CB	2.41	0.92
1:B:140:GLU:HB3	1:B:145:VAL:HG22	1.52	0.91
1:D:140:GLU:HB3	1:D:145:VAL:HG22	1.52	0.91
1:F:160:ARG:HG3	1:F:256:GLU:OE1	1.70	0.91
1:C:140:GLU:CB	1:C:145:VAL:HG22	2.00	0.91
1:D:140:GLU:CB	1:D:145:VAL:HG22	2.00	0.91
1:B:140:GLU:CB	1:B:145:VAL:HG22	2.01	0.90
1:A:484:ASP:OD2	1:A:504:SER:HA	1.73	0.89
1:C:394:MET:HG3	1:D:391:ASN:OD1	1.71	0.88
1:E:271:THR:CG2	1:E:294:LEU:CD1	2.52	0.88
1:F:140:GLU:CB	1:F:145:VAL:HG22	2.03	0.88
1:G:88:MET:HE1	1:G:98:PHE:HB2	1.56	0.87
1:F:202:SER:HA	7:F:720:HOH:O	1.75	0.87
1:D:268:VAL:CG1	1:D:297:SER:HB3	2.05	0.85
1:F:140:GLU:HB3	1:F:145:VAL:HG22	1.55	0.85
1:D:462:GLU:HG2	7:D:796:HOH:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:453:THR:HG22	1:G:167:ASP:HA	1.59	0.84
1:D:145:VAL:HG23	7:D:723:HOH:O	1.78	0.84
1:B:208:PRO:HG3	3:B:604:NAG:C6	2.08	0.83
1:C:77:LEU:HD23	1:C:77:LEU:C	2.00	0.82
1:H:23:ARG:HD2	1:H:325:TRP:CZ2	2.15	0.82
1:H:330:TYR:CG	1:H:343:LEU:HD21	2.15	0.82
1:H:330:TYR:CD2	1:H:343:LEU:HD21	2.15	0.82
1:G:77:LEU:C	1:G:77:LEU:HD23	2.01	0.81
1:D:501:GLU:C	1:D:501:GLU:OE1	2.18	0.81
1:H:77:LEU:C	1:H:77:LEU:HD23	2.01	0.80
1:E:24:ASN:CB	1:E:266:THR:HG22	2.10	0.79
1:A:61:ARG:HD2	1:A:310:GLU:OE2	1.83	0.78
1:B:459:GLN:HG2	1:G:384:PHE:CZ	2.20	0.77
1:G:88:MET:CE	1:G:88:MET:HA	2.15	0.76
3:H:604:NAG:H61	3:H:605:NAG:O5	1.85	0.76
1:G:88:MET:HE2	1:G:98:PHE:HB3	1.69	0.74
1:H:272:SER:O	1:H:292:GLU:HG2	1.88	0.74
1:F:160:ARG:O	1:F:164:GLN:HG2	1.88	0.74
1:C:299:PRO:O	3:C:606:NAG:H62	1.88	0.73
1:G:160:ARG:HB2	1:G:256:GLU:OE1	1.89	0.72
1:C:304:ARG:HG3	1:C:307:GLN:CD	2.10	0.72
1:B:460:LEU:HD11	1:G:463:MET:HE1	1.72	0.71
1:G:77:LEU:HD22	1:G:78:LEU:HG	1.72	0.71
1:A:304:ARG:HG3	1:A:307:GLN:CD	2.10	0.71
1:E:88:MET:HE3	1:E:92:HIS:HB2	1.71	0.71
1:H:77:LEU:HD22	1:H:78:LEU:HG	1.72	0.71
3:H:604:NAG:O3	3:H:605:NAG:C7	2.38	0.71
1:E:304:ARG:HG3	1:E:307:GLN:CD	2.11	0.71
1:G:88:MET:HE1	1:G:98:PHE:C	2.11	0.70
1:G:88:MET:CE	1:G:98:PHE:C	2.60	0.70
1:C:23:ARG:NH2	1:C:300:GLU:OE1	2.24	0.70
1:D:117:ARG:HD3	1:D:166:GLN:OE1	1.92	0.70
1:G:304:ARG:HG3	1:G:307:GLN:CD	2.11	0.70
1:H:69:SER:HB2	1:H:368:HIS:ND1	2.07	0.70
1:A:88:MET:HE3	1:A:92:HIS:HB2	1.73	0.69
1:B:77:LEU:CD1	1:B:318:LEU:HD23	2.21	0.69
1:C:77:LEU:HD22	1:C:78:LEU:HG	1.73	0.69
1:G:61:ARG:HD2	1:G:310:GLU:OE2	1.92	0.69
1:H:438:LEU:HD23	1:H:439:TYR:N	2.07	0.69
1:G:105:ARG:NH1	1:G:109:LEU:HD21	2.07	0.69
1:B:117:ARG:HD3	1:B:166:GLN:OE1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ASN:O	1:A:394[B]:MET:HG2	1.93	0.69
1:A:117:ARG:HD3	1:A:166:GLN:OE1	1.93	0.68
1:H:343:LEU:N	1:H:343:LEU:HD22	2.08	0.68
1:B:61:ARG:NH2	3:B:601:NAG:O3	2.27	0.68
1:E:117:ARG:HD3	1:E:166:GLN:OE1	1.94	0.68
1:B:460:LEU:CD1	1:G:463:MET:CE	2.72	0.68
1:F:160:ARG:CG	1:F:256:GLU:OE1	2.41	0.68
1:C:88:MET:HE3	1:C:92:HIS:HB2	1.75	0.68
1:E:51:ASP:O	1:E:55:ARG:CD	2.43	0.67
1:B:460:LEU:HD11	1:G:463:MET:CE	2.25	0.67
1:A:304:ARG:HG3	1:A:307:GLN:OE1	1.95	0.67
1:E:214:ALA:HA	7:E:704:HOH:O	1.95	0.66
1:C:77:LEU:HD23	1:C:78:LEU:N	2.11	0.66
1:C:167:ASP:O	1:C:168:ASP:HB2	1.95	0.66
1:G:117:ARG:HD3	1:G:166:GLN:OE1	1.94	0.66
1:B:71:SER:HB2	1:B:72:PRO:HD3	1.78	0.66
1:D:71:SER:HB2	1:D:72:PRO:HD3	1.77	0.66
1:E:452:ALA:O	1:G:168:ASP:CB	2.43	0.66
1:C:304:ARG:HG3	1:C:307:GLN:OE1	1.95	0.66
1:H:71:SER:HB2	1:H:72:PRO:HD3	1.78	0.66
1:C:71:SER:HB2	1:C:72:PRO:HD3	1.78	0.66
1:G:88:MET:HE2	1:G:88:MET:HA	1.77	0.65
1:G:71:SER:HB2	1:G:72:PRO:HD3	1.78	0.65
1:E:71:SER:HB2	1:E:72:PRO:HD3	1.78	0.65
1:E:304:ARG:HG3	1:E:307:GLN:OE1	1.95	0.65
3:H:603:NAG:H2	3:H:603:NAG:C6	2.26	0.65
1:D:61:ARG:NE	1:D:310:GLU:OE2	2.30	0.65
1:F:71:SER:HB2	1:F:72:PRO:HD3	1.78	0.65
1:D:140:GLU:CB	1:D:145:VAL:CG2	2.74	0.65
1:A:71:SER:HB2	1:A:72:PRO:HD3	1.78	0.64
1:F:287:TRP:HB3	1:F:288:PRO:HD3	1.79	0.64
1:F:418:GLY:O	1:G:102:ASP:HB3	1.97	0.64
1:B:460:LEU:CD1	1:G:463:MET:HE3	2.28	0.64
1:A:287:TRP:HB3	1:A:288:PRO:HD3	1.80	0.64
1:H:77:LEU:HD23	1:H:78:LEU:N	2.13	0.63
1:F:418:GLY:HA3	7:G:712:HOH:O	1.97	0.63
1:G:287:TRP:HB3	1:G:288:PRO:HD3	1.80	0.63
1:G:77:LEU:HD23	1:G:78:LEU:N	2.12	0.63
1:A:167:ASP:O	1:A:168:ASP:HB2	1.97	0.63
1:G:304:ARG:HG3	1:G:307:GLN:OE1	1.98	0.63
1:G:109:LEU:HD22	7:G:705:HOH:O	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:TRP:HB3	1:E:288:PRO:HD3	1.80	0.63
1:F:201:GLU:OE1	1:F:201:GLU:N	2.32	0.63
1:H:287:TRP:HB3	1:H:288:PRO:HD3	1.81	0.63
1:B:140:GLU:CB	1:B:145:VAL:CG2	2.75	0.62
1:C:140:GLU:CB	1:C:145:VAL:CG2	2.75	0.62
1:H:330:TYR:CD2	1:H:343:LEU:CD2	2.82	0.62
1:D:287:TRP:HB3	1:D:288:PRO:HD3	1.82	0.62
1:G:416:THR:HG21	1:H:499:HIS:CE1	2.34	0.62
1:C:287:TRP:HB3	1:C:288:PRO:HD3	1.81	0.61
1:B:287:TRP:HB3	1:B:288:PRO:HD3	1.81	0.61
1:B:57:SER:HB3	1:B:297:SER:HB2	1.82	0.61
1:F:140:GLU:CB	1:F:145:VAL:CG2	2.77	0.61
1:B:501:GLU:O	1:B:502:LEU:HD23	2.01	0.61
1:H:438:LEU:HD23	1:H:438:LEU:C	2.21	0.61
1:H:31:ASP:O	1:H:180:PRO:HD2	2.01	0.60
1:G:319:THR:HB	1:G:320:PRO:HD3	1.83	0.60
1:H:23:ARG:HG3	1:H:325:TRP:NE1	2.16	0.60
1:H:319:THR:HB	1:H:320:PRO:HD3	1.82	0.60
1:B:459:GLN:HB3	1:G:460:LEU:HD11	1.82	0.60
1:A:441:ARG:NH1	1:A:445:PRO:O	2.35	0.60
1:H:272:SER:HB3	1:H:292:GLU:HG3	1.84	0.60
1:F:70:FGP:HOG	1:F:125:HIS:CE1	2.18	0.59
1:F:319:THR:HB	1:F:320:PRO:HD3	1.83	0.59
1:C:77:LEU:CD2	1:C:78:LEU:HG	2.33	0.59
1:D:319:THR:HB	1:D:320:PRO:HD3	1.84	0.59
1:B:44:ALA:HB2	1:B:221:LEU:HD13	1.85	0.59
1:C:319:THR:HB	1:C:320:PRO:HD3	1.84	0.59
1:B:424:TYR:CZ	1:B:425:LYS:HD2	2.38	0.59
1:A:319:THR:HB	1:A:320:PRO:HD3	1.84	0.59
1:H:44:ALA:HB2	1:H:221:LEU:HD13	1.83	0.59
1:B:44:ALA:CB	1:B:221:LEU:HD13	2.32	0.59
1:D:23:ARG:O	1:D:170:PRO:HB3	2.03	0.59
1:B:23:ARG:O	1:B:170:PRO:HB3	2.02	0.59
1:D:424:TYR:CZ	1:D:425:LYS:HD2	2.38	0.59
1:G:77:LEU:CD2	1:G:78:LEU:HG	2.32	0.59
1:A:424:TYR:CZ	1:A:425:LYS:HD2	2.38	0.59
1:H:77:LEU:CD2	1:H:78:LEU:HG	2.31	0.59
1:E:424:TYR:CZ	1:E:425:LYS:HD2	2.38	0.59
1:E:319:THR:HB	1:E:320:PRO:HD3	1.84	0.59
1:F:424:TYR:CZ	1:F:425:LYS:HD2	2.38	0.59
1:G:88:MET:HE1	1:G:98:PHE:CA	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:THR:HB	1:B:320:PRO:HD3	1.85	0.58
1:G:441:ARG:NH1	1:G:445:PRO:O	2.36	0.58
1:F:201:GLU:CA	1:F:201:GLU:OE1	2.51	0.58
1:H:424:TYR:CZ	1:H:425:LYS:HD2	2.38	0.58
1:E:24:ASN:HB2	1:E:266:THR:HG23	1.80	0.58
3:H:603:NAG:C2	3:H:603:NAG:C6	2.82	0.58
1:C:140:GLU:HB3	1:C:145:VAL:CG2	2.31	0.58
1:F:160:ARG:HG3	1:F:256:GLU:CD	2.22	0.58
1:H:105:ARG:NH2	1:H:333:TYR:HB3	2.19	0.58
1:C:424:TYR:CZ	1:C:425:LYS:HD2	2.39	0.58
1:B:140:GLU:HB3	1:B:145:VAL:CG2	2.31	0.57
1:F:70:FGP:OG1	1:F:125:HIS:ND1	2.30	0.57
1:B:501:GLU:O	1:B:501:GLU:HG2	2.04	0.57
1:D:44:ALA:CB	1:D:221:LEU:HD13	2.34	0.57
1:H:23:ARG:O	1:H:170:PRO:HB3	2.05	0.57
1:B:77:LEU:HD13	1:B:318:LEU:HD23	1.85	0.57
1:E:441:ARG:NH1	1:E:445:PRO:O	2.37	0.57
1:D:140:GLU:HB2	1:D:145:VAL:CG2	2.34	0.57
1:C:441:ARG:NH1	1:C:445:PRO:O	2.37	0.57
1:F:125:HIS:HA	7:F:726:HOH:O	2.05	0.57
1:F:140:GLU:HB2	1:F:145:VAL:CG2	2.35	0.57
1:D:140:GLU:HB3	1:D:145:VAL:CG2	2.31	0.57
1:D:44:ALA:HB2	1:D:221:LEU:HD13	1.87	0.56
1:E:271:THR:CG2	1:E:294:LEU:HD12	2.35	0.56
1:H:438:LEU:CD2	1:H:438:LEU:C	2.74	0.56
1:H:262:VAL:HG12	1:H:262:VAL:O	2.05	0.56
1:C:140:GLU:HB2	1:C:145:VAL:CG2	2.35	0.56
1:F:278:PHE:HB3	1:F:279:PRO:HD2	1.88	0.56
1:A:278:PHE:HB3	1:A:279:PRO:HD2	1.88	0.56
1:D:437:GLU:HG2	6:D:609:PEG:H22	1.88	0.56
1:G:278:PHE:HB3	1:G:279:PRO:HD2	1.88	0.56
1:D:278:PHE:HB3	1:D:279:PRO:HD2	1.88	0.56
1:E:278:PHE:HB3	1:E:279:PRO:HD2	1.88	0.56
1:H:44:ALA:CB	1:H:221:LEU:HD13	2.36	0.55
1:H:171:PHE:HE2	1:H:262:VAL:HG11	1.71	0.55
1:G:274:ASN:HA	1:G:292:GLU:OE2	2.06	0.55
1:B:140:GLU:HB2	1:B:145:VAL:CG2	2.35	0.55
1:A:274:ASN:HA	1:A:292:GLU:OE2	2.07	0.55
1:G:107:LEU:N	1:G:108:PRO:HD2	2.21	0.55
3:H:605:NAG:O3	3:H:605:NAG:H82	2.07	0.55
1:H:171:PHE:CE2	1:H:262:VAL:HG11	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:PHE:HB3	1:C:279:PRO:HD2	1.88	0.55
1:B:355:GLU:H	1:G:492:SER:CB	2.20	0.55
1:H:412:LEU:O	1:H:412:LEU:HD23	2.06	0.55
1:F:274:ASN:HA	1:F:292:GLU:OE2	2.07	0.54
3:B:603:NAG:O4	3:B:604:NAG:H4	2.07	0.54
1:E:274:ASN:HA	1:E:292:GLU:OE2	2.07	0.54
1:B:274:ASN:HA	1:B:292:GLU:OE2	2.08	0.54
1:C:274:ASN:HA	1:C:292:GLU:OE2	2.08	0.54
1:H:278:PHE:HB3	1:H:279:PRO:HD2	1.88	0.54
1:D:274:ASN:HA	1:D:292:GLU:OE2	2.08	0.54
1:B:278:PHE:HB3	1:B:279:PRO:HD2	1.89	0.54
1:C:492:SER:HA	1:C:493:PRO:C	2.29	0.53
1:E:270:PHE:O	1:E:271:THR:HG23	2.08	0.53
1:D:107:LEU:N	1:D:108:PRO:HD2	2.23	0.53
1:A:409:GLN:HB3	4:A:608:NAG:H82	1.90	0.53
1:A:107:LEU:N	1:A:108:PRO:HD2	2.23	0.53
1:D:77:LEU:C	1:D:77:LEU:HD12	2.28	0.53
1:G:88:MET:HE3	1:G:98:PHE:C	2.29	0.53
1:H:343:LEU:HD22	1:H:343:LEU:H	1.72	0.53
3:B:605:NAG:H61	3:B:606:NAG:C1	2.39	0.53
1:H:107:LEU:HB3	1:H:108:PRO:CD	2.39	0.53
1:H:107:LEU:N	1:H:108:PRO:HD2	2.24	0.53
1:G:77:LEU:C	1:G:77:LEU:CD2	2.75	0.52
1:A:107:LEU:HB3	1:A:108:PRO:CD	2.40	0.52
1:F:107:LEU:N	1:F:108:PRO:HD2	2.24	0.52
1:F:94:ASP:OD1	1:F:95:VAL:N	2.39	0.52
1:G:94:ASP:OD1	1:G:95:VAL:N	2.38	0.52
1:C:23:ARG:O	1:C:170:PRO:HB3	2.10	0.52
1:A:192:THR:HG23	1:A:193:PHE:HD1	1.75	0.52
1:B:107:LEU:N	1:B:108:PRO:HD2	2.24	0.52
1:B:459:GLN:CB	1:G:460:LEU:HD11	2.40	0.52
1:E:271:THR:HG22	1:E:294:LEU:HD13	1.87	0.52
1:D:107:LEU:HB3	1:D:108:PRO:CD	2.40	0.52
1:F:107:LEU:HB3	1:F:108:PRO:CD	2.40	0.52
1:B:107:LEU:HB3	1:B:108:PRO:CD	2.39	0.52
1:C:94:ASP:OD1	1:C:95:VAL:N	2.37	0.52
1:G:55:ARG:NE	1:G:55:ARG:HA	2.25	0.52
1:B:459:GLN:HG2	1:G:384:PHE:CE2	2.45	0.51
1:B:179:ASP:OD2	1:B:245:ARG:HD2	2.11	0.51
1:G:107:LEU:HB3	1:G:108:PRO:CD	2.40	0.51
1:H:23:ARG:O	1:H:24:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:282:ARG:O	1:H:283:THR:CB	2.58	0.51
1:G:395:PRO:HG3	1:H:502:LEU:HD11	1.92	0.51
1:B:287:TRP:N	1:B:288:PRO:CD	2.73	0.51
1:C:107:LEU:N	1:C:108:PRO:HD2	2.26	0.51
1:E:107:LEU:N	1:E:108:PRO:HD2	2.25	0.51
1:G:393:LYS:HB2	1:H:394:MET:SD	2.50	0.50
1:F:140:GLU:HB3	1:F:145:VAL:CG2	2.34	0.50
1:C:287:TRP:N	1:C:288:PRO:CD	2.73	0.50
1:C:107:LEU:HB3	1:C:108:PRO:CD	2.40	0.50
1:H:262:VAL:CG1	1:H:262:VAL:O	2.58	0.50
1:H:192:THR:HG23	1:H:193:PHE:HD1	1.76	0.50
1:E:107:LEU:HB3	1:E:108:PRO:CD	2.40	0.50
1:H:500:ASN:OD1	1:H:502:LEU:HB2	2.12	0.50
1:F:31:ASP:O	1:F:180:PRO:HD2	2.12	0.50
1:C:221:LEU:O	1:C:223:PRO:HD3	2.11	0.50
1:A:31:ASP:O	1:A:180:PRO:HD2	2.11	0.50
1:D:31:ASP:O	1:D:180:PRO:HD2	2.11	0.50
1:D:179:ASP:OD2	1:D:245:ARG:HD2	2.12	0.50
1:E:31:ASP:O	1:E:180:PRO:HD2	2.11	0.50
1:E:287:TRP:N	1:E:288:PRO:CD	2.74	0.50
1:A:94:ASP:OD1	1:A:95:VAL:N	2.43	0.50
1:G:88:MET:HE3	1:G:88:MET:HA	1.94	0.50
1:F:179:ASP:OD2	1:F:245:ARG:HD2	2.12	0.50
3:H:604:NAG:C6	3:H:605:NAG:O5	2.58	0.49
1:B:59:LEU:C	1:B:59:LEU:HD23	2.33	0.49
1:A:488:GLU:OE1	1:A:490:LYS:NZ	2.46	0.49
1:F:59:LEU:HD23	1:F:59:LEU:C	2.32	0.49
1:A:287:TRP:N	1:A:288:PRO:CD	2.74	0.49
1:A:221:LEU:O	1:A:223:PRO:HD3	2.12	0.49
1:H:343:LEU:H	1:H:343:LEU:CD2	2.26	0.49
1:G:287:TRP:N	1:G:288:PRO:CD	2.75	0.49
1:A:229:THR:O	1:A:233:ARG:HG3	2.13	0.49
1:E:394:MET:SD	1:F:393:LYS:HB2	2.52	0.49
1:D:349:LEU:N	1:D:350:PRO:CD	2.75	0.49
1:H:343:LEU:N	1:H:343:LEU:CD2	2.74	0.49
1:H:221:LEU:O	1:H:223:PRO:HD3	2.12	0.49
1:F:192:THR:HG23	1:F:193:PHE:HD1	1.77	0.49
1:A:59:LEU:C	1:A:59:LEU:HD23	2.33	0.49
1:H:179:ASP:OD2	1:H:245:ARG:HD2	2.13	0.49
1:D:94:ASP:OD1	1:D:95:VAL:N	2.38	0.49
1:E:31:ASP:O	1:E:32:ASP:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:THR:O	1:C:233:ARG:HG3	2.13	0.49
1:E:258:ARG:HG3	1:E:263:LEU:HD22	1.95	0.49
1:H:330:TYR:CD1	1:H:343:LEU:HD21	2.48	0.49
1:D:287:TRP:N	1:D:288:PRO:CD	2.75	0.49
1:G:416:THR:HG21	1:H:499:HIS:ND1	2.27	0.49
1:B:349:LEU:HB2	1:B:350:PRO:HD3	1.95	0.49
1:F:258:ARG:HG3	1:F:263:LEU:HD22	1.95	0.49
1:A:504:SER:CB	7:A:746:HOH:O	2.61	0.48
1:C:59:LEU:HD23	1:C:59:LEU:C	2.34	0.48
1:E:271:THR:HG22	1:E:294:LEU:CD1	2.39	0.48
1:B:349:LEU:N	1:B:350:PRO:CD	2.76	0.48
1:G:312:TYR:CZ	1:G:382:ARG:HA	2.48	0.48
1:H:59:LEU:HD23	1:H:59:LEU:C	2.33	0.48
1:D:282:ARG:O	1:D:283:THR:OG1	2.25	0.48
1:E:349:LEU:HB2	1:E:350:PRO:HD3	1.95	0.48
1:E:271:THR:HG23	1:E:294:LEU:CD1	2.41	0.48
1:B:94:ASP:OD1	1:B:95:VAL:N	2.40	0.48
1:G:278:PHE:HB3	1:G:279:PRO:CD	2.44	0.48
1:A:492:SER:HA	1:A:493:PRO:C	2.33	0.48
1:B:31:ASP:O	1:B:180:PRO:HD2	2.14	0.48
1:C:380:GLN:OE1	1:C:385:ARG:HD2	2.14	0.48
1:F:278:PHE:HB3	1:F:279:PRO:CD	2.44	0.47
1:H:107:LEU:HB3	1:H:108:PRO:HD3	1.96	0.47
1:H:287:TRP:N	1:H:288:PRO:CD	2.77	0.47
1:G:349:LEU:N	1:G:350:PRO:CD	2.77	0.47
1:H:349:LEU:HB2	1:H:350:PRO:HD3	1.95	0.47
1:H:69:SER:OG	1:H:72:PRO:HG2	2.13	0.47
1:E:492:SER:HA	1:E:493:PRO:C	2.34	0.47
1:G:59:LEU:C	1:G:59:LEU:HD23	2.34	0.47
1:G:88:MET:HE1	1:G:98:PHE:O	2.14	0.47
1:D:221:LEU:O	1:D:223:PRO:HD3	2.15	0.47
1:A:349:LEU:HB2	1:A:350:PRO:HD3	1.96	0.47
1:E:392:PHE:O	7:E:702:HOH:O	2.20	0.47
1:C:349:LEU:N	1:C:350:PRO:CD	2.77	0.47
1:E:160:ARG:O	1:E:164:GLN:HG3	2.14	0.47
1:G:349:LEU:HB2	1:G:350:PRO:HD3	1.96	0.47
1:A:258:ARG:HG3	1:A:263:LEU:HD22	1.96	0.47
1:G:229:THR:O	1:G:233:ARG:HG3	2.14	0.47
1:F:287:TRP:N	1:F:288:PRO:CD	2.77	0.47
1:C:278:PHE:HB3	1:C:279:PRO:CD	2.45	0.47
1:C:349:LEU:HB2	1:C:350:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:LEU:N	1:F:350:PRO:CD	2.78	0.47
1:E:271:THR:HG23	1:E:294:LEU:HD12	1.97	0.47
1:B:221:LEU:O	1:B:223:PRO:HD3	2.14	0.47
1:E:278:PHE:HB3	1:E:279:PRO:CD	2.45	0.47
1:F:274:ASN:C	1:F:292:GLU:OE2	2.54	0.47
1:B:107:LEU:HB3	1:B:108:PRO:HD3	1.97	0.47
1:D:274:ASN:C	1:D:292:GLU:OE2	2.53	0.47
1:E:302:PRO:HA	1:E:305:TRP:CD1	2.50	0.47
1:C:77:LEU:CD2	1:C:77:LEU:C	2.74	0.47
1:A:302:PRO:HA	1:A:305:TRP:CD1	2.50	0.47
1:D:59:LEU:HD23	1:D:59:LEU:C	2.35	0.47
1:C:394:MET:HE1	1:D:390:LEU:O	2.14	0.46
1:D:349:LEU:HB2	1:D:350:PRO:HD3	1.97	0.46
1:G:31:ASP:O	1:G:32:ASP:HB2	2.15	0.46
1:G:221:LEU:O	1:G:223:PRO:HD3	2.15	0.46
1:H:278:PHE:HB3	1:H:279:PRO:CD	2.44	0.46
1:D:31:ASP:O	1:D:32:ASP:HB2	2.15	0.46
1:C:31:ASP:O	1:C:32:ASP:HB2	2.15	0.46
1:C:302:PRO:HA	1:C:305:TRP:CD1	2.50	0.46
1:B:31:ASP:O	1:B:32:ASP:HB2	2.14	0.46
1:E:146:LEU:HD22	1:E:197:PHE:CZ	2.50	0.46
1:E:221:LEU:O	1:E:223:PRO:HD3	2.14	0.46
1:H:94:ASP:OD1	1:H:95:VAL:N	2.40	0.46
1:C:31:ASP:O	1:C:180:PRO:HD2	2.16	0.46
1:F:302:PRO:HA	1:F:305:TRP:CD1	2.50	0.46
1:F:221:LEU:O	1:F:223:PRO:HD3	2.16	0.46
1:B:278:PHE:HB3	1:B:279:PRO:CD	2.46	0.46
1:F:31:ASP:O	1:F:32:ASP:HB2	2.14	0.46
1:D:278:PHE:HB3	1:D:279:PRO:CD	2.45	0.46
1:H:302:PRO:HA	1:H:305:TRP:CD1	2.50	0.46
1:H:77:LEU:C	1:H:77:LEU:CD2	2.75	0.46
1:A:409:GLN:CB	4:A:608:NAG:H82	2.46	0.46
1:C:107:LEU:HB3	1:C:108:PRO:HD3	1.98	0.46
1:C:409:GLN:CB	4:C:608:NAG:H82	2.46	0.46
1:E:94:ASP:OD1	1:E:95:VAL:N	2.44	0.46
1:A:394[A]:MET:SD	1:B:393:LYS:HB2	2.56	0.45
1:F:107:LEU:HB3	1:F:108:PRO:HD3	1.97	0.45
1:F:349:LEU:HB2	1:F:350:PRO:HD3	1.97	0.45
1:C:146:LEU:HD22	1:C:197:PHE:CZ	2.51	0.45
1:A:125:HIS:HA	7:A:794:HOH:O	2.16	0.45
1:C:61:ARG:NE	1:C:310:GLU:OE2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:HD22	1:A:197:PHE:CZ	2.50	0.45
1:A:278:PHE:HB3	1:A:279:PRO:CD	2.45	0.45
1:A:274:ASN:C	1:A:292:GLU:OE2	2.55	0.45
1:G:492:SER:HA	1:G:493:PRO:C	2.37	0.45
1:A:312:TYR:CZ	1:A:382:ARG:HA	2.51	0.45
1:D:23:ARG:NH2	1:D:300:GLU:OE2	2.45	0.45
1:A:107:LEU:HB3	1:A:108:PRO:HD3	1.97	0.45
1:D:302:PRO:HA	1:D:305:TRP:CD1	2.51	0.45
1:E:64:PHE:O	1:E:314:SER:HA	2.15	0.45
3:B:604:NAG:O5	3:B:604:NAG:O7	2.34	0.45
3:H:604:NAG:H4	3:H:605:NAG:H2	1.52	0.45
1:E:107:LEU:HB3	1:E:108:PRO:HD3	1.98	0.45
1:B:381:HIS:NE2	1:G:466:ASP:OD2	2.49	0.45
1:E:274:ASN:C	1:E:292:GLU:OE2	2.55	0.45
1:D:229:THR:O	1:D:233:ARG:HG3	2.17	0.45
1:F:312:TYR:CZ	1:F:382:ARG:HA	2.52	0.45
1:C:274:ASN:C	1:C:292:GLU:OE2	2.55	0.45
1:D:290:THR:O	1:D:292:GLU:HG2	2.16	0.45
1:E:32:ASP:HB3	1:E:277:PRO:HD3	1.98	0.45
1:C:304:ARG:CG	1:C:307:GLN:OE1	2.65	0.45
1:B:355:GLU:H	1:G:492:SER:HB2	1.80	0.45
1:B:274:ASN:C	1:B:292:GLU:OE2	2.55	0.45
1:A:31:ASP:O	1:A:32:ASP:HB2	2.16	0.45
1:E:349:LEU:N	1:E:350:PRO:CD	2.78	0.45
1:H:349:LEU:N	1:H:350:PRO:CD	2.79	0.45
3:G:602:NAG:H61	3:G:603:NAG:C1	2.46	0.45
1:B:23:ARG:NH2	1:B:300:GLU:OE2	2.39	0.45
1:G:336:PHE:CE1	1:H:94:ASP:HA	2.51	0.45
1:B:167:ASP:OD1	1:B:167:ASP:N	2.50	0.45
1:H:292:GLU:HG3	1:H:293:PRO:HD2	1.99	0.45
1:B:355:GLU:H	1:G:492:SER:HB3	1.79	0.45
1:F:57:SER:OG	1:F:297:SER:HB2	2.16	0.45
1:B:282:ARG:O	1:B:283:THR:OG1	2.24	0.45
1:A:304:ARG:CG	1:A:307:GLN:OE1	2.64	0.45
1:A:349:LEU:N	1:A:350:PRO:CD	2.79	0.45
1:B:160:ARG:O	1:B:164:GLN:HG3	2.17	0.44
1:H:330:TYR:CE2	1:H:343:LEU:HD21	2.51	0.44
1:C:282:ARG:O	1:C:283:THR:OG1	2.24	0.44
1:G:107:LEU:HB3	1:G:108:PRO:HD3	1.98	0.44
1:A:88:MET:CE	1:A:92:HIS:HB2	2.45	0.44
1:D:107:LEU:HB3	1:D:108:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:160:ARG:O	1:H:164:GLN:HG3	2.17	0.44
1:G:302:PRO:HA	1:G:305:TRP:CD1	2.53	0.44
1:F:167:ASP:C	1:F:169:ARG:H	2.21	0.44
1:A:319:THR:N	1:A:320:PRO:CD	2.80	0.44
1:H:412:LEU:C	1:H:412:LEU:HD23	2.38	0.44
1:A:484:ASP:N	1:A:484:ASP:OD1	2.48	0.44
1:B:229:THR:O	1:B:233:ARG:HG3	2.18	0.44
1:E:117:ARG:CD	1:E:166:GLN:OE1	2.65	0.44
1:F:319:THR:N	1:F:320:PRO:CD	2.81	0.44
1:D:319:THR:N	1:D:320:PRO:CD	2.81	0.44
1:G:274:ASN:C	1:G:292:GLU:OE2	2.56	0.44
1:E:312:TYR:CZ	1:E:382:ARG:HA	2.52	0.44
1:B:312:TYR:CZ	1:B:382:ARG:HA	2.52	0.44
1:E:271:THR:HG22	1:E:294:LEU:HA	2.00	0.44
1:G:319:THR:N	1:G:320:PRO:CD	2.81	0.43
1:E:88:MET:CE	1:E:92:HIS:HB2	2.45	0.43
1:D:117:ARG:CD	1:D:166:GLN:OE1	2.64	0.43
1:E:94:ASP:HA	1:F:336:PHE:CE1	2.53	0.43
1:A:504:SER:HB3	7:A:746:HOH:O	2.19	0.43
1:C:88:MET:CE	1:C:92:HIS:HB2	2.45	0.43
1:D:274:ASN:CA	1:D:292:GLU:OE2	2.67	0.43
1:H:312:TYR:CZ	1:H:382:ARG:HA	2.54	0.43
1:A:88:MET:HE1	1:A:98:PHE:O	2.18	0.43
1:B:117:ARG:CD	1:B:166:GLN:OE1	2.63	0.43
1:A:117:ARG:CD	1:A:166:GLN:OE1	2.65	0.43
1:H:31:ASP:O	1:H:32:ASP:HB2	2.19	0.43
1:B:319:THR:N	1:B:320:PRO:CD	2.82	0.43
1:B:484:ASP:OD1	1:B:484:ASP:N	2.48	0.43
1:C:484:ASP:OD1	1:C:484:ASP:N	2.47	0.43
1:A:274:ASN:CA	1:A:292:GLU:OE2	2.67	0.43
1:D:119:GLY:HA2	1:D:136:PHE:O	2.19	0.43
1:G:496:GLN:HB3	1:H:403:TYR:OH	2.19	0.43
1:G:105:ARG:NH1	1:G:109:LEU:CD2	2.81	0.43
1:F:279:PRO:O	1:F:280:SER:HB2	2.19	0.43
1:B:302:PRO:HA	1:B:305:TRP:CD1	2.53	0.43
1:C:491:LEU:HD13	1:C:496:GLN:NE2	2.34	0.43
1:B:197:PHE:O	1:B:245:ARG:NH2	2.52	0.43
1:A:491:LEU:HD13	1:A:496:GLN:NE2	2.34	0.43
1:E:491:LEU:HD13	1:E:496:GLN:NE2	2.34	0.43
1:G:390:LEU:O	1:H:394:MET:HE1	2.19	0.42
1:G:304:ARG:CG	1:G:307:GLN:OE1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:GLU:O	1:B:501:GLU:CG	2.66	0.42
1:C:319:THR:N	1:C:320:PRO:CD	2.82	0.42
1:H:64:PHE:O	1:H:314:SER:HA	2.18	0.42
3:C:606:NAG:H61	3:C:607:NAG:C7	2.49	0.42
1:E:393:LYS:HB2	1:F:394:MET:SD	2.59	0.42
1:C:88:MET:HE1	1:C:98:PHE:O	2.19	0.42
1:E:319:THR:N	1:E:320:PRO:CD	2.83	0.42
1:H:105:ARG:HH21	1:H:333:TYR:HB3	1.83	0.42
1:G:274:ASN:CA	1:G:292:GLU:OE2	2.67	0.42
1:E:304:ARG:CG	1:E:307:GLN:OE1	2.65	0.42
1:E:279:PRO:O	1:E:280:SER:HB2	2.19	0.42
1:C:312:TYR:CZ	1:C:382:ARG:HA	2.54	0.42
1:G:119:GLY:HA2	1:G:136:PHE:O	2.20	0.42
1:E:203:GLY:O	1:E:204:MET:HE2	2.20	0.42
1:G:88:MET:HE2	1:G:88:MET:CA	2.46	0.42
1:A:290:THR:O	1:A:292:GLU:HG2	2.19	0.42
1:F:274:ASN:CA	1:F:292:GLU:OE2	2.67	0.42
1:D:454:ASP:OD1	1:D:456:ARG:HD3	2.18	0.42
1:D:167:ASP:N	1:D:167:ASP:OD1	2.53	0.42
1:D:156:LYS:HG3	1:D:157:LEU:N	2.34	0.42
1:B:119:GLY:HA2	1:B:136:PHE:O	2.19	0.42
1:G:88:MET:CE	1:G:98:PHE:O	2.68	0.42
1:H:105:ARG:NE	1:H:333:TYR:CG	2.88	0.42
1:E:274:ASN:CA	1:E:292:GLU:OE2	2.67	0.42
1:A:488:GLU:HB2	1:A:491:LEU:HD11	2.02	0.42
1:C:207:ILE:HA	1:C:208:PRO:HD2	1.92	0.42
1:A:425:LYS:CE	7:A:752:HOH:O	2.67	0.41
1:H:105:ARG:HD3	1:H:333:TYR:CE2	2.55	0.41
1:E:290:THR:O	1:E:292:GLU:HG2	2.19	0.41
1:H:492:SER:HA	1:H:493:PRO:C	2.39	0.41
1:E:88:MET:HE1	1:E:98:PHE:O	2.19	0.41
1:G:290:THR:O	1:G:292:GLU:HG2	2.20	0.41
1:A:32:ASP:HB3	1:A:277:PRO:HD3	2.02	0.41
1:B:32:ASP:HB3	1:B:277:PRO:HD3	2.02	0.41
1:C:146:LEU:HD22	1:C:197:PHE:CE2	2.55	0.41
1:F:167:ASP:N	1:F:167:ASP:OD1	2.53	0.41
1:C:21:ARG:HA	1:C:22:PRO:HD2	1.89	0.41
3:F:603:NAG:H61	3:F:604:NAG:C1	2.51	0.41
1:B:290:THR:O	1:B:292:GLU:HG2	2.21	0.41
1:D:346:ARG:HG2	1:D:346:ARG:O	2.19	0.41
1:B:274:ASN:CA	1:B:292:GLU:OE2	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:THR:O	1:C:292:GLU:HG2	2.20	0.41
1:C:147:GLN:O	1:C:151:ASN:HB3	2.21	0.41
1:F:492:SER:HA	1:F:493:PRO:C	2.40	0.41
1:E:167:ASP:C	1:E:169:ARG:H	2.24	0.41
1:A:119:GLY:HA2	1:A:136:PHE:O	2.21	0.41
1:F:207:ILE:HG13	3:F:603:NAG:H82	2.03	0.41
1:F:83:GLN:OE1	1:F:89:TYR:HA	2.21	0.41
1:E:488:GLU:HB2	1:E:491:LEU:HD11	2.03	0.41
1:F:206:ARG:N	3:F:603:NAG:H83	2.35	0.41
1:F:22:PRO:O	1:F:265:ASP:HB3	2.21	0.41
1:C:140:GLU:HB2	1:C:145:VAL:HG22	1.89	0.41
3:B:603:NAG:H61	3:B:604:NAG:H2	2.02	0.41
1:C:274:ASN:CA	1:C:292:GLU:OE2	2.68	0.41
1:C:409:GLN:HB2	4:C:608:NAG:H82	2.03	0.41
1:A:427:LEU:HA	1:A:427:LEU:HD23	1.87	0.41
1:H:83:GLN:OE1	1:H:89:TYR:HA	2.21	0.41
1:B:83:GLN:OE1	1:B:89:TYR:HA	2.21	0.41
1:F:360:THR:HA	1:F:380:GLN:O	2.21	0.41
1:A:486:VAL:CG2	1:A:498:LEU:HD21	2.51	0.41
1:D:312:TYR:CZ	1:D:382:ARG:HA	2.55	0.41
1:C:394:MET:SD	1:D:393:LYS:HB2	2.61	0.40
1:H:23:ARG:C	1:H:24:ASN:ND2	2.75	0.40
1:G:117:ARG:CD	1:G:166:GLN:OE1	2.66	0.40
1:C:119:GLY:HA2	1:C:136:PHE:O	2.21	0.40
1:B:77:LEU:HD13	1:B:318:LEU:CD2	2.52	0.40
1:A:317:ASP:C	1:A:320:PRO:HD2	2.41	0.40
1:A:394[A]:MET:HE3	1:A:395:PRO:HD2	2.04	0.40
1:H:167:ASP:C	1:H:169:ARG:H	2.25	0.40
1:H:154:ARG:HA	1:H:154:ARG:NE	2.36	0.40
1:D:427:LEU:HD23	1:D:427:LEU:HA	1.88	0.40
1:F:229:THR:O	1:F:233:ARG:HG3	2.21	0.40
1:F:105:ARG:HG3	1:F:109:LEU:HD23	2.04	0.40
1:A:83:GLN:OE1	1:A:89:TYR:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	484/510 (95%)	472 (98%)	11 (2%)	1 (0%)	52	69
1	B	480/510 (94%)	464 (97%)	15 (3%)	1 (0%)	52	69
1	C	481/510 (94%)	469 (98%)	10 (2%)	2 (0%)	39	56
1	D	478/510 (94%)	463 (97%)	13 (3%)	2 (0%)	39	56
1	E	480/510 (94%)	468 (98%)	11 (2%)	1 (0%)	52	69
1	F	473/510 (93%)	459 (97%)	11 (2%)	3 (1%)	30	43
1	G	474/510 (93%)	460 (97%)	13 (3%)	1 (0%)	52	69
1	H	479/510 (94%)	466 (97%)	12 (2%)	1 (0%)	52	69
All	All	3829/4080 (94%)	3721 (97%)	96 (2%)	12 (0%)	46	63

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	B	94	ASP
1	C	94	ASP
1	D	94	ASP
1	E	94	ASP
1	F	94	ASP
1	G	94	ASP
1	H	94	ASP
1	F	168	ASP
1	F	339	LYS
1	D	339	LYS
1	C	339	LYS

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	410/442 (93%)	404 (98%)	6 (2%)	72 87
1	B	414/442 (94%)	408 (99%)	6 (1%)	74 88
1	C	408/442 (92%)	400 (98%)	8 (2%)	63 81
1	D	404/442 (91%)	397 (98%)	7 (2%)	68 85
1	E	326/442 (74%)	320 (98%)	6 (2%)	66 84
1	F	363/442 (82%)	359 (99%)	4 (1%)	80 92
1	G	359/442 (81%)	351 (98%)	8 (2%)	60 79
1	H	334/442 (76%)	326 (98%)	8 (2%)	57 76
All	All	3018/3536 (85%)	2965 (98%)	53 (2%)	66 84

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	146	LEU
1	A	274	ASN
1	A	304	ARG
1	A	424	TYR
1	A	490	LYS
1	B	95	VAL
1	B	206	ARG
1	B	274	ASN
1	B	318	LEU
1	B	424	TYR
1	B	456	ARG
1	C	77	LEU
1	C	95	VAL
1	C	146	LEU
1	C	194	CYS
1	C	274	ASN
1	C	304	ARG
1	C	385	ARG
1	C	424	TYR
1	D	77	LEU
1	D	95	VAL
1	D	156	LYS

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Mol	Chain	Res	Type
1	D	424	TYR
1	D	428	ARG
1	D	462	GLU
1	D	501	GLU
1	E	146	LEU
1	E	206	ARG
1	E	266	THR
1	E	274	ASN
1	E	304	ARG
1	E	424	TYR
1	F	201	GLU
1	F	274	ASN
1	F	424	TYR
1	F	456	ARG
1	G	77	LEU
1	G	88	MET
1	G	93	GLN
1	G	105	ARG
1	G	274	ASN
1	G	304	ARG
1	G	424	TYR
1	G	460	LEU
1	H	77	LEU
1	H	105	ARG
1	H	117	ARG
1	H	274	ASN
1	H	343	LEU
1	H	424	TYR
1	H	438	LEU
1	H	446	HIS

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	FGP	A	70	1,2	7,10,11	0.88	0	7,14,16	1.56	1 (14%)
1	FGP	B	70	1,2	7,10,11	0.85	0	7,14,16	1.55	1 (14%)
1	FGP	C	70	1,2	7,10,11	0.88	0	7,14,16	1.41	1 (14%)
1	FGP	D	70	1,2	7,10,11	0.89	0	7,14,16	1.48	1 (14%)
1	FGP	E	70	1,2	7,10,11	0.87	0	7,14,16	1.34	1 (14%)
1	FGP	F	70	1,2	7,10,11	0.84	0	7,14,16	1.50	1 (14%)
1	FGP	G	70	1,2	2,6,11	0.88	0	1,7,16	0.29	0
1	FGP	H	70	1,2	2,6,11	0.90	0	1,7,16	0.37	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
1	FGP	A	70	1,2	-	0/5/11/13	0/0/0/0
1	FGP	B	70	1,2	-	0/5/11/13	0/0/0/0
1	FGP	C	70	1,2	-	0/5/11/13	0/0/0/0
1	FGP	D	70	1,2	-	0/5/11/13	0/0/0/0
1	FGP	E	70	1,2	-	0/5/11/13	0/0/0/0
1	FGP	F	70	1,2	-	0/5/11/13	0/0/0/0
1	FGP	G	70	1,2	-	0/0/6/13	0/0/0/0
1	FGP	H	70	1,2	-	0/0/6/13	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	FGP	O-C-CA	-3.06	117.36	125.44
1	B	70	FGP	O-C-CA	-3.02	117.46	125.44
1	D	70	FGP	O-C-CA	-2.99	117.54	125.44
1	F	70	FGP	O-C-CA	-2.94	117.67	125.44
1	C	70	FGP	O-C-CA	-2.66	118.41	125.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	70	FGP	O-C-CA	-2.45	118.96	125.44

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
1	F	70	FGP	2	0

5.5 Carbohydrates (i)

38 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	$\#\|Z\| > 2$
3	NAG	A	602	1,3	14,14,15	0.54	0	15,19,21	0.73	0
3	NAG	A	603	3	14,14,15	0.53	0	15,19,21	0.74	0
3	NAG	A	604	1,3	14,14,15	0.57	0	15,19,21	0.66	0
3	NAG	A	605	3	14,14,15	0.57	0	15,19,21	0.66	0
3	NAG	A	606	1,3	14,14,15	0.41	0	15,19,21	0.72	0
3	NAG	A	607	3	14,14,15	0.51	0	15,19,21	0.71	0
3	NAG	B	601	1,3	14,14,15	0.49	0	15,19,21	0.85	0
3	NAG	B	602	3	14,14,15	0.52	0	15,19,21	0.63	0
3	NAG	B	603	1,3	14,14,15	0.59	0	15,19,21	0.95	1 (6%)
3	NAG	B	604	3	13,13,15	0.45	0	15,18,21	1.23	2 (13%)
3	NAG	B	605	1,3	14,14,15	0.53	0	15,19,21	0.83	1 (6%)
3	NAG	B	606	3	14,14,15	0.52	0	15,19,21	0.64	0
3	NAG	C	602	1,3	14,14,15	0.46	0	15,19,21	0.59	0
3	NAG	C	603	3	13,13,15	0.63	0	15,18,21	1.62	2 (13%)
3	NAG	C	604	1,3	14,14,15	0.56	0	15,19,21	0.69	0
3	NAG	C	605	3	13,13,15	0.49	0	15,18,21	0.81	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	C	606	1,3	14,14,15	0.50	0	15,19,21	0.62	0
3	NAG	C	607	3	14,14,15	0.54	0	15,19,21	0.63	0
3	NAG	D	602	1,3	14,14,15	0.52	0	15,19,21	0.72	0
3	NAG	D	603	3	14,14,15	0.48	0	15,19,21	0.91	1 (6%)
3	NAG	D	604	1,3	14,14,15	0.56	0	15,19,21	0.90	0
3	NAG	D	605	3	14,14,15	0.55	0	15,19,21	0.67	0
3	NAG	D	606	1,3	14,14,15	0.54	0	15,19,21	0.70	0
3	NAG	D	607	3	14,14,15	0.56	0	15,19,21	0.53	0
3	NAG	E	601	1,3	14,14,15	0.46	0	15,19,21	0.60	0
3	NAG	E	602	3	14,14,15	0.45	0	15,19,21	0.91	1 (6%)
3	NAG	E	603	1,3	14,14,15	0.58	0	15,19,21	0.74	0
3	NAG	E	604	3	14,14,15	0.57	0	15,19,21	0.70	0
3	NAG	F	603	1,3	14,14,15	0.55	0	15,19,21	0.69	0
3	NAG	F	604	3	14,14,15	0.53	0	15,19,21	0.71	0
3	NAG	F	606	1,3	14,14,15	0.48	0	15,19,21	1.05	1 (6%)
3	NAG	F	607	3	14,14,15	0.48	0	15,19,21	0.82	0
3	NAG	G	602	1,3	14,14,15	0.50	0	15,19,21	0.70	0
3	NAG	G	603	3	11,11,15	0.58	0	13,15,21	0.64	0
3	NAG	H	602	1,3	14,14,15	0.58	0	15,19,21	0.59	0
3	NAG	H	603	3	13,13,15	0.47	0	15,18,21	1.08	2 (13%)
3	NAG	H	604	1,3	14,14,15	0.47	0	15,19,21	0.82	1 (6%)
3	NAG	H	605	3	14,14,15	0.54	0	15,19,21	0.59	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
3	NAG	A	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	603	3	-	0/6/23/26	0/1/1/1
3	NAG	A	604	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	605	3	-	0/6/23/26	0/1/1/1
3	NAG	A	606	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	607	3	-	0/6/23/26	0/1/1/1
3	NAG	B	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	602	3	-	0/6/23/26	0/1/1/1
3	NAG	B	603	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	604	3	-	0/4/21/26	0/1/1/1
3	NAG	B	605	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	606	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	603	3	-	0/4/21/26	0/1/1/1
3	NAG	C	604	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	605	3	-	0/4/21/26	0/1/1/1
3	NAG	C	606	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	607	3	-	0/6/23/26	0/1/1/1
3	NAG	D	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	603	3	-	0/6/23/26	0/1/1/1
3	NAG	D	604	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	605	3	-	0/6/23/26	0/1/1/1
3	NAG	D	606	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	607	3	-	0/6/23/26	0/1/1/1
3	NAG	E	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	602	3	-	0/6/23/26	0/1/1/1
3	NAG	E	603	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	604	3	-	0/6/23/26	0/1/1/1
3	NAG	F	603	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	604	3	-	0/6/23/26	0/1/1/1
3	NAG	F	606	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	607	3	-	0/6/23/26	0/1/1/1
3	NAG	G	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	603	3	-	0/2/19/26	0/1/1/1
3	NAG	H	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	603	3	-	0/4/21/26	0/1/1/1
3	NAG	H	604	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	605	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	604	NAG	C4-C3-C2	-2.96	106.62	111.23
3	E	602	NAG	C4-C3-C2	-2.32	107.63	111.23
3	B	605	NAG	C2-N2-C7	-2.28	120.10	123.04
3	H	604	NAG	C4-C3-C2	-2.12	107.93	111.23
3	D	603	NAG	C1-O5-C5	2.04	114.84	112.25
3	C	605	NAG	O5-C5-C6	2.30	109.93	106.13
3	B	604	NAG	O5-C5-C6	2.36	110.03	106.13
3	H	603	NAG	C1-O5-C5	2.40	116.09	112.38
3	H	603	NAG	O5-C5-C6	2.44	110.17	106.13
3	B	603	NAG	C4-C3-C2	2.61	115.29	111.23
3	F	606	NAG	C1-O5-C5	2.80	115.81	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	603	NAG	O5-C5-C4	3.21	115.10	109.53
3	C	603	NAG	C3-C4-C5	4.40	117.14	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	NAG	1	0
3	B	603	NAG	2	0
3	B	604	NAG	4	0
3	B	605	NAG	1	0
3	B	606	NAG	1	0
3	C	606	NAG	2	0
3	C	607	NAG	1	0
3	F	603	NAG	3	0
3	F	604	NAG	1	0
3	G	602	NAG	1	0
3	G	603	NAG	1	0
3	H	603	NAG	2	0
3	H	604	NAG	4	0
3	H	605	NAG	5	0

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 10 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	$\#\|Z\| > 2$
4	NAG	A	608	1	14,14,15	0.52	0	15,19,21	0.80	0
4	NAG	B	607	1	14,14,15	0.52	0	15,19,21	0.90	1 (6%)
4	NAG	C	608	1	14,14,15	0.54	0	15,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	D	608	1	14,14,15	0.49	0	15,19,21	1.44	1 (6%)
6	PEG	D	609	-	4,4,6	0.59	0	3,3,5	0.24	0
4	NAG	F	602	1	14,14,15	0.46	0	15,19,21	0.81	0
4	NAG	F	605	1	14,14,15	0.48	0	15,19,21	0.61	0
4	NAG	G	604	1	14,14,15	0.51	0	15,19,21	0.86	1 (6%)
4	NAG	G	605	1	10,10,15	0.54	0	13,14,21	0.85	1 (7%)
4	NAG	H	606	1	14,14,15	0.46	0	15,19,21	0.80	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	NAG	A	608	1	-	0/6/23/26	0/1/1/1
4	NAG	B	607	1	-	0/6/23/26	0/1/1/1
4	NAG	C	608	1	-	0/6/23/26	0/1/1/1
4	NAG	D	608	1	-	0/6/23/26	0/1/1/1
6	PEG	D	609	-	-	0/2/2/4	0/0/0/0
4	NAG	F	602	1	-	0/6/23/26	0/1/1/1
4	NAG	F	605	1	-	0/6/23/26	0/1/1/1
4	NAG	G	604	1	-	0/6/23/26	0/1/1/1
4	NAG	G	605	1	-	0/0/17/26	0/1/1/1
4	NAG	H	606	1	-	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(^{o})	Ideal(^{o})
4	G	605	NAG	O5-C5-C6	2.18	109.73	106.13
4	B	607	NAG	C1-O5-C5	2.30	115.17	112.25
4	G	604	NAG	C1-O5-C5	2.41	115.31	112.25
4	D	608	NAG	C1-O5-C5	4.61	118.10	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	608	NAG	2	0
4	C	608	NAG	2	0
6	D	609	PEG	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	483/510 (94%)	-0.15	2 (0%) 93 93	26, 48, 70, 100	0
1	B	480/510 (94%)	-0.13	2 (0%) 93 93	22, 41, 71, 101	0
1	C	483/510 (94%)	-0.05	7 (1%) 78 77	28, 46, 75, 105	0
1	D	479/510 (93%)	-0.20	2 (0%) 93 93	26, 42, 67, 114	0
1	E	482/510 (94%)	0.48	39 (8%) 15 14	54, 83, 119, 135	0
1	F	477/510 (93%)	0.28	23 (4%) 34 35	53, 75, 99, 126	0
1	G	478/510 (93%)	0.45	39 (8%) 14 14	44, 77, 122, 160	0
1	H	481/510 (94%)	0.76	60 (12%) 5 5	62, 91, 128, 142	0
All	All	3843/4080 (94%)	0.18	174 (4%) 37 38	22, 63, 111, 160	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	184	GLY	7.0
1	E	349	LEU	5.8
1	G	231	ALA	5.1
1	E	354	ALA	5.1
1	F	217	PRO	5.0
1	G	191	GLY	4.8
1	E	420	PRO	4.7
1	E	230	PRO	4.6
1	G	370	VAL	4.5
1	H	418	GLY	4.4
1	H	329	PRO	4.4
1	H	470	LYS	4.3
1	H	466	ASP	4.2
1	H	467	GLN	4.2
1	B	502	LEU	4.2
1	H	370	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	416	THR	4.1
1	H	463	MET	4.1
1	H	361	VAL	4.0
1	H	266	THR	4.0
1	B	200	GLY	3.9
1	F	203	GLY	3.8
1	E	352	LEU	3.8
1	E	418	GLY	3.8
1	G	115	GLY	3.8
1	H	455	PRO	3.7
1	E	353	GLU	3.7
1	A	203	GLY	3.6
1	E	325	TRP	3.6
1	G	186	SER	3.5
1	H	412	LEU	3.5
1	E	224	TYR	3.5
1	G	234	ALA	3.5
1	G	200	GLY	3.4
1	H	328	ILE	3.3
1	H	44	ALA	3.3
1	E	312	TYR	3.3
1	F	237	ALA	3.3
1	H	469	ALA	3.3
1	H	326	PHE	3.2
1	H	299	PRO	3.2
1	G	366	SER	3.2
1	H	454	ASP	3.2
1	G	90	GLY	3.2
1	H	465	ARG	3.2
1	G	114	ALA	3.2
1	G	367	HIS	3.1
1	F	24	ASN	3.1
1	C	479	TRP	3.1
1	E	493	PRO	3.1
1	H	203	GLY	3.1
1	G	72	PRO	3.0
1	G	88	MET	3.0
1	G	188	PRO	3.0
1	G	157	LEU	3.0
1	H	218	LEU	3.0
1	H	471	TRP	2.9
1	H	417	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	67	VAL	2.9
1	H	219	ASP	2.9
1	G	197	PHE	2.9
1	C	185	HIS	2.9
1	E	459	GLN	2.9
1	F	168	ASP	2.9
1	G	259	ASP	2.8
1	E	403	TYR	2.8
1	E	463	MET	2.8
1	H	215	TYR	2.8
1	E	322	ILE	2.7
1	D	370	VAL	2.7
1	G	430	TYR	2.7
1	H	186	SER	2.7
1	E	491	LEU	2.7
1	H	110	LEU	2.7
1	H	114	ALA	2.7
1	E	445	PRO	2.7
1	G	201	GLU	2.7
1	F	95	VAL	2.7
1	H	231	ALA	2.7
1	E	350	PRO	2.7
1	H	320	PRO	2.7
1	E	458	ALA	2.6
1	G	185	HIS	2.6
1	F	406	PRO	2.6
1	H	298	SER	2.6
1	H	98	PHE	2.6
1	C	478	PRO	2.6
1	E	91	LEU	2.6
1	G	202	SER	2.6
1	F	153	THR	2.6
1	E	473	TRP	2.6
1	H	453	THR	2.6
1	G	238	ALA	2.6
1	G	368	HIS	2.6
1	F	232	ALA	2.5
1	E	370	VAL	2.5
1	H	373	SER	2.5
1	H	216	ASP	2.5
1	F	90	GLY	2.5
1	G	180	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	161	LYS	2.5
1	E	326	PHE	2.5
1	G	218	LEU	2.5
1	H	45	ILE	2.5
1	H	202	SER	2.5
1	H	366	SER	2.5
1	G	373	SER	2.4
1	F	91	LEU	2.4
1	E	457	PHE	2.4
1	G	230	PRO	2.4
1	E	68	SER	2.4
1	E	384	PHE	2.4
1	E	406	PRO	2.4
1	H	479	TRP	2.4
1	G	193	PHE	2.4
1	H	171	PHE	2.4
1	H	384	PHE	2.4
1	E	168	ASP	2.4
1	E	357	LEU	2.4
1	H	323	LEU	2.4
1	F	165	THR	2.4
1	E	348	LEU	2.3
1	C	186	SER	2.3
1	E	444	ASP	2.3
1	F	216	ASP	2.3
1	H	90	GLY	2.3
1	F	22	PRO	2.3
1	F	214	ALA	2.3
1	C	491	LEU	2.3
1	G	126	VAL	2.3
1	F	134	PHE	2.3
1	H	357	LEU	2.3
1	G	241	THR	2.3
1	F	209	ASP	2.2
1	C	366	SER	2.2
1	C	480	VAL	2.2
1	E	100	SER	2.2
1	G	96	HIS	2.2
1	F	170	PRO	2.2
1	G	67	VAL	2.2
1	G	203	GLY	2.2
1	E	419	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	187	GLN	2.2
1	H	419	GLN	2.2
1	H	170	PRO	2.2
1	D	366	SER	2.2
1	E	442	SER	2.2
1	E	492	SER	2.2
1	H	46	ALA	2.2
1	H	272	SER	2.2
1	G	410	ASP	2.2
1	E	448	THR	2.1
1	F	202	SER	2.1
1	F	162	PHE	2.1
1	H	91	LEU	2.1
1	H	92	HIS	2.1
1	F	159	VAL	2.1
1	F	171	PHE	2.1
1	H	468	LEU	2.1
1	H	438	LEU	2.1
1	H	283	THR	2.1
1	H	43	SER	2.1
1	E	186	SER	2.1
1	H	324	ASP	2.1
1	H	296	VAL	2.1
1	G	432	TYR	2.1
1	A	366	SER	2.1
1	G	166	GLN	2.0
1	H	268	VAL	2.0
1	E	495	CYS	2.0
1	G	196	LYS	2.0
1	E	311	ALA	2.0
1	G	198	GLY	2.0
1	H	478	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	FGP	E	70	11/12	0.88	0.22	-	68,80,139,144	0
1	FGP	C	70	11/12	0.94	0.17	-	32,40,91,115	0
1	FGP	A	70	11/12	0.94	0.15	-	33,50,105,123	0
1	FGP	H	70	7/12	0.94	0.22	-	66,68,70,75	0
1	FGP	D	70	11/12	0.93	0.16	-	29,40,93,95	0
1	FGP	F	70	11/12	0.91	0.17	-	61,72,131,141	0
1	FGP	B	70	11/12	0.94	0.16	-	26,34,85,101	0
1	FGP	G	70	7/12	0.84	0.24	-	72,75,80,83	0

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(Å^2)	Q<0.9
3	NAG	D	602	14/15	0.78	0.17	2.75	48,80,128,145	0
3	NAG	A	602	14/15	0.78	0.18	1.36	60,98,132,137	0
3	NAG	B	603	14/15	0.90	0.20	1.17	44,65,85,107	0
3	NAG	B	601	14/15	0.87	0.13	0.69	49,64,88,90	0
3	NAG	E	601	14/15	0.83	0.17	0.26	80,128,152,152	0
3	NAG	C	602	14/15	0.82	0.15	0.15	55,78,105,130	0
3	NAG	E	603	14/15	0.94	0.13	-0.35	49,63,77,79	0
3	NAG	C	604	14/15	0.96	0.12	-0.39	39,49,67,68	0
3	NAG	G	602	14/15	0.88	0.15	-0.47	52,80,105,114	0
3	NAG	H	602	14/15	0.93	0.16	-0.50	47,64,74,77	0
3	NAG	A	604	14/15	0.94	0.12	-0.65	36,48,61,70	0
3	NAG	F	603	14/15	0.88	0.14	-0.72	44,78,94,95	0
3	NAG	D	604	14/15	0.96	0.10	-1.11	36,43,61,69	0
3	NAG	D	603	14/15	0.77	0.36	-	71,104,136,136	0
3	NAG	C	607	14/15	0.79	0.29	-	80,116,146,150	0
3	NAG	D	607	14/15	0.88	0.17	-	72,101,118,120	0
3	NAG	D	606	14/15	0.94	0.13	-	56,65,92,100	0
3	NAG	B	605	14/15	0.94	0.07	-	48,63,78,81	0
3	NAG	A	605	14/15	0.86	0.18	-	47,83,104,116	0
3	NAG	H	605	14/15	0.75	0.35	-	86,132,149,150	0
3	NAG	E	602	14/15	0.74	0.25	-	71,119,139,145	0
3	NAG	F	607	14/15	0.90	0.26	-	60,75,94,100	0
3	NAG	G	603	11/15	0.89	0.15	-	80,116,138,142	0
3	NAG	E	604	14/15	0.92	0.14	-	56,77,85,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	H	603	13/15	0.86	0.31	-	69,98,115,115	0
3	NAG	D	605	14/15	0.86	0.17	-	53,76,115,118	0
3	NAG	C	605	13/15	0.90	0.21	-	60,92,106,120	0
3	NAG	F	604	14/15	0.84	0.17	-	58,74,92,96	0
3	NAG	A	606	14/15	0.89	0.13	-	54,72,94,97	0
3	NAG	H	604	14/15	0.81	0.28	-	76,127,145,153	0
3	NAG	A	607	14/15	0.74	0.25	-	74,102,124,126	0
3	NAG	B	604	13/15	0.88	0.21	-	55,103,128,139	0
3	NAG	C	603	13/15	0.83	0.26	-	84,105,126,132	0
3	NAG	B	606	14/15	0.88	0.23	-	70,87,99,104	0
3	NAG	B	602	14/15	0.83	0.23	-	73,97,111,114	0
3	NAG	F	606	14/15	0.88	0.18	-	58,73,85,86	0
3	NAG	A	603	14/15	0.79	0.29	-	78,106,134,140	0
3	NAG	C	606	14/15	0.78	0.24	-	71,112,124,129	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	PEG	D	609	5/7	0.90	0.22	4.91	27,33,49,54	0
4	NAG	G	604	14/15	0.79	0.21	-0.17	61,83,117,120	0
2	CA	G	601	1/1	0.81	0.10	-2.23	107,107,107,107	0
2	CA	D	601	1/1	0.98	0.06	-2.60	43,43,43,43	0
2	CA	H	601	1/1	0.96	0.04	-2.78	75,75,75,75	0
2	CA	E	600	1/1	0.98	0.04	-2.91	69,69,69,69	0
2	CA	A	601	1/1	0.98	0.05	-3.05	57,57,57,57	0
2	CA	B	600	1/1	0.97	0.06	-3.42	52,52,52,52	0
2	CA	C	601	1/1	0.97	0.04	-4.24	50,50,50,50	0
2	CA	F	601	1/1	0.85	0.06	-5.49	73,73,73,73	0
5	CL	C	609	1/1	0.98	0.37	-	64,64,64,64	0
4	NAG	F	602	14/15	0.85	0.13	-	63,87,110,118	0
4	NAG	F	605	14/15	0.91	0.18	-	77,105,120,129	0
5	CL	A	609	1/1	0.98	0.11	-	43,43,43,43	0
4	NAG	B	607	14/15	0.87	0.16	-	50,71,89,101	0
4	NAG	H	606	14/15	0.88	0.23	-	81,99,115,117	0
4	NAG	G	605	10/15	0.79	0.19	-	72,88,104,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	D	608	14/15	0.87	0.12	-	37,62,87,91	0
4	NAG	A	608	14/15	0.75	0.26	-	73,114,126,128	0
4	NAG	C	608	14/15	0.83	0.29	-	56,79,108,112	0

6.5 Other polymers (i)

There are no such residues in this entry.