



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:20 AM GMT

PDB ID : 2GJX  
Title : Crystallographic structure of human beta-Hexosaminidase A  
Authors : Lemieux, M.J.; Mark, B.L.; Cherney, M.M.; Withers, S.G.; Mahuran, D.J.;  
James, M.N.G.  
Deposited on : 2006-03-31  
Resolution : 2.80 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](mailto: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.

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

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

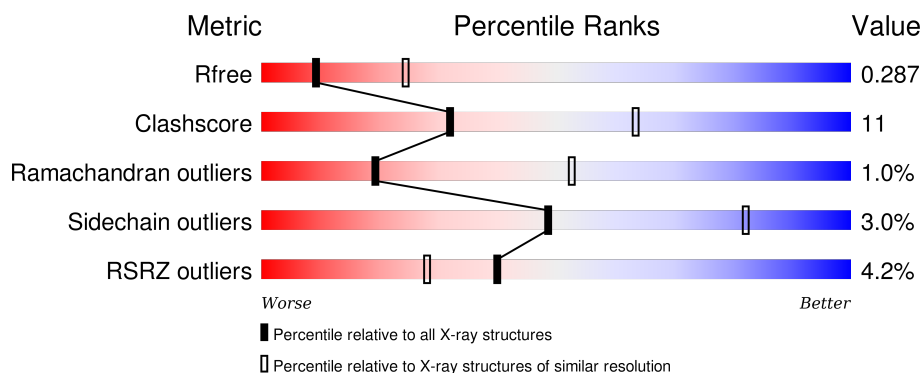
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	507	<div> <div>2%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
1	D	507	<div> <div>4%</div> <div>71%</div> <div>23%</div> <div>• • •</div> </div>
1	E	507	<div> <div>7%</div> <div>66%</div> <div>27%</div> <div>• •</div> </div>
1	H	507	<div> <div>5%</div> <div>68%</div> <div>26%</div> <div>• •</div> </div>
2	B	507	<div> <div>4%</div> <div>79%</div> <div>15%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	C	507	 2% 80% 14% • 5%
2	F	507	 4% 73% 20% • 5%
2	G	507	 4% 76% 17% • 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
6	NAG	E	21	-	-	-	X
7	SO4	A	708	-	-	-	X
7	SO4	D	717	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 32132 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 Beta-hexosaminidase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			4010	2600	650	746	14			
1	D	492	Total	C	N	O	S	0	0	0
			4010	2600	650	746	14			
1	E	492	Total	C	N	O	S	0	0	0
			4010	2600	650	746	14			
1	H	492	Total	C	N	O	S	0	0	0
			4010	2600	650	746	14			

- Molecule 2 is a protein called Beta-hexosaminidase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	480	Total	C	N	O	S	0	0	0
			3877	2505	643	716	13			
2	C	481	Total	C	N	O	S	0	0	0
			3885	2511	644	717	13			
2	F	480	Total	C	N	O	S	0	0	0
			3877	2505	643	716	13			
2	G	480	Total	C	N	O	S	0	0	0
			3877	2505	643	716	13			

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

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

- 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	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	2	Total	C	N	O	0	0
			28	16	2	10		
6	H	2	Total	C	N	O	0	0
			28	16	2	10		
6	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	34	Total	O	0	0
			34	34		
8	B	20	Total	O	0	0
			20	20		

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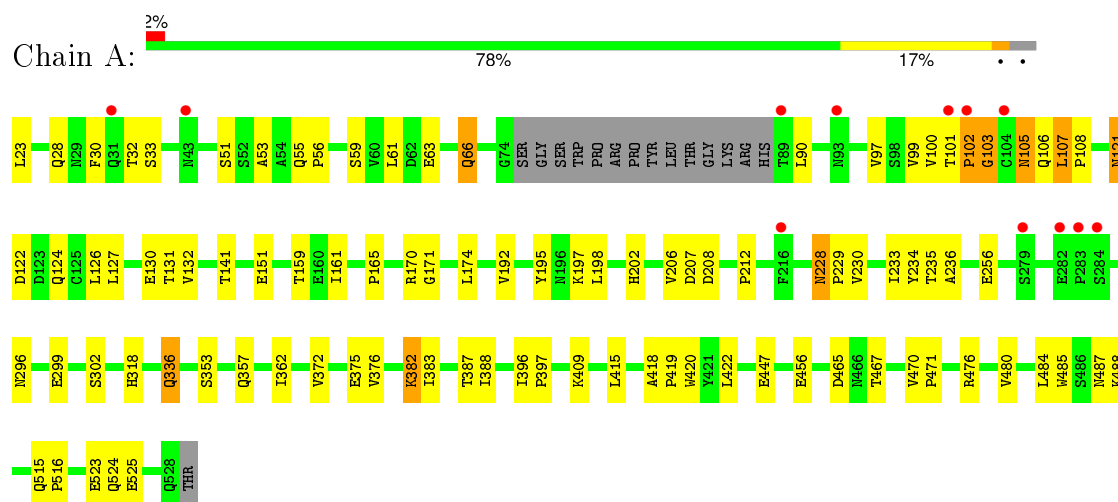
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	22	Total 22	O 22	0	0
8	D	18	Total 18	O 18	0	0
8	E	20	Total 20	O 20	0	0
8	F	11	Total 11	O 11	0	0
8	G	17	Total 17	O 17	0	0
8	H	6	Total 6	O 6	0	0

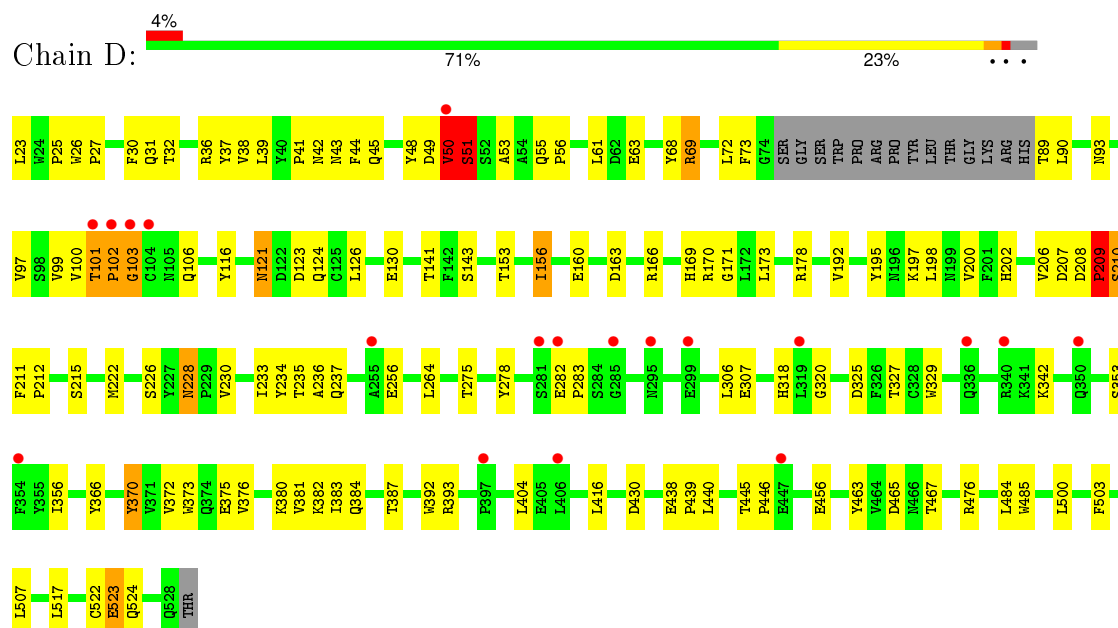
### 3 Residue-property plots

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: Beta-hexosaminidase alpha chain

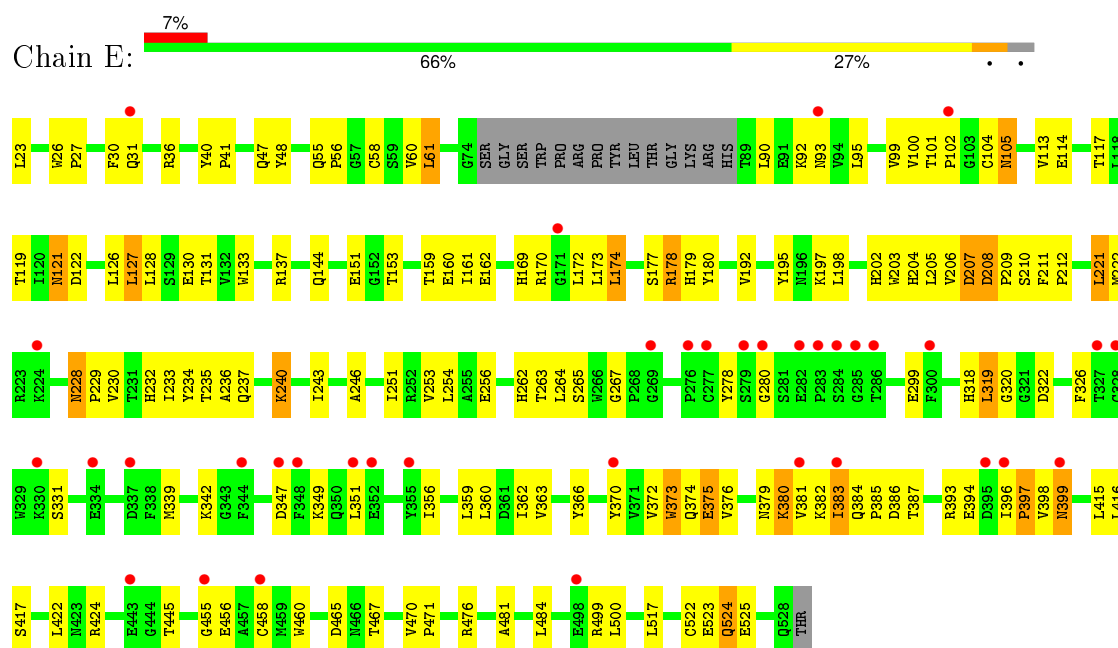


- Molecule 1: Beta-hexosaminidase alpha chain

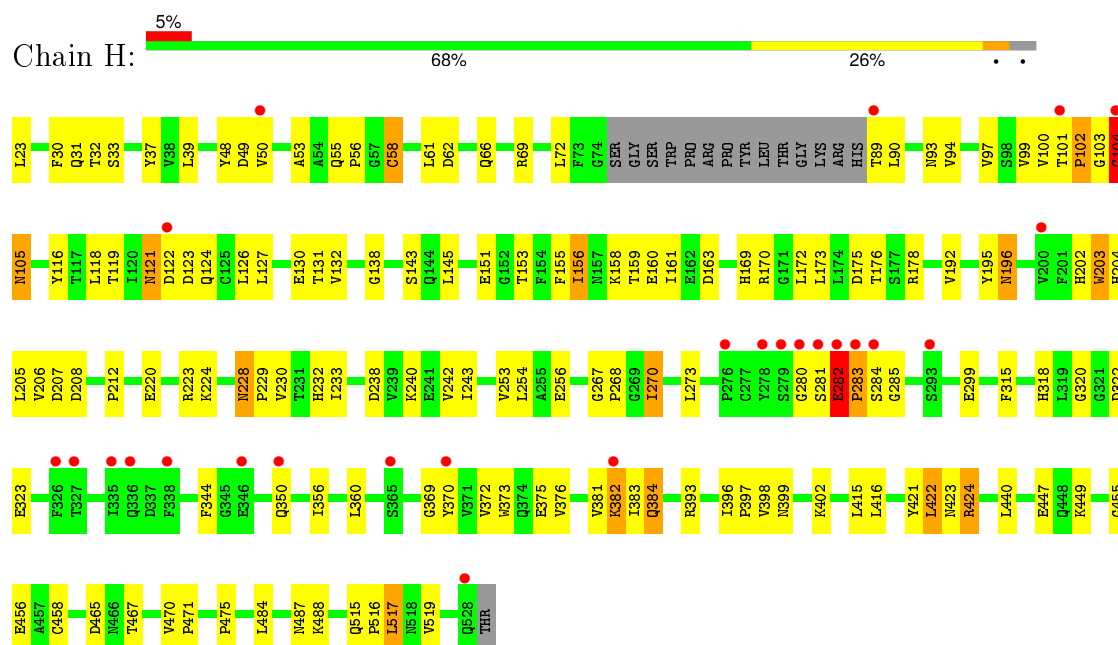


- Molecule 1: Beta-hexosaminidase alpha chain

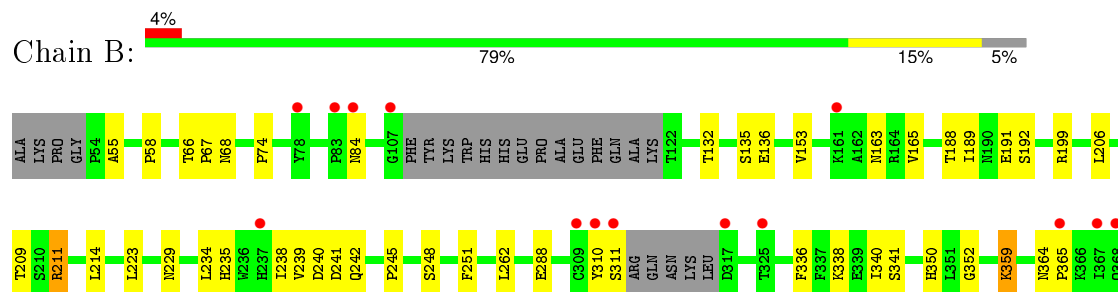


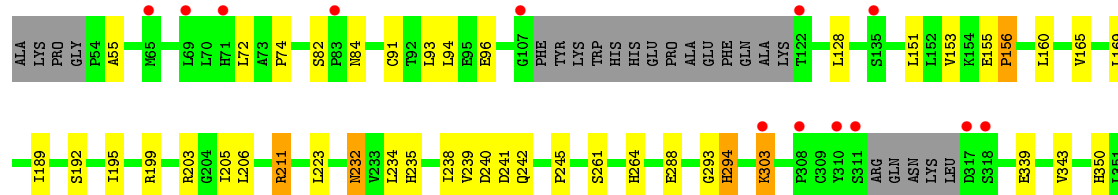


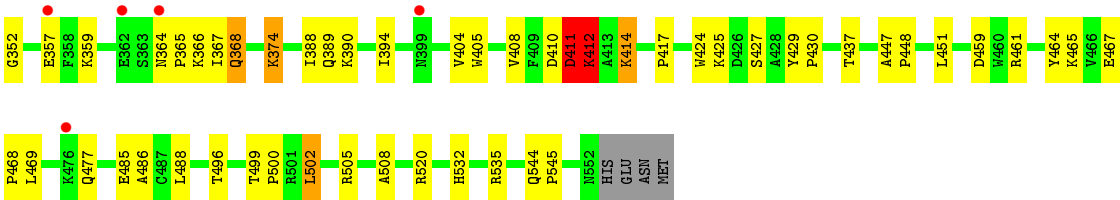
• Molecule 1: Beta-hexosaminidase alpha chain



• Molecule 2: Beta-hexosaminidase beta chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	321.09Å 110.54Å 129.67Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	39.87 – 2.80 39.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.87-2.80) 99.7 (39.87-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.269 , 0.288 0.267 , 0.287	Depositor DCC
$R_{free}$ test set	5525 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.9	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.2	EDS
Estimated twinning fraction	0.009 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 111509 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	32132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, NDG, SO4

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	0.35	1/4132 (0.0%)	0.43	0/5633
1	D	0.43	4/4132 (0.1%)	0.48	2/5633 (0.0%)
1	E	0.31	0/4132	0.43	0/5633
1	H	0.38	2/4132 (0.0%)	0.47	3/5633 (0.1%)
2	B	0.27	0/3988	0.39	0/5423
2	C	0.27	0/3996	0.40	0/5434
2	F	0.28	0/3988	0.41	1/5423 (0.0%)
2	G	0.38	3/3988 (0.1%)	0.42	0/5423
All	All	0.34	10/32488 (0.0%)	0.43	6/44235 (0.0%)

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	D	0	3
2	G	0	2
All	All	0	5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	411	ASP	CA-C	12.40	1.85	1.52
1	D	210	SER	N-CA	11.89	1.70	1.46
1	A	51	SER	CB-OG	11.22	1.56	1.42
1	H	422	LEU	C-O	9.77	1.42	1.23
1	D	209	PRO	CA-C	8.49	1.69	1.52
1	D	50	VAL	C-N	6.47	1.49	1.34
2	G	411	ASP	CB-CG	5.67	1.63	1.51
2	G	412	LYS	CE-NZ	5.42	1.62	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	209	PRO	CA-CB	5.31	1.64	1.53
1	H	58	CYS	CB-SG	-5.09	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	51	SER	N-CA-C	-8.43	88.24	111.00
1	H	282	GLU	C-N-CD	-8.15	102.66	120.60
1	H	422	LEU	O-C-N	-6.93	111.62	122.70
2	F	503	TRP	N-CA-C	5.53	125.94	111.00
1	D	51	SER	N-CA-CB	5.50	118.75	110.50
1	H	282	GLU	C-N-CA	5.23	143.97	122.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	209	PRO	Mainchain,Peptide
1	D	50	VAL	Peptide
2	G	411	ASP	Mainchain,Peptide

## 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	4010	0	3840	73	0
1	D	4010	0	3840	106	0
1	E	4010	0	3841	136	0
1	H	4010	0	3841	115	0
2	B	3877	0	3783	56	0
2	C	3885	0	3794	49	0
2	F	3877	0	3783	83	0
2	G	3877	0	3782	74	0
3	A	78	0	68	0	0
3	D	39	0	34	1	0
4	A	14	0	13	0	0
4	D	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	14	0	13	0	0
4	G	14	0	13	0	0
5	B	39	0	34	1	0
6	C	28	0	25	0	0
6	D	28	0	25	1	0
6	E	56	0	50	1	0
6	G	28	0	25	0	0
6	H	56	0	50	2	0
7	A	5	0	0	0	0
7	D	5	0	0	0	0
7	H	10	0	0	1	0
8	A	34	0	0	0	0
8	B	20	0	0	2	0
8	C	22	0	0	1	0
8	D	18	0	0	0	0
8	E	20	0	0	2	0
8	F	11	0	0	0	0
8	G	17	0	0	0	0
8	H	6	0	0	0	0
All	All	32132	0	30867	664	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 11.

All (664) 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:D:210:SER:N	1:D:210:SER:CA	1.70	1.53
2:G:411:ASP:CA	2:G:411:ASP:C	1.85	1.46
1:E:55:GLN:HG3	1:E:56:PRO:HD2	1.29	1.13
1:H:424:ARG:HH11	1:H:424:ARG:HG2	1.08	1.12
1:H:53:ALA:HB1	1:H:101:THR:HA	1.33	1.10
1:E:383:ILE:HD11	1:E:387:THR:HB	1.32	1.06
2:G:242:GLN:HG2	1:H:519:VAL:HG21	1.37	1.05
1:D:55:GLN:HG3	1:D:56:PRO:HD2	1.36	1.03
2:G:411:ASP:HA	2:G:412:LYS:HE3	1.39	1.02
1:A:66:GLN:OE1	1:A:66:GLN:HA	1.59	1.00
1:A:55:GLN:HG3	1:A:56:PRO:HD2	1.47	0.95
1:H:55:GLN:HG3	1:H:56:PRO:HD2	1.47	0.94
1:H:424:ARG:NH1	1:H:424:ARG:HG2	1.80	0.94
1:D:380:LYS:HE2	1:D:380:LYS:HA	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:504:PRO:HG3	2:F:544:GLN:HG2	1.49	0.92
2:C:131:ILE:HG21	2:C:135:SER:HB3	1.50	0.92
2:F:504:PRO:CG	2:F:544:GLN:HG2	2.01	0.91
1:D:100:VAL:HG12	1:D:102:PRO:HD2	1.52	0.90
1:E:222:MET:SD	8:E:734:HOH:O	2.30	0.90
1:A:382:LYS:HE3	1:A:382:LYS:HA	1.55	0.89
2:B:425:LYS:HG3	8:B:574:HOH:O	1.71	0.89
1:D:89:THR:HG22	1:D:90:LEU:HD23	1.54	0.87
1:H:53:ALA:CB	1:H:101:THR:HA	2.05	0.86
1:H:360:LEU:HD13	1:H:383:ILE:HG12	1.59	0.84
2:C:532:HIS:HD2	2:C:535:ARG:HH21	1.21	0.84
1:A:467:THR:HG21	2:B:544:GLN:HA	1.57	0.84
1:D:170:ARG:HG2	1:D:484:LEU:HB3	1.59	0.84
2:G:303:LYS:HE2	2:G:303:LYS:H	1.42	0.84
1:D:465:ASP:OD2	1:D:467:THR:HG22	1.79	0.82
1:H:100:VAL:HG12	1:H:102:PRO:HD2	1.62	0.82
1:A:372:VAL:HG21	1:A:376:VAL:HG21	1.61	0.82
1:D:228:ASN:HD22	1:D:230:VAL:H	1.29	0.80
1:H:282:GLU:OE1	1:H:283:PRO:HD3	1.82	0.80
1:E:393:ARG:HD2	1:E:396:ILE:HB	1.63	0.79
1:E:393:ARG:HD2	1:E:397:PRO:HD3	1.63	0.79
1:A:170:ARG:HG2	1:A:484:LEU:HB3	1.65	0.79
2:C:532:HIS:CD2	2:C:535:ARG:HH21	2.00	0.78
2:F:352:GLY:HA2	2:F:405:TRP:CD1	2.18	0.78
1:E:26:TRP:HB2	1:E:499:ARG:HH21	1.47	0.78
2:G:94:LEU:HD21	2:G:165:VAL:HG23	1.66	0.78
1:A:396:ILE:HD12	1:A:397:PRO:HA	1.65	0.78
2:G:303:LYS:HE2	2:G:303:LYS:N	1.97	0.77
2:G:429:TYR:N	2:G:430:PRO:HD2	1.99	0.77
1:A:228:ASN:HD22	1:A:230:VAL:H	1.31	0.77
2:G:368:GLN:HE21	2:G:368:GLN:HA	1.50	0.76
2:F:135:SER:O	2:F:136:GLU:HG2	1.86	0.76
1:E:342:LYS:HA	1:E:342:LYS:HE2	1.67	0.75
1:D:209:PRO:C	1:D:210:SER:CA	2.55	0.74
1:A:170:ARG:NH2	1:A:197:LYS:O	2.21	0.74
1:A:30:PHE:HD2	1:A:161:ILE:HG12	1.51	0.74
1:E:228:ASN:HD22	1:E:230:VAL:H	1.34	0.73
2:F:390:LYS:O	2:F:394:ILE:HG12	1.88	0.73
1:D:210:SER:N	1:D:210:SER:C	2.42	0.73
1:H:97:VAL:HG12	1:H:126:LEU:HD11	1.70	0.73
1:H:58:CYS:C	1:H:104:CYS:SG	2.67	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:H	1:A:107:LEU:HD13	1.53	0.72
1:H:121:ASN:ND2	1:H:124:GLN:H	1.87	0.72
1:E:55:GLN:HG3	1:E:56:PRO:CD	2.15	0.72
1:E:170:ARG:NH2	1:E:197:LYS:O	2.23	0.72
1:A:465:ASP:OD2	1:A:467:THR:HG22	1.91	0.71
1:D:49:ASP:OD2	1:D:97:VAL:HB	1.90	0.70
1:E:254:LEU:HD21	1:E:318:HIS:HB2	1.72	0.70
2:F:532:HIS:HD2	2:F:535:ARG:HH21	1.37	0.70
1:H:240:LYS:HA	1:H:240:LYS:HE2	1.73	0.70
1:E:100:VAL:HG12	1:E:102:PRO:HD2	1.72	0.70
2:B:341:SER:OG	2:B:398:ILE:HD12	1.91	0.70
2:G:155:GLU:HG3	2:G:156:PRO:HD3	1.74	0.69
1:E:170:ARG:HG2	1:E:484:LEU:HB3	1.74	0.69
1:A:121:ASN:ND2	1:A:124:GLN:H	1.90	0.69
2:C:488:LEU:HD22	2:C:502:LEU:HG	1.74	0.68
1:D:49:ASP:CG	1:D:51:SER:HB2	2.14	0.68
1:A:101:THR:N	1:A:102:PRO:HD2	2.09	0.68
1:E:153:THR:HG23	1:H:151:GLU:HB3	1.76	0.67
1:H:205:LEU:H	1:H:205:LEU:HD12	1.58	0.67
2:G:91:CYS:SG	2:G:94:LEU:HD23	2.34	0.67
1:H:121:ASN:HD22	1:H:123:ASP:H	1.42	0.67
1:D:49:ASP:O	1:D:51:SER:N	2.27	0.67
1:E:113:VAL:O	1:E:131:THR:HG22	1.94	0.67
1:H:228:ASN:ND2	1:H:230:VAL:HG12	2.09	0.67
2:F:147:GLU:HB2	2:F:198:PRO:HG3	1.77	0.67
2:C:346:ASP:O	2:C:400:LYS:NZ	2.26	0.67
2:G:411:ASP:HA	2:G:412:LYS:CE	2.21	0.67
1:A:100:VAL:HG12	1:A:102:PRO:HD2	1.77	0.66
1:A:131:THR:HG22	1:A:132:VAL:H	1.60	0.66
2:F:352:GLY:HA2	2:F:405:TRP:HD1	1.60	0.66
1:H:424:ARG:CG	1:H:424:ARG:HH11	1.95	0.66
1:A:131:THR:HG22	1:A:132:VAL:N	2.11	0.66
1:H:383:ILE:HG13	1:H:384:GLN:NE2	2.11	0.66
1:D:209:PRO:HB2	1:D:210:SER:HB2	1.77	0.65
2:F:56:LEU:O	2:F:528:ARG:NH1	2.29	0.65
1:H:202:HIS:NE2	1:H:256:GLU:OE1	2.20	0.65
2:G:451:LEU:O	2:G:505:ARG:NH2	2.29	0.65
2:C:534:CYS:O	2:C:538:GLU:HG2	1.96	0.65
1:E:100:VAL:HG12	1:E:102:PRO:HG2	1.77	0.65
1:H:228:ASN:HD21	1:H:230:VAL:HG12	1.61	0.65
1:D:383:ILE:HD11	1:D:387:THR:HG21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:372:VAL:HG21	1:H:376:VAL:HG21	1.78	0.65
1:H:61:LEU:HD13	1:H:132:VAL:HG13	1.80	0.64
1:D:202:HIS:HE1	1:D:256:GLU:OE1	1.80	0.64
2:F:459:ASP:OD2	2:F:505:ARG:NH1	2.29	0.64
1:E:525:GLU:HG2	2:F:264:HIS:HE1	1.62	0.64
1:D:192:VAL:HA	1:D:195:TYR:CD2	2.32	0.64
1:H:421:TYR:OH	7:H:534:SO4:O1	2.15	0.63
1:A:23:LEU:HD21	1:A:141:THR:HG23	1.81	0.63
1:D:121:ASN:HD22	1:D:123:ASP:H	1.47	0.63
1:E:278:TYR:O	1:E:331:SER:HB2	1.98	0.63
2:B:262:LEU:CD2	1:D:69:ARG:HH22	2.11	0.63
1:D:282:GLU:OE1	1:D:282:GLU:HA	1.99	0.63
1:A:372:VAL:CG2	1:A:376:VAL:HG21	2.28	0.62
1:E:172:LEU:CD1	1:E:174:LEU:HD13	2.29	0.62
2:G:544:GLN:HA	1:H:467:THR:HG21	1.81	0.62
1:A:524:GLN:HG2	1:A:524:GLN:O	1.99	0.62
1:D:170:ARG:NH2	1:D:485:TRP:HE3	1.98	0.62
1:E:204:HIS:HD2	1:E:256:GLU:CD	2.02	0.62
1:H:72:LEU:HD11	1:H:143:SER:HB2	1.82	0.62
2:F:451:LEU:O	2:F:505:ARG:NH2	2.32	0.61
2:C:240:ASP:OD2	2:C:241:ASP:N	2.26	0.61
2:C:551:CYS:O	2:C:552:ASN:HB2	1.99	0.61
1:A:192:VAL:HA	1:A:195:TYR:CD2	2.35	0.61
1:D:372:VAL:HG21	1:D:376:VAL:HG21	1.82	0.61
2:G:94:LEU:CD2	2:G:165:VAL:HG23	2.30	0.61
1:E:467:THR:HG21	2:F:544:GLN:HA	1.83	0.61
1:E:318:HIS:HE1	1:E:373:TRP:NE1	1.99	0.61
1:D:380:LYS:CE	1:D:380:LYS:HA	2.25	0.61
2:G:223:LEU:HD21	2:G:234:LEU:HD22	1.81	0.61
1:D:100:VAL:HG12	1:D:102:PRO:CD	2.26	0.61
1:H:360:LEU:CD1	1:H:383:ILE:HG12	2.29	0.61
1:E:383:ILE:CD1	1:E:387:THR:HB	2.22	0.61
2:F:100:ARG:HG2	2:F:104:TYR:HE2	1.65	0.61
2:B:262:LEU:HD22	1:D:69:ARG:HH22	1.66	0.61
1:H:103:GLY:HA3	1:H:132:VAL:HG21	1.83	0.60
1:D:101:THR:O	1:D:102:PRO:C	2.40	0.60
1:E:26:TRP:HB2	1:E:499:ARG:NH2	2.13	0.60
2:F:240:ASP:OD2	2:F:241:ASP:N	2.31	0.60
1:E:208:ASP:OD2	1:E:262:HIS:HA	2.01	0.60
2:F:504:PRO:HG2	2:F:544:GLN:HG2	1.81	0.60
1:E:192:VAL:HA	1:E:195:TYR:CD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:85:SER:HB2	2:F:130:SER:HA	1.83	0.60
2:G:242:GLN:CG	1:H:519:VAL:HG21	2.25	0.60
1:E:318:HIS:C	1:E:320:GLY:H	2.05	0.60
1:E:393:ARG:CD	1:E:396:ILE:HB	2.32	0.60
1:E:372:VAL:HG11	1:E:376:VAL:HG21	1.83	0.60
1:H:176:THR:HG1	1:H:203:TRP:HZ3	1.50	0.60
1:E:211:PHE:CE1	1:E:221:LEU:HD13	2.37	0.60
1:E:318:HIS:HE1	1:E:373:TRP:CD1	2.20	0.59
2:B:58:PRO:HB3	2:B:511:GLU:HA	1.84	0.59
2:F:154:LYS:HB3	2:F:156:PRO:HD2	1.84	0.59
2:B:451:LEU:O	2:B:505:ARG:NH2	2.35	0.59
1:D:39:LEU:HG	1:D:156:ILE:HD11	1.85	0.59
1:H:131:THR:HG22	1:H:132:VAL:H	1.66	0.59
1:A:170:ARG:HG2	1:A:484:LEU:CB	2.31	0.59
1:E:172:LEU:HD11	1:E:174:LEU:HD13	1.83	0.59
1:D:31:GLN:HB2	1:D:160:GLU:HB3	1.84	0.59
2:B:499:THR:HB	2:B:500:PRO:HD3	1.85	0.59
2:F:58:PRO:HB3	2:F:511:GLU:HA	1.84	0.58
1:E:100:VAL:HG12	1:E:102:PRO:CD	2.33	0.58
2:B:310:TYR:O	2:B:311:SER:HB3	2.02	0.58
2:F:134:GLN:OE1	2:F:134:GLN:HA	2.03	0.58
1:E:383:ILE:HD11	1:E:387:THR:CB	2.21	0.58
1:H:131:THR:HG22	1:H:132:VAL:N	2.16	0.58
2:C:154:LYS:O	2:C:154:LYS:HE3	2.03	0.58
2:G:374:LYS:NZ	2:G:374:LYS:HA	2.18	0.58
2:F:203:ARG:HG2	2:F:513:LEU:HB3	1.86	0.58
2:F:532:HIS:CD2	2:F:535:ARG:HH21	2.19	0.58
2:F:173:GLU:O	2:F:177:GLN:HG3	2.03	0.58
1:H:196:ASN:N	1:H:196:ASN:HD22	2.01	0.58
1:E:100:VAL:CG1	1:E:102:PRO:HD2	2.33	0.58
1:E:101:THR:N	1:E:102:PRO:HD2	2.18	0.58
2:B:262:LEU:CD2	1:D:69:ARG:NH2	2.67	0.58
1:A:61:LEU:CD1	1:A:132:VAL:HG23	2.34	0.58
1:E:384:GLN:OE1	1:E:384:GLN:N	2.31	0.58
1:A:383:ILE:HD11	1:A:387:THR:HB	1.85	0.58
2:F:488:LEU:HD22	2:F:502:LEU:HB2	1.86	0.58
2:G:240:ASP:OD2	2:G:241:ASP:N	2.27	0.57
1:H:243:ILE:HA	1:H:253:VAL:HG21	1.86	0.57
1:E:356:ILE:HD13	1:E:376:VAL:HG22	1.86	0.57
2:C:239:VAL:HG12	2:C:245:PRO:HD2	1.86	0.57
2:F:362:GLU:O	2:F:368:GLN:NE2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:532:HIS:HD2	2:B:535:ARG:HH21	1.53	0.57
2:G:464:TYR:HB2	2:G:508:ALA:HB1	1.87	0.57
2:G:239:VAL:HG12	2:G:245:PRO:HD2	1.85	0.57
1:E:205:LEU:HD12	1:E:205:LEU:H	1.70	0.57
1:E:235:THR:HG22	1:E:236:ALA:N	2.20	0.57
1:E:30:PHE:CD2	1:E:161:ILE:HG12	2.39	0.57
1:D:370:TYR:OH	1:D:384:GLN:HG3	2.03	0.57
1:H:465:ASP:OD2	1:H:467:THR:HG22	2.04	0.57
1:D:325:ASP:OD1	1:D:327:THR:HG22	2.04	0.57
2:G:411:ASP:O	2:G:412:LYS:HB2	2.04	0.57
1:A:66:GLN:OE1	1:A:66:GLN:CA	2.41	0.57
1:E:114:GLU:OE2	1:E:170:ARG:NH1	2.38	0.57
1:D:30:PHE:HE2	1:D:32:THR:HB	1.69	0.57
2:G:411:ASP:N	2:G:411:ASP:OD1	2.37	0.57
1:H:270:ILE:O	1:H:270:ILE:HG23	2.03	0.57
2:B:406:GLN:HE22	2:B:423:VAL:HG13	1.70	0.56
2:F:135:SER:C	2:F:136:GLU:HG2	2.24	0.56
2:F:66:THR:HB	2:F:191:GLU:O	2.04	0.56
1:H:383:ILE:HG13	1:H:384:GLN:H	1.69	0.56
1:E:30:PHE:HD2	1:E:161:ILE:HG12	1.69	0.56
1:D:101:THR:N	1:D:102:PRO:HD2	2.21	0.56
2:B:429:TYR:N	2:B:430:PRO:CD	2.69	0.56
1:D:222:MET:CG	1:D:233:ILE:HD12	2.36	0.56
2:C:58:PRO:HB3	2:C:511:GLU:HA	1.86	0.56
2:G:411:ASP:CA	2:G:412:LYS:N	2.66	0.56
1:E:58:CYS:SG	1:E:61:LEU:HB2	2.46	0.56
1:E:422:LEU:O	1:E:476:ARG:NH2	2.39	0.56
2:F:153:VAL:HB	2:F:192:SER:H	1.70	0.56
2:C:429:TYR:N	2:C:430:PRO:CD	2.68	0.56
1:E:381:VAL:O	1:E:383:ILE:N	2.40	0.55
2:B:262:LEU:HD23	1:D:69:ARG:NH2	2.21	0.55
2:F:429:TYR:N	2:F:430:PRO:CD	2.69	0.55
1:E:100:VAL:HG12	1:E:102:PRO:CG	2.36	0.55
1:H:475:PRO:HG2	1:H:517:LEU:CD1	2.37	0.55
2:F:389:GLN:HA	2:F:392:LEU:CD2	2.37	0.55
1:A:409:LYS:HB2	1:A:409:LYS:HZ2	1.71	0.55
1:E:36:ARG:HD2	6:E:21:NAG:H62	1.88	0.55
1:E:90:LEU:H	1:E:90:LEU:HD23	1.72	0.55
1:D:25:PRO:HD2	1:D:197:LYS:HD3	1.89	0.55
1:A:55:GLN:HG3	1:A:56:PRO:CD	2.30	0.55
1:A:105:ASN:OD1	1:A:105:ASN:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:173:LEU:HA	1:H:202:HIS:HB3	1.89	0.55
1:H:196:ASN:H	1:H:196:ASN:HD22	1.53	0.55
2:F:267:THR:CG2	1:H:66:GLN:HG3	2.37	0.55
1:E:347:ASP:OD1	1:E:349:LYS:HG2	2.07	0.55
1:H:229:PRO:HA	1:H:233:ILE:HD11	1.89	0.55
1:E:500:LEU:HG	1:E:517:LEU:HD11	1.89	0.55
1:D:171:GLY:HA2	1:D:200:VAL:O	2.07	0.55
1:A:207:ASP:OD2	1:A:208:ASP:N	2.31	0.55
1:H:99:VAL:HG22	1:H:130:GLU:HA	1.89	0.55
1:A:151:GLU:HG3	1:D:38:VAL:HG11	1.88	0.54
1:A:151:GLU:HB3	1:D:153:THR:HG23	1.88	0.54
2:B:364:ASN:HD22	2:B:365:PRO:HD2	1.72	0.54
2:G:429:TYR:N	2:G:430:PRO:CD	2.69	0.54
1:H:202:HIS:ND1	1:H:456:GLU:OE1	2.41	0.54
2:G:240:ASP:OD2	2:G:294:HIS:HB3	2.07	0.54
1:H:487:ASN:OD1	1:H:488:LYS:N	2.41	0.54
1:E:235:THR:HG22	1:E:237:GLN:H	1.73	0.54
2:C:327:ASN:HD22	2:C:328:THR:N	2.05	0.54
2:F:91:CYS:O	2:F:95:GLU:HG2	2.07	0.54
1:E:254:LEU:CD2	1:E:318:HIS:HB2	2.38	0.54
1:H:356:ILE:HD13	1:H:376:VAL:HG22	1.88	0.54
2:B:406:GLN:NE2	2:B:423:VAL:HG13	2.22	0.54
1:H:118:LEU:HD13	1:H:127:LEU:HD23	1.90	0.54
1:H:30:PHE:CE2	1:H:32:THR:HB	2.43	0.54
2:F:532:HIS:HD2	2:F:535:ARG:NH2	2.05	0.54
2:G:153:VAL:HB	2:G:192:SER:H	1.73	0.54
2:C:258:GLY:HA2	2:C:300:LYS:HE3	1.90	0.54
1:D:170:ARG:HG2	1:D:484:LEU:CB	2.34	0.53
2:B:240:ASP:OD1	2:B:241:ASP:N	2.30	0.53
2:B:239:VAL:HG12	2:B:245:PRO:HD2	1.90	0.53
1:A:61:LEU:HD13	1:A:132:VAL:HG23	1.90	0.53
2:C:211:ARG:HD2	2:C:242:GLN:OE1	2.08	0.53
1:A:382:LYS:HA	1:A:382:LYS:CE	2.34	0.53
1:D:41:PRO:HB3	1:D:73:PHE:CD1	2.44	0.53
2:C:154:LYS:HE3	2:C:154:LYS:C	2.29	0.53
1:E:384:GLN:O	1:E:386:ASP:N	2.36	0.53
1:E:222:MET:SD	1:E:233:ILE:HD12	2.49	0.53
1:D:170:ARG:NH2	1:D:485:TRP:CE3	2.77	0.53
2:G:261:SER:OG	2:G:264:HIS:HD2	1.92	0.52
2:G:203:ARG:H	2:G:232:ASN:HD21	1.56	0.52
1:A:235:THR:HG22	1:A:236:ALA:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:390:LYS:NZ	2:C:390:LYS:HB3	2.24	0.52
1:E:237:GLN:HB3	2:G:96:GLU:OE2	2.10	0.52
1:E:206:VAL:HG12	1:E:211:PHE:HA	1.92	0.52
1:A:418:ALA:HB3	1:A:419:PRO:HD3	1.92	0.52
2:B:425:LYS:O	2:B:429:TYR:HB3	2.10	0.52
1:H:416:LEU:O	1:H:455:GLY:HA3	2.09	0.52
6:H:532:NAG:H62	6:H:533:NAG:HN2	1.75	0.52
1:E:467:THR:CG2	2:F:544:GLN:HA	2.40	0.52
1:E:137:ARG:HB3	1:E:197:LYS:HE3	1.92	0.52
1:E:318:HIS:C	1:E:320:GLY:N	2.62	0.52
1:H:31:GLN:HB2	1:H:160:GLU:HB3	1.92	0.52
1:D:524:GLN:HG2	1:D:524:GLN:O	2.10	0.52
2:G:357:GLU:HB3	2:G:359:LYS:HG2	1.92	0.52
1:D:206:VAL:HG12	1:D:212:PRO:HD2	1.91	0.52
2:F:499:THR:HB	2:F:500:PRO:HD3	1.92	0.52
2:F:317:ASP:OD2	2:F:318:SER:N	2.43	0.52
2:F:502:LEU:HD23	2:F:506:ALA:HB2	1.92	0.51
2:F:475:GLN:O	2:F:479:GLN:HG3	2.10	0.51
2:B:135:SER:HB2	2:B:165:VAL:HG23	1.92	0.51
2:F:135:SER:O	2:F:136:GLU:CG	2.58	0.51
1:H:344:PHE:HA	1:H:350:GLN:HE21	1.75	0.51
1:E:322:ASP:HB3	1:E:373:TRP:CD1	2.45	0.51
1:A:235:THR:HG22	1:A:236:ALA:N	2.25	0.51
1:D:53:ALA:HB1	1:D:101:THR:CG2	2.41	0.51
1:H:33:SER:HB3	1:H:158:LYS:HB3	1.92	0.51
2:G:72:LEU:HD11	2:G:189:ILE:HG22	1.91	0.51
1:D:235:THR:HG22	1:D:237:GLN:H	1.75	0.51
2:G:410:ASP:O	2:G:412:LYS:HG3	2.10	0.51
1:E:105:ASN:OD1	1:E:105:ASN:N	2.44	0.51
1:A:256:GLU:HB2	1:A:318:HIS:HB3	1.93	0.51
1:E:465:ASP:OD1	1:E:467:THR:HG22	2.11	0.51
1:H:282:GLU:O	1:H:282:GLU:CD	2.49	0.51
2:F:404:VAL:HG11	2:F:408:VAL:HB	1.93	0.51
2:B:532:HIS:CD2	2:B:535:ARG:HH21	2.28	0.51
1:H:170:ARG:HG2	1:H:484:LEU:HB3	1.93	0.51
2:B:209:THR:HG22	2:B:214:LEU:HD12	1.92	0.51
1:D:45:GLN:HG3	1:D:93:ASN:HD22	1.76	0.51
1:E:525:GLU:CG	2:F:264:HIS:HE1	2.24	0.50
1:E:179:HIS:HB3	1:E:465:ASP:HB3	1.93	0.50
2:C:499:THR:HB	2:C:500:PRO:HD3	1.93	0.50
1:A:171:GLY:HA3	1:A:456:GLU:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:368:GLN:NE2	2:G:368:GLN:HA	2.23	0.50
1:A:202:HIS:ND1	1:A:456:GLU:OE1	2.45	0.50
2:B:425:LYS:N	8:B:574:HOH:O	2.44	0.50
2:F:155:GLU:N	2:F:156:PRO:HD2	2.26	0.50
2:B:490:GLY:HA2	2:B:493:VAL:HB	1.94	0.50
1:E:322:ASP:HB3	1:E:373:TRP:CG	2.47	0.50
2:F:64:LYS:O	2:F:192:SER:OG	2.23	0.50
1:H:254:LEU:CD2	1:H:318:HIS:HB2	2.41	0.50
1:E:263:THR:C	1:E:265:SER:H	2.16	0.50
1:E:318:HIS:ND1	1:E:320:GLY:HA2	2.27	0.49
1:D:72:LEU:HD11	1:D:143:SER:HB2	1.93	0.49
2:C:362:GLU:HG2	2:C:380:PHE:CE2	2.46	0.49
1:D:97:VAL:HG12	1:D:126:LEU:HD11	1.92	0.49
2:G:411:ASP:CA	2:G:411:ASP:O	2.52	0.49
1:E:131:THR:HG23	1:E:133:TRP:H	1.77	0.49
1:E:207:ASP:OD1	1:E:262:HIS:CD2	2.65	0.49
2:C:242:GLN:OE1	2:C:242:GLN:N	2.44	0.49
1:A:28:GLN:HE22	1:A:487:ASN:HD22	1.60	0.49
2:F:211:ARG:HD2	2:F:242:GLN:OE1	2.13	0.49
1:A:99:VAL:HG22	1:A:130:GLU:HA	1.94	0.49
1:H:281:SER:O	1:H:282:GLU:HB2	2.12	0.49
1:E:372:VAL:HG11	1:E:376:VAL:CG2	2.41	0.49
1:H:224:LYS:HB3	1:H:268:PRO:HB2	1.94	0.49
2:C:135:SER:HB2	2:C:165:VAL:HB	1.93	0.49
2:C:199:ARG:HH21	2:C:469:LEU:HD12	1.77	0.49
1:H:48:TYR:CD1	1:H:56:PRO:HD3	2.47	0.49
1:E:318:HIS:CE1	1:E:373:TRP:NE1	2.80	0.49
1:D:353:SER:HA	1:D:381:VAL:HG13	1.94	0.49
2:G:414:LYS:HD2	2:G:414:LYS:H	1.77	0.49
2:F:362:GLU:HG2	2:F:380:PHE:CE2	2.48	0.49
2:G:93:LEU:HD21	2:G:169:LEU:HD21	1.95	0.49
1:D:48:TYR:CD1	1:D:56:PRO:HD3	2.47	0.48
1:H:93:ASN:OD1	1:H:94:VAL:N	2.45	0.48
1:A:206:VAL:HG12	1:A:212:PRO:HD2	1.94	0.48
2:B:352:GLY:HA2	2:B:405:TRP:CD1	2.48	0.48
1:A:447:GLU:H	1:A:447:GLU:CD	2.16	0.48
2:B:235:HIS:NE2	2:B:288:GLU:OE1	2.24	0.48
3:D:13:NAG:H61	3:D:14:NAG:H83	1.95	0.48
1:E:467:THR:HG21	2:F:533:ARG:HH21	1.78	0.48
1:D:53:ALA:HB1	1:D:101:THR:HA	1.94	0.48
1:D:500:LEU:HG	1:D:517:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:VAL:HB	2:B:192:SER:H	1.78	0.48
1:D:178:ARG:HA	1:D:209:PRO:HG3	1.95	0.48
2:C:532:HIS:HD2	2:C:535:ARG:NH2	1.99	0.48
1:E:246:ALA:HB1	1:E:251:ILE:HB	1.94	0.48
1:A:131:THR:CG2	1:A:132:VAL:H	2.27	0.48
2:G:374:LYS:HZ2	2:G:374:LYS:HA	1.78	0.48
2:B:238:ILE:HG23	2:B:239:VAL:HG13	1.95	0.48
1:H:55:GLN:O	1:H:58:CYS:HB2	2.13	0.48
1:H:281:SER:O	1:H:282:GLU:CB	2.62	0.48
1:H:207:ASP:OD2	1:H:208:ASP:N	2.36	0.48
2:C:206:LEU:HA	2:C:235:HIS:HB3	1.94	0.48
2:F:100:ARG:HG2	2:F:104:TYR:CE2	2.46	0.48
1:H:206:VAL:HG12	1:H:212:PRO:HD2	1.95	0.48
1:D:30:PHE:CE2	1:D:32:THR:HB	2.48	0.48
2:F:89:PRO:HA	2:F:95:GLU:OE2	2.14	0.48
1:D:356:ILE:HD12	1:D:381:VAL:HG21	1.95	0.48
1:E:299:GLU:OE1	1:E:299:GLU:HA	2.14	0.48
1:H:103:GLY:HA3	1:H:132:VAL:CG2	2.44	0.47
1:A:422:LEU:O	1:A:476:ARG:NH2	2.42	0.47
1:E:229:PRO:HA	8:E:734:HOH:O	2.15	0.47
1:A:375:GLU:OE1	1:A:375:GLU:N	2.45	0.47
2:G:82:SER:HA	2:G:128:LEU:HD22	1.95	0.47
2:F:206:LEU:HB3	2:F:487:CYS:HA	1.95	0.47
1:H:39:LEU:HG	1:H:156:ILE:HD11	1.96	0.47
2:C:188:THR:HG22	2:C:189:ILE:N	2.30	0.47
1:D:306:LEU:HG	1:D:366:TYR:CE2	2.49	0.47
1:D:382:LYS:NZ	1:D:382:LYS:HB2	2.29	0.47
2:G:499:THR:HB	2:G:500:PRO:HD3	1.96	0.47
1:D:210:SER:N	1:D:210:SER:CB	2.67	0.47
2:G:414:LYS:N	2:G:414:LYS:HD2	2.29	0.47
1:E:47:GLN:CD	1:E:93:ASN:HD21	2.18	0.47
2:F:404:VAL:HG12	2:F:405:TRP:O	2.15	0.47
2:F:459:ASP:N	2:F:459:ASP:OD1	2.47	0.47
2:G:437:THR:HB	2:G:477:GLN:HB3	1.97	0.47
1:D:50:VAL:CG2	1:D:51:SER:OG	2.63	0.47
1:H:175:ASP:OD2	1:H:178:ARG:HD3	2.15	0.47
1:E:342:LYS:HA	1:E:342:LYS:CE	2.43	0.46
1:E:525:GLU:HG2	2:F:264:HIS:CE1	2.47	0.46
1:E:208:ASP:HB2	1:E:209:PRO:HD3	1.96	0.46
2:F:302:GLN:HG3	2:F:305:LEU:HB2	1.97	0.46
1:D:102:PRO:O	1:D:103:GLY:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:LEU:HB3	1:E:458:CYS:HA	1.96	0.46
1:D:68:TYR:O	1:D:72:LEU:HD13	2.15	0.46
2:F:223:LEU:HD21	2:F:234:LEU:HD22	1.98	0.46
1:H:192:VAL:HA	1:H:195:TYR:CD2	2.50	0.46
1:H:151:GLU:OE1	1:H:151:GLU:N	2.46	0.46
2:F:352:GLY:CA	2:F:405:TRP:HD1	2.28	0.46
1:A:121:ASN:HD21	1:A:124:GLN:H	1.63	0.46
1:H:228:ASN:HD22	1:H:228:ASN:C	2.18	0.46
1:H:203:TRP:HE3	1:H:204:HIS:N	2.14	0.46
1:D:99:VAL:HG22	1:D:130:GLU:HA	1.98	0.46
1:H:315:PHE:O	1:H:369:GLY:N	2.39	0.46
2:G:411:ASP:N	2:G:411:ASP:C	2.61	0.46
1:D:44:PHE:O	1:D:69:ARG:NH1	2.49	0.46
2:F:267:THR:HB	2:F:268:PRO:HD2	1.97	0.46
2:B:223:LEU:HD21	2:B:234:LEU:HD22	1.97	0.46
1:H:515:GLN:HB2	1:H:516:PRO:HD2	1.97	0.46
1:D:522:CYS:O	1:D:523:GLU:C	2.53	0.46
2:C:398:ILE:O	2:C:398:ILE:HG22	2.15	0.46
1:H:220:GLU:HA	1:H:223:ARG:HB2	1.98	0.46
1:E:278:TYR:HB2	1:E:331:SER:O	2.16	0.46
1:H:440:LEU:HD22	1:H:449:LYS:HB3	1.98	0.46
2:F:205:ILE:HD13	2:F:486:ALA:HB3	1.97	0.46
2:C:536:MET:HB3	2:C:541:ILE:HB	1.98	0.46
2:G:242:GLN:HG2	1:H:519:VAL:CG2	2.27	0.46
1:D:256:GLU:HB2	1:D:318:HIS:HB3	1.98	0.46
2:B:359:LYS:HB2	2:B:359:LYS:NZ	2.30	0.46
2:C:203:ARG:HG2	2:C:513:LEU:HB3	1.98	0.46
2:F:267:THR:HG21	1:H:66:GLN:HG3	1.98	0.46
1:E:207:ASP:OD1	1:E:262:HIS:HD2	1.99	0.46
2:C:366:LYS:HD2	2:C:366:LYS:H	1.81	0.46
1:H:53:ALA:HB1	1:H:101:THR:CA	2.23	0.46
1:E:100:VAL:CG1	1:E:102:PRO:HG2	2.42	0.46
2:B:67:PRO:HB3	5:B:8:NDG:H8C1	1.97	0.45
2:G:195:ILE:N	2:G:195:ILE:HD12	2.32	0.45
1:E:221:LEU:HD12	1:E:222:MET:N	2.31	0.45
1:E:173:LEU:HD23	1:E:173:LEU:C	2.36	0.45
2:F:458:GLN:HB3	2:F:460:TRP:NE1	2.32	0.45
1:D:215:SER:OG	1:D:307:GLU:OE2	2.33	0.45
2:C:135:SER:O	2:C:136:GLU:C	2.55	0.45
1:H:320:GLY:HA2	1:H:373:TRP:CD1	2.52	0.45
1:E:180:TYR:HB3	1:E:232:HIS:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:ARG:HH21	2:B:469:LEU:HD12	1.80	0.45
1:A:467:THR:CG2	2:B:544:GLN:HA	2.38	0.45
1:H:176:THR:OG1	1:H:203:TRP:HZ3	1.99	0.45
1:H:270:ILE:HD12	1:H:273:LEU:HB2	1.98	0.45
1:E:117:THR:OG1	1:E:128:LEU:HG	2.16	0.45
1:D:23:LEU:HD11	1:D:141:THR:HG23	1.96	0.45
1:E:396:ILE:HD12	1:E:396:ILE:N	2.31	0.45
1:E:228:ASN:ND2	1:E:230:VAL:H	2.09	0.45
2:G:364:ASN:OD1	2:G:367:ILE:HG13	2.17	0.45
2:G:205:ILE:HD13	2:G:486:ALA:HB3	1.98	0.45
1:H:382:LYS:HD3	1:H:382:LYS:O	2.17	0.45
2:G:411:ASP:C	2:G:411:ASP:CB	2.78	0.45
1:E:204:HIS:CD2	1:E:256:GLU:CD	2.88	0.45
1:E:101:THR:O	1:E:102:PRO:C	2.54	0.45
1:D:72:LEU:HD11	1:D:143:SER:CB	2.46	0.45
1:E:522:CYS:O	1:E:523:GLU:C	2.54	0.45
2:B:188:THR:HG22	2:B:189:ILE:N	2.31	0.45
1:E:524:GLN:NE2	1:E:524:GLN:O	2.50	0.45
1:H:104:CYS:C	1:H:105:ASN:HD22	2.21	0.45
1:E:318:HIS:CE1	1:E:320:GLY:HA2	2.52	0.45
1:A:131:THR:CG2	1:A:132:VAL:N	2.79	0.45
1:D:235:THR:HG22	1:D:236:ALA:N	2.30	0.45
2:G:151:LEU:HD13	2:G:160:LEU:HD13	1.99	0.45
2:C:481:PHE:O	8:C:577:HOH:O	2.21	0.45
1:D:202:HIS:CE1	1:D:256:GLU:OE1	2.66	0.45
1:E:178:ARG:HH11	1:E:460:TRP:HE3	1.63	0.45
1:E:169:HIS:ND1	1:E:415:LEU:HD11	2.32	0.45
2:F:206:LEU:HD23	2:F:206:LEU:C	2.37	0.45
2:G:388:ILE:HD12	2:G:389:GLN:N	2.32	0.45
1:A:470:VAL:N	1:A:471:PRO:HD2	2.32	0.45
1:H:103:GLY:O	1:H:105:ASN:N	2.50	0.44
2:F:544:GLN:HB2	2:F:545:PRO:HD2	1.99	0.44
1:H:173:LEU:HB3	1:H:458:CYS:HA	1.99	0.44
2:B:229:ASN:OD1	2:B:532:HIS:HE1	1.99	0.44
1:A:302:SER:HA	1:A:362:ILE:HG21	1.99	0.44
2:F:155:GLU:N	2:F:156:PRO:CD	2.80	0.44
2:F:105:ILE:HG23	2:F:179:VAL:HG21	1.99	0.44
2:F:287:PRO:HG3	2:F:344:PHE:CG	2.53	0.44
1:E:26:TRP:HA	1:E:27:PRO:HD3	1.86	0.44
1:H:196:ASN:N	1:H:196:ASN:ND2	2.66	0.44
1:D:169:HIS:CD2	1:D:200:VAL:HG21	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:199:ARG:HH21	2:G:469:LEU:HD12	1.81	0.44
1:E:243:ILE:HA	1:E:253:VAL:HG21	2.00	0.44
2:F:399:ASN:HD22	2:F:399:ASN:C	2.21	0.44
1:H:422:LEU:O	1:H:423:ASN:C	2.55	0.44
2:G:55:ALA:O	2:G:535:ARG:NH2	2.49	0.44
1:D:503:PHE:O	1:D:507:LEU:HG	2.16	0.44
1:E:173:LEU:HG	1:E:202:HIS:HD1	1.82	0.44
1:E:202:HIS:HE1	1:E:256:GLU:OE1	2.00	0.44
1:D:202:HIS:CD2	1:D:456:GLU:OE1	2.71	0.44
1:E:169:HIS:HE1	1:E:456:GLU:OE2	2.00	0.44
1:H:159:THR:HB	1:H:161:ILE:CD1	2.47	0.44
2:B:447:ALA:HB3	2:B:448:PRO:HD3	2.00	0.44
1:E:177:SER:O	1:E:210:SER:HB2	2.18	0.44
1:H:396:ILE:HA	1:H:397:PRO:C	2.37	0.44
2:C:229:ASN:HD22	2:C:229:ASN:N	2.16	0.44
1:D:207:ASP:OD2	1:D:208:ASP:N	2.38	0.44
1:A:100:VAL:HG12	1:A:102:PRO:CD	2.46	0.44
2:B:248:SER:HB3	2:B:251:PHE:O	2.18	0.44
1:D:211:PHE:H	1:D:226:SER:HA	1.82	0.44
2:F:504:PRO:HG3	2:F:544:GLN:CG	2.35	0.44
1:D:50:VAL:HG23	1:D:51:SER:OG	2.17	0.44
1:E:470:VAL:N	1:E:471:PRO:HD2	2.33	0.44
2:C:261:SER:OG	2:C:264:HIS:CD2	2.71	0.44
1:A:420:TRP:CD1	1:A:480:VAL:HG22	2.53	0.44
2:B:504:PRO:HD3	2:B:544:GLN:O	2.18	0.43
2:G:155:GLU:N	2:G:156:PRO:CD	2.81	0.43
2:G:544:GLN:HA	1:H:467:THR:CG2	2.47	0.43
2:B:55:ALA:O	2:B:535:ARG:NH2	2.44	0.43
1:H:169:HIS:ND1	1:H:415:LEU:HD11	2.33	0.43
2:B:153:VAL:O	2:B:191:GLU:HB2	2.18	0.43
2:B:132:THR:HB	2:B:163:ASN:HA	2.00	0.43
2:F:452:ASP:OD1	2:F:489:TRP:HD1	2.01	0.43
1:D:430:ASP:OD2	1:D:476:ARG:NH1	2.51	0.43
2:G:532:HIS:HD2	2:G:535:ARG:HE	1.66	0.43
1:H:89:THR:HG22	1:H:90:LEU:N	2.33	0.43
2:C:352:GLY:HA2	2:C:405:TRP:CD1	2.54	0.43
1:A:165:PRO:HB3	1:A:485:TRP:CE3	2.53	0.43
1:A:101:THR:N	1:A:102:PRO:CD	2.80	0.43
1:E:208:ASP:CB	1:E:209:PRO:HD3	2.49	0.43
1:E:198:LEU:HD11	1:E:481:ALA:CB	2.48	0.43
1:A:32:THR:OG1	1:A:33:SER:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:385:SER:O	2:C:389:GLN:HG3	2.18	0.43
2:C:504:PRO:HD3	2:C:544:GLN:O	2.18	0.43
1:E:212:PRO:HB2	1:E:234:TYR:CD1	2.53	0.43
1:E:359:LEU:HD23	1:E:359:LEU:O	2.18	0.43
1:E:40:TYR:HA	1:E:41:PRO:HD2	1.73	0.43
2:B:469:LEU:HD22	2:B:478:LYS:HD2	2.00	0.43
1:D:275:THR:HG21	1:D:329:TRP:HD1	1.84	0.43
1:D:445:THR:HB	1:D:446:PRO:HD2	1.99	0.43
1:E:235:THR:CG2	1:E:236:ALA:N	2.81	0.43
1:H:232:HIS:O	1:H:233:ILE:HD13	2.18	0.43
1:D:116:TYR:CE1	1:D:163:ASP:HB3	2.52	0.43
2:F:466:VAL:O	2:F:512:ARG:HD3	2.18	0.43
2:B:206:LEU:HD23	2:B:206:LEU:C	2.39	0.43
2:G:352:GLY:HA2	2:G:405:TRP:CD1	2.53	0.43
1:A:336:GLN:HA	1:A:336:GLN:HE21	1.84	0.43
1:H:103:GLY:O	1:H:105:ASN:ND2	2.52	0.43
2:G:459:ASP:OD2	2:G:505:ARG:NH1	2.51	0.43
1:H:393:ARG:HD3	1:H:396:ILE:O	2.18	0.43
1:E:60:VAL:HG23	1:E:104:CYS:O	2.18	0.43
1:A:97:VAL:CG1	1:A:126:LEU:HD21	2.49	0.43
1:D:166:ARG:HH21	1:D:440:LEU:HD12	1.84	0.43
1:E:179:HIS:CE1	2:F:548:ALA:HA	2.54	0.43
1:D:100:VAL:HG12	1:D:102:PRO:HG2	2.00	0.43
2:B:406:GLN:HE21	2:B:423:VAL:HA	1.84	0.43
1:D:233:ILE:HG22	1:D:234:TYR:N	2.34	0.43
1:H:254:LEU:HD21	1:H:318:HIS:HB2	2.00	0.43
2:G:390:LYS:O	2:G:394:ILE:HG13	2.19	0.43
1:H:375:GLU:N	1:H:375:GLU:OE1	2.50	0.43
1:A:121:ASN:HD21	1:A:124:GLN:HG2	1.83	0.43
2:B:262:LEU:HD23	1:D:69:ARG:HH22	1.83	0.43
2:F:502:LEU:HD23	2:F:502:LEU:C	2.39	0.43
2:B:68:ASN:HB3	2:B:191:GLU:HG2	2.01	0.43
2:G:447:ALA:HB3	2:G:448:PRO:HD3	2.00	0.43
2:F:195:ILE:HD12	2:F:195:ILE:N	2.34	0.43
6:H:532:NAG:H62	6:H:533:NAG:N2	2.33	0.42
2:B:350:HIS:CD2	2:B:352:GLY:H	2.37	0.42
2:G:339:GLU:O	2:G:343:VAL:HG23	2.19	0.42
1:H:470:VAL:N	1:H:471:PRO:HD2	2.34	0.42
2:G:206:LEU:HA	2:G:235:HIS:HB3	2.00	0.42
1:E:198:LEU:HD11	1:E:481:ALA:HB2	1.99	0.42
2:C:251:PHE:HB3	2:C:254:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:404:VAL:HG21	2:G:408:VAL:HG21	2.01	0.42
1:H:66:GLN:HA	1:H:69:ARG:HG2	2.02	0.42
1:H:90:LEU:N	1:H:90:LEU:HD23	2.34	0.42
1:E:151:GLU:HB3	1:H:153:THR:HG23	2.01	0.42
1:E:339:MET:SD	1:E:351:LEU:HD22	2.59	0.42
1:E:256:GLU:HB2	1:E:318:HIS:HB3	2.00	0.42
1:A:100:VAL:HG12	1:A:102:PRO:HG2	2.00	0.42
1:H:127:LEU:HD21	1:H:138:GLY:HA3	2.01	0.42
2:G:488:LEU:HD22	2:G:502:LEU:HG	2.01	0.42
1:A:102:PRO:O	1:A:103:GLY:O	2.36	0.42
1:D:208:ASP:OD1	1:D:264:LEU:HB2	2.19	0.42
1:D:36:ARG:HD2	6:D:17:NAG:H62	2.02	0.42
1:H:23:LEU:HD12	1:H:145:LEU:HD21	2.01	0.42
1:D:375:GLU:OE1	1:D:375:GLU:N	2.53	0.42
2:C:457:GLY:HA2	1:D:463:TYR:CZ	2.55	0.42
2:G:544:GLN:HB2	2:G:545:PRO:HD2	2.00	0.42
1:A:126:LEU:HD23	1:A:127:LEU:N	2.34	0.42
2:C:465:LYS:HA	2:C:520:ARG:NH1	2.35	0.42
2:C:336:PHE:O	2:C:340:ILE:HG12	2.20	0.42
1:A:388:ILE:HG21	1:A:415:LEU:CD2	2.50	0.42
2:F:261:SER:OG	2:F:264:HIS:HD2	2.02	0.42
2:C:551:CYS:O	2:C:552:ASN:CB	2.68	0.42
2:B:404:VAL:HG21	2:B:408:VAL:HG21	2.02	0.42
1:H:238:ASP:O	1:H:242:VAL:HG23	2.20	0.42
2:G:467:GLU:HA	2:G:468:PRO:HD2	1.92	0.42
1:E:126:LEU:HD23	1:E:127:LEU:N	2.34	0.42
1:E:121:ASN:C	1:E:121:ASN:HD22	2.23	0.42
1:E:55:GLN:CG	1:E:56:PRO:HD2	2.22	0.42
1:E:172:LEU:HD11	1:E:174:LEU:CD1	2.49	0.42
1:A:151:GLU:HG3	1:D:38:VAL:CG1	2.49	0.42
2:B:135:SER:O	2:B:136:GLU:HB2	2.20	0.42
2:G:424:TRP:CZ2	2:G:425:LYS:HE3	2.54	0.42
1:H:402:LYS:HA	1:H:402:LYS:HE2	2.02	0.42
2:C:245:PRO:HB2	2:C:266:TYR:CD2	2.55	0.42
1:H:37:TYR:O	1:H:155:PHE:HA	2.20	0.42
1:E:416:LEU:O	1:E:455:GLY:CA	2.67	0.42
1:E:40:TYR:HE2	1:E:90:LEU:HB2	1.84	0.41
1:D:26:TRP:HA	1:D:27:PRO:HD3	1.84	0.41
2:B:211:ARG:HD2	2:B:242:GLN:OE1	2.20	0.41
1:D:228:ASN:ND2	1:D:230:VAL:H	2.07	0.41
2:G:496:THR:OG1	1:H:515:GLN:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:398:VAL:HG22	1:H:399:ASN:H	1.86	0.41
1:E:240:LYS:NZ	1:E:240:LYS:HB2	2.35	0.41
1:E:48:TYR:CD1	1:E:56:PRO:HD3	2.55	0.41
2:G:288:GLU:HB2	2:G:350:HIS:HB3	2.03	0.41
1:E:394:GLU:O	1:E:399:ASN:HA	2.19	0.41
2:C:246:TYR:O	2:C:255:SER:HB3	2.20	0.41
2:G:366:LYS:N	2:G:366:LYS:HD2	2.35	0.41
1:A:228:ASN:ND2	1:A:230:VAL:H	2.09	0.41
1:E:372:VAL:HG12	1:E:373:TRP:N	2.35	0.41
1:D:121:ASN:ND2	1:D:124:GLN:H	2.18	0.41
2:G:235:HIS:HB2	2:G:485:GLU:OE2	2.20	0.41
1:D:53:ALA:HB1	1:D:101:THR:HG22	2.03	0.41
1:A:515:GLN:HB2	1:A:516:PRO:HD2	2.01	0.41
1:D:320:GLY:HA2	1:D:373:TRP:CD1	2.55	0.41
1:D:100:VAL:HG12	1:D:102:PRO:CG	2.51	0.41
1:H:383:ILE:HG13	1:H:384:GLN:N	2.35	0.41
1:H:322:ASP:HB3	1:H:373:TRP:CD1	2.55	0.41
2:F:286:LEU:HD21	2:F:403:ILE:HD12	2.02	0.41
2:F:204:GLY:HA2	2:F:233:VAL:O	2.21	0.41
1:D:404:LEU:HD11	1:D:416:LEU:HD13	2.03	0.41
2:C:275:ILE:HD13	2:C:345:PRO:HD3	2.02	0.41
2:G:364:ASN:HA	2:G:365:PRO:HD2	1.87	0.41
2:C:285:VAL:O	2:C:287:PRO:HD3	2.21	0.41
2:F:346:ASP:OD2	2:F:347:GLN:N	2.53	0.41
1:E:318:HIS:O	1:E:320:GLY:N	2.53	0.41
2:B:407:GLU:OE2	2:B:424:TRP:HZ2	2.04	0.41
1:E:393:ARG:HG2	1:E:396:ILE:HD13	2.03	0.41
1:A:53:ALA:HB1	1:A:101:THR:HA	2.01	0.41
1:D:202:HIS:HD2	1:D:456:GLU:OE1	2.04	0.41
1:D:37:TYR:O	1:D:156:ILE:HD12	2.21	0.41
1:D:25:PRO:CD	1:D:197:LYS:HD3	2.49	0.41
1:A:487:ASN:OD1	1:A:488:LYS:N	2.54	0.41
1:A:59:SER:O	1:A:63:GLU:HG2	2.21	0.41
2:B:467:GLU:HA	2:B:468:PRO:HD2	1.87	0.41
1:E:95:LEU:HD12	1:E:95:LEU:N	2.36	0.41
1:E:362:ILE:HG22	1:E:366:TYR:CE1	2.56	0.41
2:F:323:ASN:HA	2:F:324:PRO:HD3	1.88	0.41
1:A:228:ASN:HA	1:A:229:PRO:HD3	1.82	0.41
1:D:278:TYR:HA	1:D:283:PRO:HA	2.01	0.41
2:F:458:GLN:HB3	2:F:460:TRP:CD1	2.56	0.41
2:C:73:ALA:HB3	2:C:76:ASN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:TRP:CE2	1:D:393:ARG:HG2	2.56	0.41
2:F:183:SER:O	2:G:74:PRO:HD2	2.21	0.41
2:B:336:PHE:O	2:B:340:ILE:HG12	2.20	0.41
1:D:42:ASN:O	1:D:43:ASN:ND2	2.54	0.41
2:G:211:ARG:O	1:H:519:VAL:HG23	2.21	0.40
1:D:282:GLU:HB3	1:D:283:PRO:HD2	2.02	0.40
2:B:364:ASN:HA	2:B:365:PRO:HD2	1.80	0.40
1:H:398:VAL:HG22	1:H:399:ASN:N	2.36	0.40
2:G:461:ARG:O	2:G:465:LYS:HB2	2.20	0.40
2:F:303:LYS:HB2	2:F:303:LYS:NZ	2.36	0.40
2:B:398:ILE:HG12	2:B:398:ILE:H	1.77	0.40
2:G:238:ILE:HG23	2:G:239:VAL:HG13	2.02	0.40
1:E:203:TRP:CD1	1:E:205:LEU:HG	2.56	0.40
2:B:66:THR:HA	2:B:67:PRO:HD3	1.87	0.40
1:A:353:SER:O	1:A:357:GLN:HG3	2.21	0.40
2:C:149:TYR:CZ	2:C:196:ASP:HB3	2.56	0.40
2:F:390:LYS:NZ	2:F:390:LYS:HB3	2.36	0.40
1:A:107:LEU:HB2	1:A:108:PRO:HD2	2.04	0.40
2:C:206:LEU:C	2:C:206:LEU:HD23	2.42	0.40
1:E:99:VAL:HG22	1:E:130:GLU:HA	2.03	0.40
1:E:23:LEU:HA	1:E:144:GLN:OE1	2.22	0.40
1:D:438:GLU:HA	1:D:439:PRO:HD3	1.83	0.40
1:D:342:LYS:NZ	1:D:342:LYS:HB3	2.36	0.40
1:E:319:LEU:HD21	1:E:363:VAL:HG11	2.03	0.40
1:H:173:LEU:HD23	1:H:173:LEU:C	2.42	0.40
2:C:70:LEU:HD11	2:C:154:LYS:HA	2.02	0.40
2:F:170:ARG:HH21	2:F:232:ASN:HB3	1.85	0.40
1:H:116:TYR:CE1	1:H:163:ASP:HB3	2.56	0.40
1:H:49:ASP:OD1	1:H:50:VAL:N	2.55	0.40
1:E:31:GLN:HB2	1:E:160:GLU:HB3	2.04	0.40
1:H:282:GLU:CD	1:H:283:PRO:HD3	2.41	0.40
1:E:374:GLN:O	1:E:375:GLU:C	2.60	0.40
2:F:59:LEU:HA	2:F:60:PRO:HD3	1.89	0.40
2:F:149:TYR:CZ	2:F:196:ASP:HB3	2.56	0.40
1:A:233:ILE:HG22	1:A:234:TYR:N	2.35	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	488/507 (96%)	453 (93%)	33 (7%)	2 (0%)	39	74
1	D	488/507 (96%)	449 (92%)	36 (7%)	3 (1%)	30	65
1	E	488/507 (96%)	435 (89%)	39 (8%)	14 (3%)	6	19
1	H	488/507 (96%)	447 (92%)	31 (6%)	10 (2%)	9	30
2	B	474/507 (94%)	447 (94%)	26 (6%)	1 (0%)	52	84
2	C	475/507 (94%)	450 (95%)	25 (5%)	0	100	100
2	F	474/507 (94%)	434 (92%)	36 (8%)	4 (1%)	24	58
2	G	474/507 (94%)	442 (93%)	26 (6%)	6 (1%)	15	44
All	All	3849/4056 (95%)	3557 (92%)	252 (6%)	40 (1%)	19	52

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	PRO
1	A	103	GLY
1	D	50	VAL
1	D	103	GLY
1	E	382	LYS
2	G	412	LYS
1	H	104	CYS
1	H	105	ASN
1	H	283	PRO
1	H	284	SER
1	H	102	PRO
1	D	102	PRO
1	E	380	LYS
1	E	417	SER
2	F	446	SER
2	G	156	PRO
2	G	427	SER

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Mol	Chain	Res	Type
1	H	280	GLY
1	H	282	GLU
1	H	323	GLU
1	E	208	ASP
1	E	373	TRP
1	E	375	GLU
2	F	156	PRO
2	G	294	HIS
1	E	207	ASP
1	E	385	PRO
2	F	504	PRO
1	E	264	LEU
1	E	267	GLY
1	E	319	LEU
2	F	74	PRO
2	G	520	ARG
1	E	280	GLY
2	G	293	GLY
1	H	267	GLY
2	B	74	PRO
1	E	397	PRO
1	H	285	GLY
1	E	398	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	441/454 (97%)	424 (96%)	17 (4%)	39	74
1	D	441/454 (97%)	428 (97%)	13 (3%)	50	83
1	E	441/454 (97%)	417 (95%)	24 (5%)	27	60
1	H	441/454 (97%)	422 (96%)	19 (4%)	35	70
2	B	426/449 (95%)	420 (99%)	6 (1%)	74	94
2	C	427/449 (95%)	422 (99%)	5 (1%)	78	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	426/449 (95%)	417 (98%)	9 (2%)	61	90
2	G	426/449 (95%)	416 (98%)	10 (2%)	58	88
All	All	3469/3612 (96%)	3366 (97%)	103 (3%)	48	82

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	90	LEU
1	A	105	ASN
1	A	106	GLN
1	A	107	LEU
1	A	121	ASN
1	A	122	ASP
1	A	159	THR
1	A	174	LEU
1	A	198	LEU
1	A	228	ASN
1	A	296	ASN
1	A	299	GLU
1	A	336	GLN
1	A	382	LYS
1	A	523	GLU
1	A	525	GLU
2	B	84	ASN
2	B	211	ARG
2	B	338	LYS
2	B	359	LYS
2	B	384	GLU
2	B	522	MET
2	C	154	LYS
2	C	155	GLU
2	C	211	ARG
2	C	327	ASN
2	C	502	LEU
1	D	51	SER
1	D	61	LEU
1	D	63	GLU
1	D	69	ARG
1	D	101	THR
1	D	106	GLN

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Mol	Chain	Res	Type
1	D	121	ASN
1	D	156	ILE
1	D	173	LEU
1	D	198	LEU
1	D	228	ASN
1	D	370	TYR
1	D	523	GLU
1	E	61	LEU
1	E	92	LYS
1	E	105	ASN
1	E	119	THR
1	E	121	ASN
1	E	122	ASP
1	E	127	LEU
1	E	159	THR
1	E	162	GLU
1	E	174	LEU
1	E	178	ARG
1	E	221	LEU
1	E	228	ASN
1	E	240	LYS
1	E	326	PHE
1	E	360	LEU
1	E	370	TYR
1	E	379	ASN
1	E	380	LYS
1	E	383	ILE
1	E	399	ASN
1	E	424	ARG
1	E	445	THR
1	E	524	GLN
2	F	64	LYS
2	F	65	MET
2	F	211	ARG
2	F	303	LYS
2	F	373	GLN
2	F	399	ASN
2	F	412	LYS
2	F	475	GLN
2	F	512	ARG
2	G	84	ASN
2	G	211	ARG

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Mol	Chain	Res	Type
2	G	232	ASN
2	G	303	LYS
2	G	368	GLN
2	G	374	LYS
2	G	411	ASP
2	G	414	LYS
2	G	417	PRO
2	G	502	LEU
1	H	62	ASP
1	H	104	CYS
1	H	119	THR
1	H	121	ASN
1	H	122	ASP
1	H	156	ILE
1	H	172	LEU
1	H	196	ASN
1	H	203	TRP
1	H	228	ASN
1	H	270	ILE
1	H	299	GLU
1	H	370	TYR
1	H	381	VAL
1	H	382	LYS
1	H	384	GLN
1	H	424	ARG
1	H	447	GLU
1	H	517	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	47	GLN
1	A	55	GLN
1	A	106	GLN
1	A	121	ASN
1	A	124	GLN
1	A	204	HIS
1	A	228	ASN
1	A	336	GLN
1	A	350	GLN
1	A	357	GLN

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Mol	Chain	Res	Type
1	A	399	ASN
1	A	448	GLN
1	A	466	ASN
1	A	513	GLN
2	B	84	ASN
2	B	102	HIS
2	B	123	GLN
2	B	126	GLN
2	B	134	GLN
2	B	237	HIS
2	B	264	HIS
2	B	302	GLN
2	B	350	HIS
2	B	364	ASN
2	B	406	GLN
2	B	532	HIS
2	C	68	ASN
2	C	123	GLN
2	C	126	GLN
2	C	134	GLN
2	C	237	HIS
2	C	264	HIS
2	C	327	ASN
2	C	350	HIS
2	C	368	GLN
2	C	475	GLN
2	C	479	GLN
2	C	532	HIS
1	D	28	GLN
1	D	29	ASN
1	D	43	ASN
1	D	47	GLN
1	D	55	GLN
1	D	106	GLN
1	D	121	ASN
1	D	202	HIS
1	D	228	ASN
1	D	296	ASN
1	D	399	ASN
1	D	487	ASN
1	D	513	GLN
1	E	28	GLN

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Mol	Chain	Res	Type
1	E	31	GLN
1	E	55	GLN
1	E	121	ASN
1	E	204	HIS
1	E	228	ASN
1	E	262	HIS
1	E	296	ASN
1	E	318	HIS
1	E	336	GLN
1	E	357	GLN
1	E	379	ASN
1	E	513	GLN
1	E	524	GLN
2	F	68	ASN
2	F	76	ASN
2	F	84	ASN
2	F	177	GLN
2	F	237	HIS
2	F	264	HIS
2	F	323	ASN
2	F	373	GLN
2	F	399	ASN
2	F	475	GLN
2	F	477	GLN
2	F	532	HIS
2	G	76	ASN
2	G	123	GLN
2	G	126	GLN
2	G	232	ASN
2	G	237	HIS
2	G	264	HIS
2	G	368	GLN
2	G	475	GLN
2	G	477	GLN
2	G	479	GLN
2	G	532	HIS
1	H	28	GLN
1	H	31	GLN
1	H	45	GLN
1	H	47	GLN
1	H	55	GLN
1	H	105	ASN

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Mol	Chain	Res	Type
1	H	106	GLN
1	H	121	ASN
1	H	196	ASN
1	H	204	HIS
1	H	228	ASN
1	H	295	ASN
1	H	296	ASN
1	H	350	GLN
1	H	357	GLN
1	H	384	GLN
1	H	466	ASN
1	H	513	GLN
1	H	524	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

26 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	1	1,3	14,14,15	0.60	0	15,19,21	0.65	0
3	NAG	A	2	3	14,14,15	0.51	0	15,19,21	0.57	0
3	BMA	A	3	3	11,11,12	0.55	0	14,15,17	0.67	0
3	NAG	A	4	1,3	14,14,15	0.57	0	15,19,21	0.78	0
3	NAG	A	5	3	14,14,15	0.64	0	15,19,21	0.77	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BMA	A	6	3	11,11,12	0.50	0	14,15,17	1.41	2 (14%)
5	BMA	B	10	5	11,11,12	0.59	0	14,15,17	0.94	1 (7%)
5	NDG	B	8	2,5	14,14,15	0.72	0	15,19,21	0.97	1 (6%)
5	NAG	B	9	5	14,14,15	0.59	0	15,19,21	0.63	0
6	NAG	C	11	2,6	14,14,15	0.45	0	15,19,21	0.56	0
6	NAG	C	12	6	14,14,15	0.46	0	15,19,21	0.61	0
3	NAG	D	13	1,3	14,14,15	0.79	0	15,19,21	1.09	2 (13%)
3	NAG	D	14	3	14,14,15	0.58	0	15,19,21	0.76	0
3	BMA	D	15	3	11,11,12	0.57	0	14,15,17	0.69	1 (7%)
6	NAG	D	17	1,6	14,14,15	0.66	0	15,19,21	0.99	1 (6%)
6	NAG	D	18	6	14,14,15	0.48	0	15,19,21	0.64	0
6	NAG	E	19	1,6	14,14,15	0.51	0	15,19,21	0.72	0
6	NAG	E	20	6	14,14,15	0.55	0	15,19,21	0.52	0
6	NAG	E	21	1,6	14,14,15	0.60	0	15,19,21	0.71	0
6	NAG	E	22	6	14,14,15	0.51	0	15,19,21	0.58	0
6	NAG	G	24	2,6	14,14,15	0.53	0	15,19,21	0.66	0
6	NAG	G	25	6	14,14,15	0.47	0	15,19,21	0.53	0
6	NAG	H	530	1,6	14,14,15	0.53	0	15,19,21	0.61	0
6	NAG	H	531	6	14,14,15	0.47	0	15,19,21	0.56	0
6	NAG	H	532	1,6	14,14,15	0.61	0	15,19,21	0.89	1 (6%)
6	NAG	H	533	6	14,14,15	0.47	0	15,19,21	0.56	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	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
3	BMA	A	3	3	-	0/2/19/22	0/1/1/1
3	NAG	A	4	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	5	3	-	0/6/23/26	0/1/1/1
3	BMA	A	6	3	-	0/2/19/22	0/1/1/1
5	BMA	B	10	5	-	0/2/19/22	0/1/1/1
5	NDG	B	8	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	9	5	-	0/6/23/26	0/1/1/1
6	NAG	C	11	2,6	-	0/6/23/26	0/1/1/1
6	NAG	C	12	6	-	0/6/23/26	0/1/1/1
3	NAG	D	13	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	14	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	D	15	3	-	0/2/19/22	0/1/1/1
6	NAG	D	17	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	18	6	-	0/6/23/26	0/1/1/1
6	NAG	E	19	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	20	6	-	0/6/23/26	0/1/1/1
6	NAG	E	21	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	22	6	-	0/6/23/26	0/1/1/1
6	NAG	G	24	2,6	-	0/6/23/26	0/1/1/1
6	NAG	G	25	6	-	0/6/23/26	0/1/1/1
6	NAG	H	530	1,6	-	0/6/23/26	0/1/1/1
6	NAG	H	531	6	-	0/6/23/26	0/1/1/1
6	NAG	H	532	1,6	-	0/6/23/26	0/1/1/1
6	NAG	H	533	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	15	BMA	C1-C2-C3	2.01	111.91	109.54
3	D	13	NAG	C3-C4-C5	2.01	113.69	110.20
6	H	532	NAG	C3-C4-C5	2.05	113.77	110.20
3	A	5	NAG	C4-C3-C2	2.06	114.43	111.23
3	D	13	NAG	C1-O5-C5	2.30	115.17	112.25
3	A	6	BMA	C1-O5-C5	2.42	115.32	112.25
6	D	17	NAG	C4-C3-C2	2.46	115.05	111.23
5	B	8	NDG	C4-C3-C2	2.90	115.74	111.23
5	B	10	BMA	C1-C2-C3	2.95	113.03	109.54
3	A	6	BMA	C1-C2-C3	4.03	114.31	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	8	NDG	1	0
3	D	13	NAG	1	0
3	D	14	NAG	1	0
6	D	17	NAG	1	0
6	E	21	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	532	NAG	2	0
6	H	533	NAG	2	0

## 5.6 Ligand geometry

8 ligands 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	$\# Z  > 2$
4	NAG	A	707	1	14,14,15	0.47	0	15,19,21	0.59	0
7	SO4	A	708	-	4,4,4	0.27	0	6,6,6	0.06	0
4	NAG	D	716	1	14,14,15	0.53	0	15,19,21	0.74	0
7	SO4	D	717	-	4,4,4	0.23	0	6,6,6	0.06	0
4	NAG	E	723	2	14,14,15	0.45	0	15,19,21	0.62	0
4	NAG	G	726	2	14,14,15	0.50	0	15,19,21	0.55	0
7	SO4	H	534	-	4,4,4	0.26	0	6,6,6	0.08	0
7	SO4	H	535	-	4,4,4	0.23	0	6,6,6	0.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	707	1	-	0/6/23/26	0/1/1/1
7	SO4	A	708	-	-	0/0/0/0	0/0/0/0
4	NAG	D	716	1	-	0/6/23/26	0/1/1/1
7	SO4	D	717	-	-	0/0/0/0	0/0/0/0
4	NAG	E	723	2	-	0/6/23/26	0/1/1/1
4	NAG	G	726	2	-	0/6/23/26	0/1/1/1
7	SO4	H	534	-	-	0/0/0/0	0/0/0/0
7	SO4	H	535	-	-	0/0/0/0	0/0/0/0

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
7	H	534	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	492/507 (97%)	0.31	12 (2%)	62	50	17, 59, 80, 87	0
1	D	492/507 (97%)	0.30	19 (3%)	43	31	21, 61, 81, 89	0
1	E	492/507 (97%)	0.49	37 (7%)	17	9	17, 61, 82, 90	0
1	H	492/507 (97%)	0.36	26 (5%)	30	20	17, 61, 81, 88	0
2	B	480/507 (94%)	0.34	18 (3%)	44	32	26, 63, 76, 84	0
2	C	481/507 (94%)	0.29	12 (2%)	61	48	26, 61, 75, 85	0
2	F	480/507 (94%)	0.41	20 (4%)	40	28	27, 64, 76, 83	0
2	G	480/507 (94%)	0.32	18 (3%)	44	32	17, 62, 77, 82	0
All	All	3889/4056 (95%)	0.35	162 (4%)	40	28	17, 62, 78, 90	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	317	ASP	6.5
2	C	316	LEU	6.4
2	C	311	SER	5.9
1	E	279	SER	5.7
2	G	317	ASP	5.6
2	G	311	SER	5.3
1	E	396	ILE	5.1
1	D	102	PRO	5.1
1	A	89	THR	4.4
2	B	373	GLN	4.4
1	E	102	PRO	4.4
1	H	101	THR	4.3
2	C	317	ASP	4.3
1	H	281	SER	4.2
1	E	355	TYR	4.2
1	H	528	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
2	G	310	TYR	4.1
1	A	43	ASN	4.0
1	E	351	LEU	4.0
2	B	325	THR	3.9
1	E	328	CYS	3.7
1	H	282	GLU	3.7
1	D	285	GLY	3.6
1	H	283	PRO	3.6
1	E	370	TYR	3.6
1	E	284	SER	3.6
2	G	399	ASN	3.4
1	A	101	THR	3.4
2	G	318	SER	3.4
1	H	365	SER	3.3
1	H	338	PHE	3.2
2	C	183	SER	3.2
1	H	89	THR	3.1
2	B	107	GLY	3.1
1	A	93	ASN	3.1
2	F	54	PRO	3.1
2	B	83	PRO	3.1
2	C	310	TYR	3.0
1	E	327	THR	3.0
1	H	346	GLU	3.0
2	F	440	GLY	2.9
2	F	475	GLN	2.9
1	E	337	ASP	2.9
2	G	107	GLY	2.9
2	G	65	MET	2.9
1	E	443	GLU	2.9
1	D	104	CYS	2.9
1	E	283	PRO	2.9
1	D	336	GLN	2.8
1	H	279	SER	2.8
1	H	278	TYR	2.8
1	H	370	TYR	2.8
1	D	340	ARG	2.8
1	E	286	THR	2.7
2	F	87	ALA	2.7
2	F	474	THR	2.7
1	A	283	PRO	2.7
1	E	171	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	134	GLN	2.7
2	F	125	GLN	2.7
2	B	309	CYS	2.7
1	H	335	ILE	2.7
2	F	479	GLN	2.7
2	G	122	THR	2.6
2	F	473	GLY	2.6
1	A	216	PHE	2.6
2	F	180	TYR	2.6
2	F	522	MET	2.6
2	C	134	GLN	2.6
1	E	334	GLU	2.6
2	G	362	GLU	2.6
1	E	269	GLY	2.6
1	E	282	GLU	2.6
2	G	83	PRO	2.6
2	F	122	THR	2.6
2	C	136	GLU	2.6
1	E	399	ASN	2.5
1	A	102	PRO	2.5
1	E	300	PHE	2.5
1	H	280	GLY	2.5
1	H	284	SER	2.5
2	B	431	GLU	2.5
1	E	347	ASP	2.5
1	H	327	THR	2.5
1	A	284	SER	2.4
1	D	295	ASN	2.4
1	D	350	GLN	2.4
1	E	455	GLY	2.4
2	B	368	GLN	2.4
2	G	308	PRO	2.4
1	D	406	LEU	2.4
1	E	31	GLN	2.4
2	B	367	ILE	2.4
2	G	476	LYS	2.4
1	E	383	ILE	2.4
1	E	458	CYS	2.4
1	H	293	SER	2.4
2	G	364	ASN	2.4
2	G	71	HIS	2.4
1	A	279	SER	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	447	GLU	2.3
2	B	317	ASP	2.3
1	D	397	PRO	2.3
1	D	281	SER	2.3
2	B	371	MET	2.3
2	B	161	LYS	2.3
1	E	395	ASP	2.3
1	E	280	GLY	2.3
2	F	163	ASN	2.3
1	A	282	GLU	2.3
1	H	276	PRO	2.3
1	E	348	PHE	2.3
1	D	282	GLU	2.3
2	C	413	ALA	2.3
2	B	310	TYR	2.3
1	A	31	GLN	2.2
1	D	103	GLY	2.2
1	E	344	PHE	2.2
1	D	255	ALA	2.2
1	H	336	GLN	2.2
2	F	480	LEU	2.2
2	G	69	LEU	2.2
2	B	237	HIS	2.2
2	C	364	ASN	2.2
1	D	299	GLU	2.2
1	H	50	VAL	2.2
1	H	326	PHE	2.2
2	B	365	PRO	2.2
1	E	285	GLY	2.2
1	E	330	LYS	2.2
2	C	161	LYS	2.2
2	G	357	GLU	2.2
2	C	427	SER	2.2
2	B	311	SER	2.2
1	H	382	LYS	2.2
1	D	101	THR	2.2
2	B	84	ASN	2.2
2	F	68	ASN	2.2
2	C	478	LYS	2.1
2	G	303	LYS	2.1
2	F	132	THR	2.1
1	H	200	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	93	ASN	2.1
2	B	78	TYR	2.1
1	E	498	GLU	2.1
1	E	277	CYS	2.1
1	H	122	ASP	2.1
2	B	420	ILE	2.1
1	A	104	CYS	2.1
1	H	350	GLN	2.1
2	F	181	GLN	2.1
2	F	441	PHE	2.0
1	E	224	LYS	2.0
1	D	319	LEU	2.0
1	E	381	VAL	2.0
2	F	195	ILE	2.0
1	D	354	PHE	2.0
1	E	352	GLU	2.0
1	H	104	CYS	2.0
1	D	50	VAL	2.0
1	E	276	PRO	2.0
2	G	135	SER	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	NAG	E	21	14/15	0.88	0.24	2.02	70,74,80,89	0
6	NAG	C	11	14/15	0.90	0.28	0.90	70,74,80,89	0
5	NDG	B	8	14/15	0.86	0.23	0.38	70,74,80,89	0
3	NAG	A	4	14/15	0.88	0.23	-0.27	70,74,80,89	0
6	NAG	D	17	14/15	0.86	0.18	-0.65	70,74,80,89	0
6	NAG	G	24	14/15	0.90	0.22	-0.78	70,74,80,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	H	532	14/15	0.93	0.13	-1.37	66,71,74,79	0
3	NAG	A	2	14/15	0.73	0.21	-	110,117,118,119	0
6	NAG	H	530	14/15	0.84	0.25	-	70,74,80,89	0
3	BMA	A	3	11/12	0.80	0.32	-	55,58,64,65	0
6	NAG	E	20	14/15	0.76	0.24	-	110,117,118,119	0
3	BMA	D	15	11/12	0.72	0.36	-	55,58,64,65	0
6	NAG	C	12	14/15	0.70	0.48	-	110,117,118,119	0
5	NAG	B	9	14/15	0.73	0.31	-	110,117,118,119	0
3	NAG	A	5	14/15	0.66	0.28	-	110,117,118,119	0
3	NAG	A	1	14/15	0.87	0.19	-	70,74,80,89	0
6	NAG	G	25	14/15	0.59	0.33	-	110,117,118,119	0
3	NAG	D	13	14/15	0.86	0.22	-	70,74,80,89	0
6	NAG	H	533	14/15	0.82	0.21	-	91,94,95,96	0
3	NAG	D	14	14/15	0.80	0.27	-	110,117,118,119	0
5	BMA	B	10	11/12	0.72	0.38	-	55,58,64,65	0
6	NAG	D	18	14/15	0.75	0.37	-	110,117,118,119	0
6	NAG	E	22	14/15	0.73	0.29	-	110,117,118,119	0
6	NAG	E	19	14/15	0.84	0.23	-	70,74,80,89	0
6	NAG	H	531	14/15	0.71	0.26	-	110,117,118,119	0
3	BMA	A	6	11/12	0.60	0.35	-	55,58,64,65	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
7	SO4	A	708	5/5	0.93	0.34	5.06	104,104,105,106	0
7	SO4	D	717	5/5	0.90	0.31	2.21	104,104,105,106	0
7	SO4	H	535	5/5	0.86	0.25	0.92	104,104,105,106	0
7	SO4	H	534	5/5	0.93	0.25	0.57	104,104,105,106	0
4	NAG	E	723	14/15	0.87	0.21	-0.82	70,74,80,89	0
4	NAG	D	716	14/15	0.61	0.42	-	120,122,122,122	0
4	NAG	A	707	14/15	0.72	0.41	-	90,94,95,95	0
4	NAG	G	726	14/15	0.81	0.26	-	70,74,80,89	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.