



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:47 AM GMT

PDB ID : 3KBH
Title : Crystal structure of NL63 respiratory coronavirus receptor-binding domain complexed with its human receptor
Authors : Wu, K.; Li, W.; Peng, G.; Li, F.
Deposited on : 2009-10-20
Resolution : 3.31 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

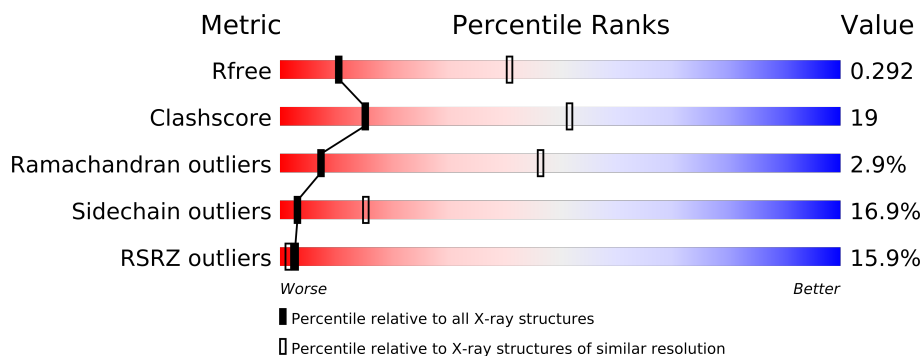
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.31 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}	66092	1372 (3.44-3.20)
Clashscore	79885	1016 (3.42-3.22)
Ramachandran outliers	78287	1699 (3.44-3.20)
Sidechain outliers	78261	1697 (3.44-3.20)
RSRZ outliers	66119	1373 (3.44-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	597	
1	B	597	
1	C	597	
1	D	597	
2	E	136	
2	F	136	
2	G	136	
2	H	136	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23024 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Angiotensin-convertingenzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	0	0
			4840	3095	802	914	29			
1	B	593	Total	C	N	O	S	0	0	0
			4840	3095	802	914	29			
1	C	593	Total	C	N	O	S	0	0	0
			4840	3095	802	914	29			
1	D	593	Total	C	N	O	S	0	0	0
			4840	3095	802	914	29			

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	110	Total	C	N	O	S	0	0	0
			860	551	142	161	6			
2	F	110	Total	C	N	O	S	0	0	0
			860	551	142	161	6			
2	G	110	Total	C	N	O	S	0	0	0
			860	551	142	161	6			
2	H	110	Total	C	N	O	S	0	0	0
			860	551	142	161	6			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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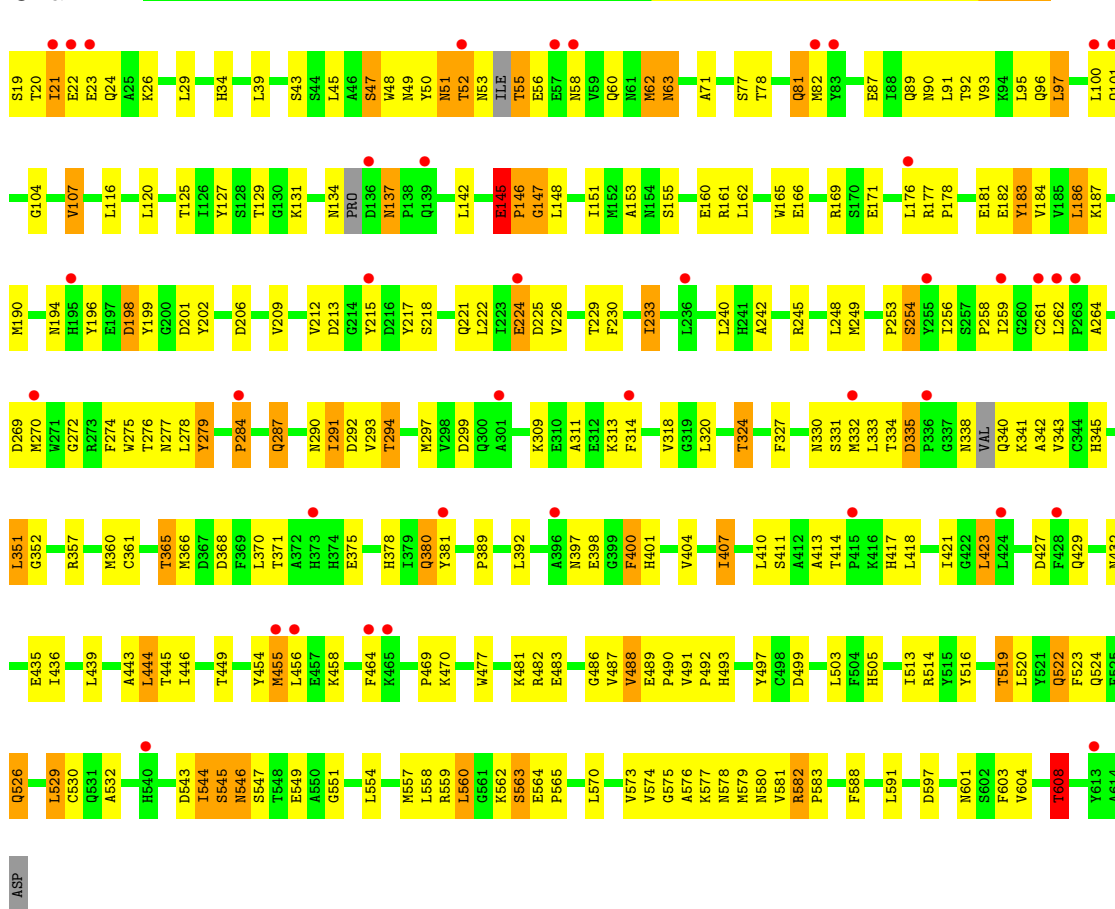
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		

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.

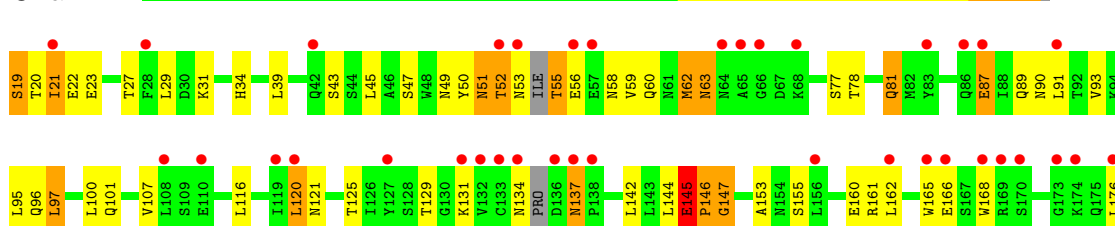
• Molecule 1: Angiotensin-convertingenzyme 2

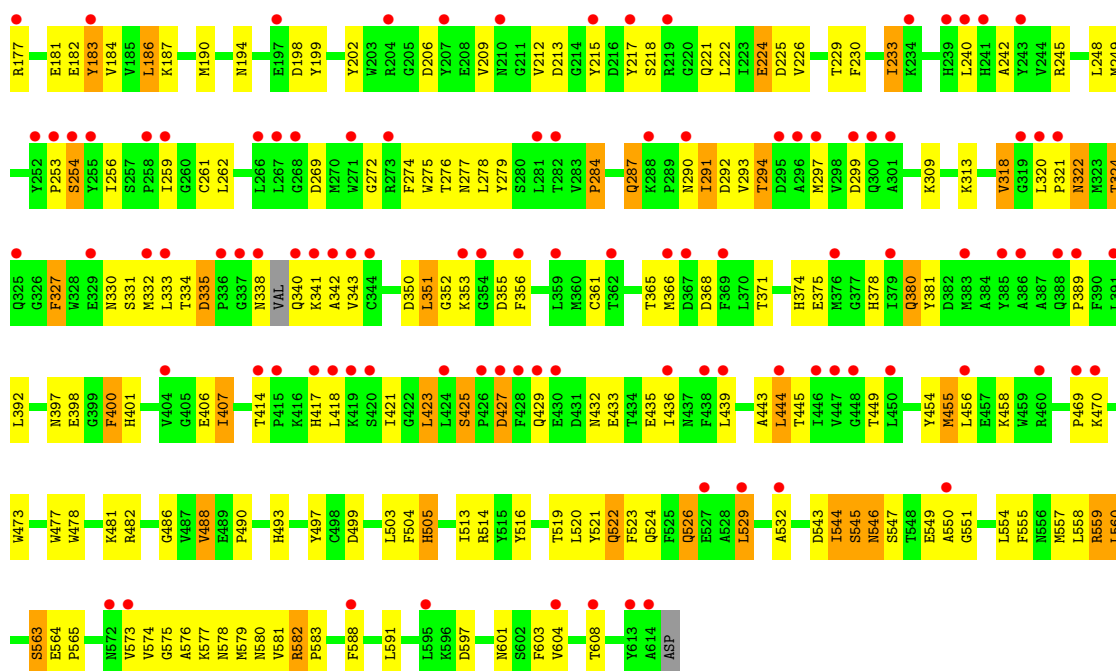
Chain A:



• Molecule 1: Angiotensin-convertingenzyme 2

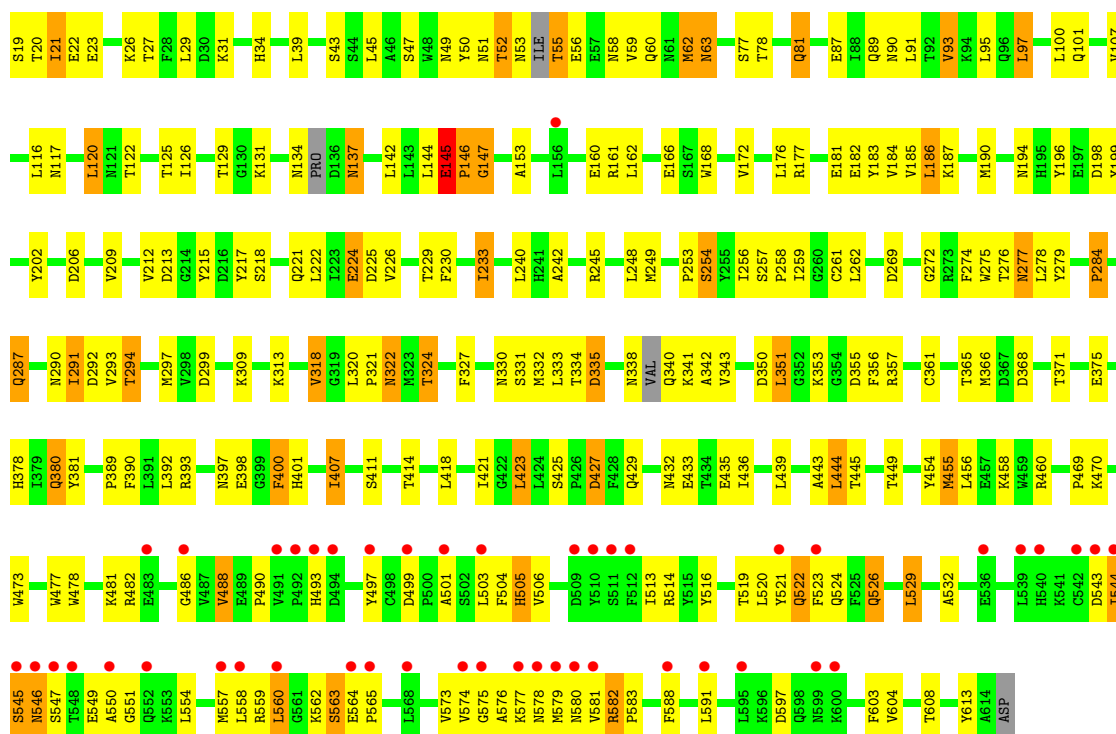
Chain B:





• Molecule 1: Angiotensin-convertingenzyme 2

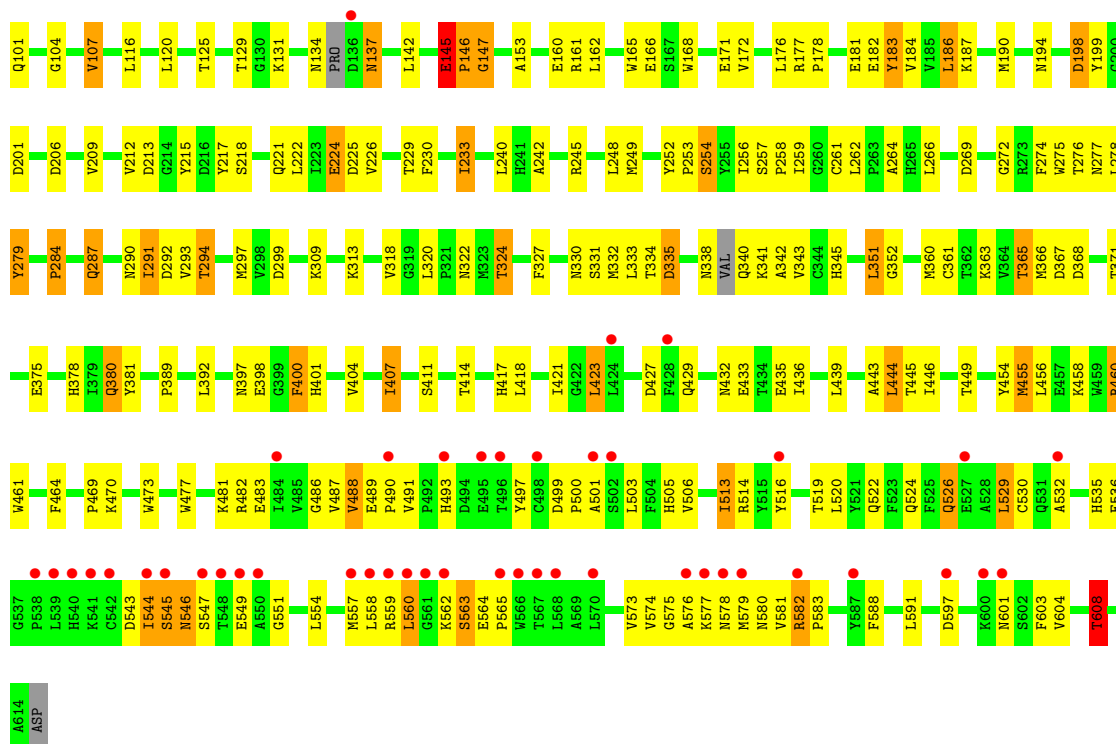
Chain C:



• Molecule 1: Angiotensin-convertingenzyme 2

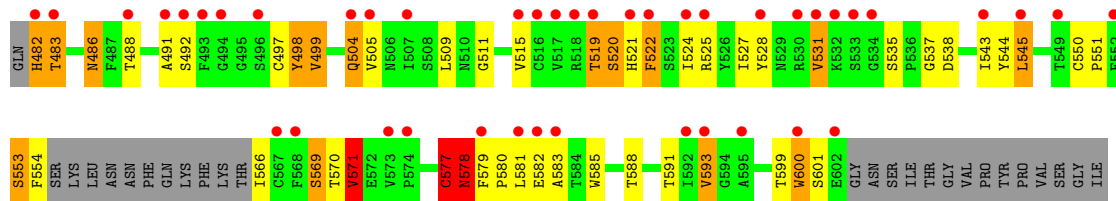
Chain D:





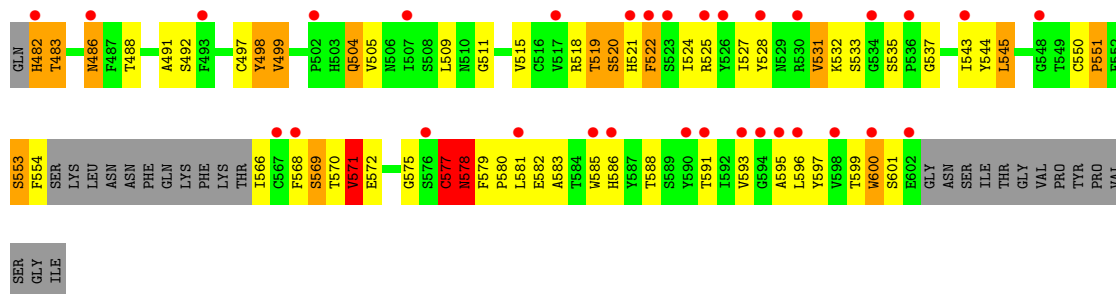
• Molecule 2: Spike glycoprotein

Chain E:



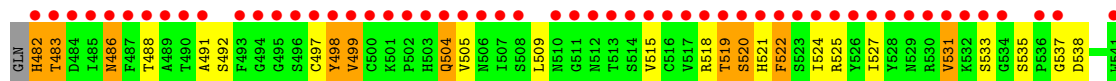
• Molecule 2: Spike glycoprotein

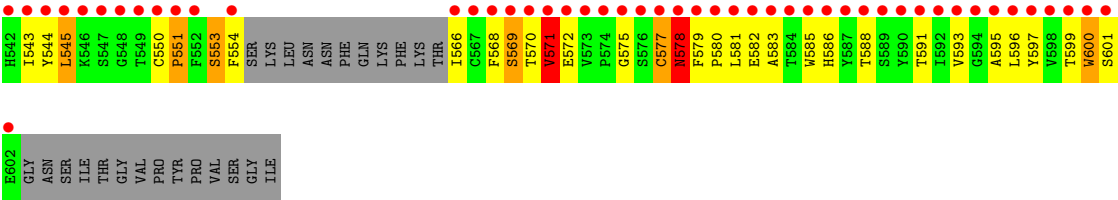
Chain F:



• Molecule 2: Spike glycoprotein

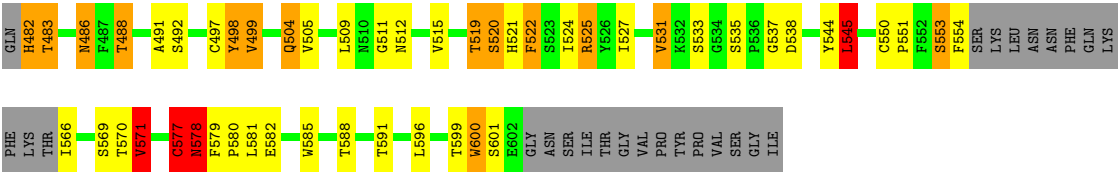
Chain G:





● Molecule 2: Spike glycoprotein

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	77.76Å 77.76Å 631.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.01 – 3.31 49.00 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.01-3.31) 88.4 (49.00-3.21)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.268 , 0.300 0.270 , 0.292	Depositor DCC
R_{free} test set	2715 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.793	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 103.1	EDS
Estimated twinning fraction	0.428 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 60292 reflections	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	23024	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.67	0/4973	0.73	0/6750
1	B	0.65	1/4973 (0.0%)	0.71	0/6750
1	C	0.64	1/4973 (0.0%)	0.71	0/6750
1	D	0.66	1/4973 (0.0%)	0.73	1/6750 (0.0%)
2	E	0.86	0/888	0.92	1/1212 (0.1%)
2	F	0.78	0/888	0.90	1/1212 (0.1%)
2	G	0.75	0/888	0.88	0/1212
2	H	0.85	0/888	0.92	2/1212 (0.2%)
All	All	0.68	3/23444 (0.0%)	0.75	5/31848 (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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
2	E	0	2
2	F	0	2
2	G	0	2
2	H	0	1
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	59	VAL	CA-CB	6.04	1.67	1.54
1	C	59	VAL	CA-CB	5.67	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	51	ASN	CB-CG	5.67	1.64	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	577	CYS	CA-CB-SG	5.90	124.61	114.00
2	H	577	CYS	CA-CB-SG	5.54	123.97	114.00
1	D	460	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	F	577	CYS	CA-CB-SG	5.13	123.24	114.00
2	H	545	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	GLU	Peptide
1	B	145	GLU	Peptide
1	C	145	GLU	Peptide
1	D	145	GLU	Peptide
2	E	520	SER	Peptide
2	E	569	SER	Peptide
2	F	520	SER	Peptide
2	F	569	SER	Peptide
2	G	520	SER	Peptide
2	G	569	SER	Peptide
2	H	520	SER	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4840	0	4607	173	2
1	B	4840	0	4607	162	0
1	C	4840	0	4607	162	0
1	D	4840	0	4607	174	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	860	0	797	47	0
2	F	860	0	797	50	2
2	G	860	0	797	44	2
2	H	860	0	797	43	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
3	E	28	0	26	1	0
3	F	28	0	26	1	0
3	G	28	0	26	0	0
3	H	28	0	26	1	0
All	All	23024	0	21824	847	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (847) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:483:THR:HG22	2:G:519:THR:HG23	1.30	1.14
2:E:483:THR:HG22	2:E:519:THR:HG23	1.27	1.13
1:D:51:ASN:HD22	1:D:343:VAL:HG22	1.13	1.10
1:B:145:GLU:HA	1:B:145:GLU:OE1	1.51	1.08
2:H:483:THR:HG22	2:H:519:THR:HG23	1.28	1.07
2:F:483:THR:HG22	2:F:519:THR:HG23	1.35	1.07
1:D:51:ASN:ND2	1:D:343:VAL:HG22	1.70	1.06
1:C:145:GLU:HA	1:C:145:GLU:OE1	1.56	1.06
1:B:53:ASN:O	1:B:55:THR:N	1.89	1.05
2:G:498:TYR:O	2:G:499:VAL:HB	1.55	1.05
1:B:51:ASN:ND2	1:B:343:VAL:HG22	1.75	1.01
2:E:498:TYR:O	2:E:499:VAL:HB	1.56	1.01
2:F:498:TYR:O	2:F:499:VAL:HB	1.57	1.00
2:E:483:THR:HG22	2:E:519:THR:CG2	1.92	0.99
2:H:498:TYR:O	2:H:499:VAL:HB	1.60	0.99
2:H:483:THR:HG22	2:H:519:THR:CG2	1.91	0.98
1:A:51:ASN:HD22	1:A:343:VAL:HG22	1.25	0.98
1:A:145:GLU:HA	1:A:145:GLU:OE1	1.61	0.98
2:G:483:THR:HG22	2:G:519:THR:CG2	1.94	0.98
1:A:51:ASN:ND2	1:A:343:VAL:HG22	1.78	0.97
1:C:51:ASN:ND2	1:C:343:VAL:HG22	1.80	0.97
1:B:81:GLN:HA	1:B:81:GLN:HE21	1.29	0.95
2:F:483:THR:HG22	2:F:519:THR:CG2	1.97	0.95

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:578:ASN:H	2:E:578:ASN:HD22	1.14	0.94
1:D:560:LEU:O	1:D:563:SER:HB3	1.68	0.93
2:H:578:ASN:H	2:H:578:ASN:HD22	1.17	0.93
1:D:145:GLU:OE1	1:D:145:GLU:HA	1.67	0.92
1:C:53:ASN:O	1:C:55:THR:N	2.01	0.91
1:C:81:GLN:HA	1:C:81:GLN:HE21	1.31	0.91
1:B:161:ARG:HH12	1:B:278:LEU:HD22	1.34	0.90
1:C:161:ARG:HH12	1:C:278:LEU:HD22	1.36	0.90
1:D:81:GLN:HE21	1:D:81:GLN:HA	1.36	0.89
1:A:81:GLN:HE21	1:A:81:GLN:HA	1.37	0.89
1:B:51:ASN:HD22	1:B:343:VAL:HG22	1.34	0.87
1:A:229:THR:HG23	1:A:516:TYR:OH	1.75	0.87
1:A:560:LEU:O	1:A:563:SER:HB3	1.75	0.86
2:G:578:ASN:HD22	2:G:578:ASN:H	1.22	0.85
1:C:560:LEU:O	1:C:563:SER:HB3	1.76	0.85
2:F:553:SER:O	2:F:554:PHE:HB2	1.77	0.85
1:D:53:ASN:O	1:D:55:THR:N	2.10	0.84
1:A:161:ARG:HH12	1:A:278:LEU:HD22	1.40	0.84
2:H:483:THR:CG2	2:H:519:THR:HG23	2.06	0.84
2:E:483:THR:CG2	2:E:519:THR:HG23	2.07	0.84
1:B:153:ALA:HA	1:B:277:ASN:OD1	1.78	0.83
2:F:578:ASN:H	2:F:578:ASN:HD22	1.23	0.83
1:C:51:ASN:HD22	1:C:343:VAL:HG22	1.38	0.83
1:C:153:ALA:HA	1:C:277:ASN:OD1	1.78	0.83
1:C:21:ILE:HD13	1:C:21:ILE:H	1.43	0.82
2:G:553:SER:O	2:G:554:PHE:HB2	1.78	0.82
1:D:327:PHE:O	1:D:331:SER:HB2	1.80	0.82
1:A:53:ASN:O	1:A:55:THR:N	2.12	0.82
1:D:229:THR:HG23	1:D:516:TYR:OH	1.80	0.81
2:G:483:THR:CG2	2:G:519:THR:HG23	2.10	0.81
1:C:327:PHE:O	1:C:331:SER:HB2	1.80	0.81
1:B:560:LEU:O	1:B:563:SER:HB3	1.80	0.81
1:B:97:LEU:O	1:B:101:GLN:HG2	1.80	0.81
1:D:21:ILE:H	1:D:21:ILE:HD13	1.45	0.80
1:A:327:PHE:O	1:A:331:SER:HB2	1.82	0.80
1:A:153:ALA:HA	1:A:277:ASN:OD1	1.82	0.80
1:A:183:TYR:O	1:A:187:LYS:HB2	1.82	0.79
1:B:21:ILE:H	1:B:21:ILE:HD13	1.45	0.79
1:A:493:HIS:HD2	1:A:499:ASP:OD1	1.65	0.79
1:C:183:TYR:O	1:C:187:LYS:HB2	1.82	0.79
1:A:21:ILE:HD13	1:A:21:ILE:H	1.45	0.79
2:E:553:SER:O	2:E:554:PHE:HB2	1.80	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:217:TYR:HE1	1:B:578:ASN:ND2	1.81	0.79
1:D:153:ALA:HA	1:D:277:ASN:OD1	1.82	0.79
2:G:566:ILE:HG12	2:G:600:TRP:HA	1.65	0.79
1:B:183:TYR:O	1:B:187:LYS:HB2	1.83	0.78
1:A:97:LEU:O	1:A:101:GLN:HG2	1.83	0.78
1:C:97:LEU:O	1:C:101:GLN:HG2	1.82	0.77
1:D:183:TYR:O	1:D:187:LYS:HB2	1.85	0.77
2:F:566:ILE:HG12	2:F:600:TRP:HA	1.66	0.77
1:D:161:ARG:HH12	1:D:278:LEU:HD22	1.49	0.77
1:D:62:MET:HG3	1:D:63:ASN:N	2.00	0.76
1:D:97:LEU:O	1:D:101:GLN:HG2	1.84	0.76
1:B:327:PHE:O	1:B:331:SER:HB2	1.86	0.75
2:H:553:SER:O	2:H:554:PHE:HB2	1.85	0.75
1:A:493:HIS:CD2	1:A:499:ASP:OD1	2.40	0.74
1:D:493:HIS:HD2	1:D:499:ASP:OD1	1.68	0.74
2:E:566:ILE:HG12	2:E:600:TRP:HA	1.70	0.74
1:A:524:GLN:NE2	1:A:580:ASN:H	1.86	0.73
1:C:544:ILE:O	1:C:547:SER:HB2	1.87	0.73
1:D:407:ILE:HD11	1:D:529:LEU:HD22	1.70	0.73
1:C:162:LEU:CD1	1:C:490:PRO:HB2	2.18	0.73
2:H:486:ASN:HB3	2:H:527:ILE:HD12	1.70	0.73
2:E:486:ASN:HB3	2:E:527:ILE:HD12	1.70	0.73
2:F:483:THR:CG2	2:F:519:THR:HG23	2.16	0.73
2:G:491:ALA:O	2:G:531:VAL:HG22	1.89	0.72
1:A:62:MET:HG3	1:A:63:ASN:N	2.03	0.72
1:B:218:SER:HB3	1:B:221:GLN:HB2	1.71	0.72
1:D:524:GLN:NE2	1:D:580:ASN:H	1.87	0.72
1:B:162:LEU:CD1	1:B:490:PRO:HB2	2.19	0.72
1:A:182:GLU:O	1:A:186:LEU:HD12	1.90	0.72
1:C:217:TYR:HE1	1:C:578:ASN:ND2	1.86	0.71
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.70	0.71
1:B:545:SER:O	1:B:546:ASN:HB2	1.90	0.71
1:B:493:HIS:HD2	1:B:499:ASP:OD1	1.73	0.71
1:C:245:ARG:HB3	1:C:262:LEU:HD21	1.72	0.71
1:B:229:THR:HG23	1:B:516:TYR:OH	1.90	0.71
1:B:245:ARG:HB3	1:B:262:LEU:HD21	1.70	0.71
2:H:566:ILE:HG12	2:H:600:TRP:HA	1.72	0.71
1:A:245:ARG:HB3	1:A:262:LEU:HD21	1.72	0.71
1:D:574:VAL:HG23	1:D:576:ALA:H	1.56	0.70
1:D:524:GLN:HG2	1:D:583:PRO:HG2	1.74	0.70
1:C:229:THR:HG23	1:C:516:TYR:OH	1.91	0.70
1:A:233:ILE:HD13	1:A:233:ILE:O	1.92	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:574:VAL:HG23	1:A:576:ALA:H	1.54	0.70
1:A:162:LEU:CD1	1:A:490:PRO:HB2	2.22	0.70
1:D:493:HIS:CD2	1:D:499:ASP:OD1	2.44	0.70
1:C:524:GLN:HG2	1:C:583:PRO:HG2	1.72	0.70
2:G:488:THR:HG22	2:G:527:ILE:HB	1.72	0.70
2:E:488:THR:HG22	2:E:527:ILE:HB	1.72	0.70
1:C:493:HIS:HD2	1:C:499:ASP:OD1	1.74	0.70
1:C:218:SER:HB3	1:C:221:GLN:HB2	1.74	0.70
2:F:491:ALA:O	2:F:531:VAL:HG22	1.92	0.69
1:B:62:MET:HG3	1:B:63:ASN:N	2.06	0.69
1:A:601:ASN:ND2	1:C:254:SER:O	2.26	0.69
1:B:493:HIS:CD2	1:B:499:ASP:OD1	2.45	0.69
1:D:182:GLU:O	1:D:186:LEU:HD12	1.92	0.69
1:B:134:ASN:HB2	1:B:137:ASN:HB3	1.75	0.69
1:B:224:GLU:HG3	1:B:225:ASP:N	2.08	0.69
2:G:486:ASN:HB3	2:G:527:ILE:HD12	1.75	0.69
1:D:545:SER:O	1:D:546:ASN:HB2	1.93	0.69
1:C:574:VAL:HG23	1:C:576:ALA:H	1.58	0.69
1:B:161:ARG:NH1	1:B:278:LEU:HD22	2.08	0.68
1:C:134:ASN:HB2	1:C:137:ASN:HB3	1.76	0.68
1:D:245:ARG:HB3	1:D:262:LEU:HD21	1.75	0.68
1:B:544:ILE:O	1:B:547:SER:HB2	1.93	0.68
1:C:545:SER:O	1:C:546:ASN:HB2	1.92	0.68
1:B:297:MET:HG3	1:B:423:LEU:HD21	1.76	0.68
1:B:414:THR:HG21	1:B:543:ASP:HB2	1.76	0.68
1:D:290:ASN:ND2	1:D:292:ASP:HB2	2.09	0.67
1:B:574:VAL:HG23	1:B:576:ALA:H	1.59	0.67
1:C:224:GLU:HG3	1:C:225:ASP:N	2.10	0.67
1:A:545:SER:O	1:A:546:ASN:HB2	1.94	0.67
1:D:162:LEU:CD1	1:D:490:PRO:HB2	2.24	0.67
1:B:125:THR:O	1:B:129:THR:HG22	1.94	0.67
1:C:125:THR:O	1:C:129:THR:HG22	1.94	0.67
2:F:488:THR:HG22	2:F:527:ILE:HB	1.75	0.67
1:B:524:GLN:HG2	1:B:583:PRO:HG2	1.77	0.67
1:A:218:SER:HB3	1:A:221:GLN:HB2	1.76	0.67
1:A:293:VAL:HB	1:A:423:LEU:HD22	1.75	0.66
1:B:81:GLN:CA	1:B:81:GLN:HE21	2.02	0.66
1:D:217:TYR:HE1	1:D:578:ASN:ND2	1.93	0.66
1:D:134:ASN:HB2	1:D:137:ASN:HB3	1.77	0.66
1:C:297:MET:HG3	1:C:423:LEU:HD21	1.76	0.66
2:H:488:THR:HG22	2:H:527:ILE:HB	1.78	0.66
1:C:62:MET:HG3	1:C:63:ASN:N	2.09	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:60:GLN:HA	1:A:63:ASN:HD21	1.60	0.66
1:C:493:HIS:CD2	1:C:499:ASP:OD1	2.49	0.66
1:A:269:ASP:OD2	1:A:272:GLY:N	2.26	0.66
1:D:81:GLN:CA	1:D:81:GLN:HE21	2.08	0.66
1:C:375:GLU:O	1:C:378:HIS:HB2	1.97	0.65
2:F:486:ASN:HB3	2:F:527:ILE:HD12	1.77	0.65
1:B:233:ILE:HD13	1:B:233:ILE:O	1.96	0.65
1:C:91:LEU:HD12	1:C:91:LEU:H	1.61	0.65
1:D:297:MET:HG3	1:D:423:LEU:HD21	1.79	0.65
1:A:107:VAL:HG11	1:A:194:ASN:OD1	1.97	0.65
1:B:290:ASN:ND2	1:B:292:ASP:HB2	2.11	0.65
1:A:407:ILE:HD11	1:A:529:LEU:HD22	1.77	0.65
1:C:81:GLN:CA	1:C:81:GLN:HE21	2.02	0.65
1:A:505:HIS:CD2	1:A:505:HIS:H	2.12	0.65
1:A:290:ASN:ND2	1:A:292:ASP:HB2	2.12	0.65
2:E:578:ASN:N	2:E:578:ASN:HD22	1.90	0.65
1:D:293:VAL:HB	1:D:423:LEU:HD22	1.79	0.65
1:D:107:VAL:HG11	1:D:194:ASN:OD1	1.96	0.65
2:H:499:VAL:HG22	2:H:585:TRP:CD2	2.32	0.64
1:D:212:VAL:HG12	1:D:215:TYR:HB2	1.79	0.64
1:D:49:ASN:HB3	1:D:58:ASN:HD22	1.63	0.64
1:C:212:VAL:HG12	1:C:215:TYR:HB2	1.80	0.64
1:A:134:ASN:HB2	1:A:137:ASN:HB3	1.80	0.64
2:G:553:SER:O	2:G:554:PHE:CB	2.45	0.64
1:C:49:ASN:HB3	1:C:58:ASN:HD22	1.63	0.64
2:F:553:SER:O	2:F:554:PHE:CB	2.45	0.64
1:A:212:VAL:HG12	1:A:215:TYR:HB2	1.79	0.64
1:C:161:ARG:NH1	1:C:278:LEU:HD22	2.09	0.64
2:E:499:VAL:HG22	2:E:585:TRP:CD2	2.33	0.64
1:D:218:SER:HB3	1:D:221:GLN:HB2	1.79	0.64
1:C:230:PHE:HA	1:C:233:ILE:HG22	1.79	0.64
1:A:81:GLN:CA	1:A:81:GLN:HE21	2.08	0.63
2:F:499:VAL:HG22	2:F:585:TRP:CD2	2.34	0.63
1:A:261:CYS:HB3	1:A:486:GLY:C	2.18	0.63
1:A:297:MET:HG3	1:A:423:LEU:HD21	1.79	0.63
1:C:414:THR:HG21	1:C:543:ASP:HB2	1.80	0.63
1:B:261:CYS:HB3	1:B:486:GLY:C	2.19	0.63
1:D:505:HIS:H	1:D:505:HIS:CD2	2.17	0.63
2:E:545:LEU:HB3	2:E:581:LEU:HD12	1.81	0.63
2:H:545:LEU:HB3	2:H:581:LEU:HD12	1.81	0.63
1:A:60:GLN:O	1:A:63:ASN:OD1	2.17	0.63
1:C:334:THR:O	1:C:335:ASP:HB3	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:578:ASN:H	2:F:578:ASN:ND2	1.96	0.62
1:B:505:HIS:H	1:B:505:HIS:CD2	2.17	0.62
1:D:375:GLU:O	1:D:378:HIS:HB2	1.99	0.62
1:C:290:ASN:ND2	1:C:292:ASP:HB2	2.14	0.62
2:G:499:VAL:HG22	2:G:585:TRP:CD2	2.34	0.62
1:C:60:GLN:HA	1:C:63:ASN:HD21	1.64	0.62
1:B:439:LEU:HD23	1:B:591:LEU:HB2	1.81	0.62
1:B:142:LEU:HD22	1:B:147:GLY:HA2	1.81	0.62
2:F:492:SER:HA	2:F:531:VAL:HG23	1.79	0.62
1:D:400:PHE:O	1:D:404:VAL:HG23	2.00	0.62
2:H:553:SER:O	2:H:554:PHE:CB	2.48	0.62
1:A:177:ARG:NH1	1:A:470:LYS:O	2.30	0.62
1:A:544:ILE:O	1:A:547:SER:HB2	1.98	0.62
1:B:212:VAL:HG12	1:B:215:TYR:HB2	1.79	0.62
1:B:230:PHE:HA	1:B:233:ILE:HG22	1.80	0.62
1:D:230:PHE:HA	1:D:233:ILE:HG22	1.81	0.62
1:A:125:THR:O	1:A:129:THR:HG22	1.99	0.62
1:A:161:ARG:NH1	1:A:278:LEU:HD22	2.14	0.62
2:F:545:LEU:HB3	2:F:581:LEU:HD12	1.80	0.62
1:C:142:LEU:HD22	1:C:147:GLY:HA2	1.82	0.61
1:C:505:HIS:H	1:C:505:HIS:CD2	2.16	0.61
1:C:439:LEU:HD23	1:C:591:LEU:HB2	1.81	0.61
1:C:293:VAL:HB	1:C:423:LEU:HD22	1.82	0.61
1:B:334:THR:O	1:B:335:ASP:HB3	2.01	0.61
2:E:491:ALA:O	2:E:531:VAL:HG22	2.00	0.61
1:C:182:GLU:O	1:C:186:LEU:HD12	2.01	0.61
2:G:492:SER:HA	2:G:531:VAL:HG23	1.81	0.61
1:A:230:PHE:HA	1:A:233:ILE:HG22	1.82	0.61
1:D:233:ILE:O	1:D:233:ILE:HD13	2.00	0.61
2:G:545:LEU:HB3	2:G:581:LEU:HD12	1.81	0.61
1:D:60:GLN:HA	1:D:63:ASN:HD21	1.65	0.60
1:D:91:LEU:H	1:D:91:LEU:HD12	1.66	0.60
1:D:261:CYS:HB3	1:D:486:GLY:C	2.21	0.60
2:G:578:ASN:ND2	2:G:578:ASN:H	1.97	0.60
2:E:553:SER:O	2:E:554:PHE:CB	2.46	0.60
1:B:293:VAL:HB	1:B:423:LEU:HD22	1.82	0.60
2:E:492:SER:HA	2:E:531:VAL:HG23	1.83	0.60
1:D:125:THR:O	1:D:129:THR:HG22	2.01	0.60
1:D:334:THR:O	1:D:335:ASP:HB3	2.01	0.60
1:B:245:ARG:O	1:B:249:MET:HG3	2.02	0.60
2:E:482:HIS:CD2	2:E:483:THR:N	2.70	0.60
1:A:334:THR:O	1:A:335:ASP:HB3	2.02	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:222:LEU:O	1:C:226:VAL:HG23	2.02	0.60
1:B:91:LEU:H	1:B:91:LEU:HD12	1.66	0.59
1:B:107:VAL:HG11	1:B:194:ASN:OD1	2.02	0.59
1:C:327:PHE:O	1:C:331:SER:CB	2.50	0.59
1:D:60:GLN:O	1:D:63:ASN:OD1	2.20	0.59
2:H:491:ALA:O	2:H:531:VAL:HG22	2.02	0.59
1:D:51:ASN:ND2	1:D:343:VAL:CG2	2.57	0.59
1:A:166:GLU:OE2	1:A:497:TYR:OH	2.17	0.59
1:C:233:ILE:O	1:C:233:ILE:HD13	2.03	0.59
1:C:524:GLN:NE2	1:C:580:ASN:H	2.01	0.58
1:C:407:ILE:HD11	1:C:529:LEU:HD22	1.85	0.58
2:F:553:SER:HA	2:F:579:PHE:HE1	1.67	0.58
1:A:327:PHE:O	1:A:331:SER:CB	2.52	0.58
1:A:276:THR:HG23	1:A:445:THR:OG1	2.02	0.58
1:A:414:THR:HG21	1:A:543:ASP:HB2	1.85	0.58
1:C:177:ARG:NH1	1:C:470:LYS:O	2.37	0.58
1:A:224:GLU:HG3	1:A:225:ASP:N	2.18	0.58
1:C:397:ASN:OD1	1:C:400:PHE:HD1	1.87	0.58
2:G:578:ASN:O	2:G:580:PRO:HD3	2.03	0.58
1:D:327:PHE:O	1:D:331:SER:CB	2.50	0.58
2:G:553:SER:HA	2:G:579:PHE:HE1	1.68	0.57
1:A:217:TYR:HE1	1:A:578:ASN:ND2	2.02	0.57
1:B:226:VAL:HA	1:B:229:THR:HG22	1.86	0.57
1:A:389:PRO:HG2	1:A:392:LEU:HD22	1.85	0.57
1:B:375:GLU:O	1:B:378:HIS:HB2	2.04	0.57
2:H:578:ASN:O	2:H:580:PRO:HD3	2.05	0.57
1:D:544:ILE:O	1:D:547:SER:HB2	2.04	0.57
1:B:60:GLN:HA	1:B:63:ASN:HD21	1.70	0.57
1:C:162:LEU:HD13	1:C:490:PRO:HB2	1.87	0.57
1:C:335:ASP:HB2	1:C:361:CYS:SG	2.44	0.57
1:C:107:VAL:HG11	1:C:194:ASN:OD1	2.05	0.57
1:A:400:PHE:O	1:A:404:VAL:HG23	2.04	0.57
1:A:418:LEU:O	1:A:421:ILE:HG22	2.05	0.57
2:G:491:ALA:O	2:G:531:VAL:CG2	2.52	0.57
1:A:456:LEU:HD23	1:A:477:TRP:HH2	1.69	0.57
2:G:578:ASN:N	2:G:578:ASN:HD22	1.95	0.56
1:D:161:ARG:NH1	1:D:278:LEU:HD22	2.19	0.56
1:B:320:LEU:HD13	1:B:380:GLN:HG2	1.86	0.56
1:A:248:LEU:HB3	1:A:256:ILE:HD13	1.87	0.56
1:D:418:LEU:O	1:D:421:ILE:HG22	2.05	0.56
1:B:182:GLU:O	1:B:186:LEU:HD12	2.04	0.56
1:D:248:LEU:HB3	1:D:256:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:49:ASN:HB3	1:A:58:ASN:HD22	1.71	0.56
1:D:245:ARG:O	1:D:249:MET:HG3	2.05	0.56
1:C:261:CYS:HB3	1:C:486:GLY:C	2.25	0.56
2:E:553:SER:HA	2:E:579:PHE:HE1	1.71	0.56
1:B:162:LEU:HD13	1:B:490:PRO:HB2	1.87	0.56
1:C:226:VAL:HA	1:C:229:THR:HG22	1.86	0.56
1:A:226:VAL:HA	1:A:229:THR:HG22	1.86	0.56
1:B:217:TYR:CE1	1:B:578:ASN:ND2	2.70	0.56
1:D:389:PRO:HG2	1:D:392:LEU:HD22	1.87	0.56
2:H:482:HIS:CD2	2:H:483:THR:N	2.74	0.56
2:H:483:THR:CG2	2:H:519:THR:CG2	2.73	0.56
2:E:483:THR:CG2	2:E:519:THR:CG2	2.75	0.55
1:D:226:VAL:HA	1:D:229:THR:HG22	1.88	0.55
1:C:320:LEU:HD13	1:C:380:GLN:HG2	1.87	0.55
1:D:324:THR:O	1:D:327:PHE:HB3	2.06	0.55
1:B:60:GLN:O	1:B:63:ASN:OD1	2.25	0.55
1:A:187:LYS:HE3	1:A:199:TYR:CZ	2.42	0.55
1:B:327:PHE:O	1:B:331:SER:CB	2.55	0.55
2:E:550:CYS:HB2	2:E:551:PRO:CD	2.36	0.55
1:B:455:MET:SD	1:B:481:LYS:HG2	2.46	0.55
1:D:181:GLU:O	1:D:184:VAL:HG22	2.06	0.55
1:A:324:THR:O	1:A:327:PHE:HB3	2.06	0.55
2:E:482:HIS:CD2	2:E:522:PHE:HA	2.42	0.55
1:C:324:THR:O	1:C:327:PHE:HB3	2.07	0.55
1:C:90:ASN:HB3	1:C:93:VAL:HG13	1.88	0.55
2:G:483:THR:CG2	2:G:519:THR:CG2	2.77	0.55
1:D:224:GLU:HG3	1:D:225:ASP:N	2.21	0.55
1:C:454:TYR:OH	1:C:458:LYS:HD3	2.07	0.55
1:A:580:ASN:HD21	1:A:582:ARG:HH12	1.52	0.55
1:D:414:THR:HG21	1:D:543:ASP:HB2	1.89	0.55
1:D:177:ARG:NH1	1:D:470:LYS:O	2.37	0.55
1:A:253:PRO:O	1:A:254:SER:HB2	2.06	0.55
1:D:455:MET:SD	1:D:481:LYS:HG2	2.46	0.55
2:H:553:SER:HA	2:H:579:PHE:HE1	1.72	0.55
1:A:51:ASN:HB3	1:A:342:ALA:HB1	1.89	0.54
2:G:504:GLN:HG2	2:G:505:VAL:N	2.22	0.54
1:C:580:ASN:HD21	1:C:582:ARG:HH12	1.56	0.54
1:A:397:ASN:OD1	1:A:400:PHE:HD1	1.90	0.54
1:B:318:VAL:O	1:B:551:GLY:HA3	2.08	0.54
2:E:578:ASN:ND2	2:E:578:ASN:H	1.95	0.54
2:G:482:HIS:HD2	2:G:522:PHE:HA	1.73	0.54
2:F:566:ILE:HA	2:F:599:THR:O	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:550:CYS:HB2	2:H:551:PRO:CD	2.38	0.54
1:C:353:LYS:HA	2:G:498:TYR:CD2	2.42	0.54
1:D:187:LYS:HE3	1:D:199:TYR:CZ	2.43	0.54
1:B:524:GLN:NE2	1:B:580:ASN:H	2.06	0.54
1:A:181:GLU:O	1:A:184:VAL:HG22	2.08	0.54
1:B:177:ARG:NH1	1:B:470:LYS:O	2.38	0.54
1:A:162:LEU:HD11	1:A:490:PRO:HB2	1.90	0.54
1:A:351:LEU:H	1:A:351:LEU:HD12	1.72	0.54
2:H:578:ASN:H	2:H:578:ASN:ND2	1.97	0.54
2:F:553:SER:HA	2:F:579:PHE:CE1	2.43	0.54
1:C:269:ASP:OD2	1:C:272:GLY:N	2.35	0.54
2:H:492:SER:HA	2:H:531:VAL:HG23	1.90	0.53
1:C:245:ARG:O	1:C:249:MET:HG3	2.08	0.53
1:B:116:LEU:O	1:B:120:LEU:HD12	2.08	0.53
1:B:580:ASN:HD21	1:B:582:ARG:HH12	1.56	0.53
1:B:90:ASN:HB3	1:B:93:VAL:HG13	1.90	0.53
2:G:566:ILE:HA	2:G:599:THR:O	2.09	0.53
1:C:60:GLN:O	1:C:63:ASN:OD1	2.27	0.53
1:B:397:ASN:OD1	1:B:400:PHE:HD1	1.90	0.53
2:E:600:TRP:O	2:E:600:TRP:HE3	1.92	0.53
1:A:455:MET:SD	1:A:481:LYS:HG2	2.49	0.53
1:B:335:ASP:HB2	1:B:361:CYS:SG	2.48	0.53
1:B:276:THR:HG23	1:B:445:THR:OG1	2.08	0.53
1:A:116:LEU:O	1:A:120:LEU:HD12	2.09	0.53
1:C:389:PRO:HG2	1:C:392:LEU:HD22	1.90	0.53
1:C:162:LEU:HD11	1:C:490:PRO:HB2	1.90	0.53
1:A:365:THR:HB	1:A:368:ASP:H	1.73	0.53
1:C:455:MET:SD	1:C:481:LYS:HG2	2.49	0.53
1:D:51:ASN:HB3	1:D:342:ALA:HB1	1.90	0.53
2:E:578:ASN:O	2:E:580:PRO:HD3	2.08	0.53
1:D:96:GLN:HG2	1:D:392:LEU:HD11	1.91	0.53
1:D:253:PRO:O	1:D:254:SER:HB2	2.09	0.53
2:G:553:SER:HA	2:G:579:PHE:CE1	2.44	0.52
1:C:116:LEU:O	1:C:120:LEU:HD12	2.09	0.52
1:C:418:LEU:O	1:C:421:ILE:HG22	2.09	0.52
1:C:456:LEU:HD23	1:C:477:TRP:HH2	1.75	0.52
1:B:407:ILE:HD11	1:B:529:LEU:HD22	1.91	0.52
1:A:142:LEU:HD22	1:A:147:GLY:HA2	1.90	0.52
1:B:52:THR:CG2	1:B:53:ASN:N	2.72	0.52
2:F:578:ASN:O	2:F:580:PRO:HD3	2.08	0.52
1:A:249:MET:HG2	1:A:256:ILE:HB	1.90	0.52
1:D:242:ALA:HA	1:D:245:ARG:HG2	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:104:GLY:O	1:D:107:VAL:HG12	2.09	0.52
2:H:498:TYR:O	2:H:499:VAL:CB	2.41	0.52
2:G:600:TRP:O	2:G:600:TRP:HE3	1.91	0.52
1:A:104:GLY:O	1:A:107:VAL:HG12	2.10	0.52
1:A:284:PRO:HG3	1:A:436:ILE:HG22	1.92	0.52
1:C:350:ASP:OD2	1:C:356:PHE:CE2	2.63	0.52
1:D:456:LEU:HD23	1:D:477:TRP:HH2	1.74	0.52
2:H:482:HIS:HD2	2:H:522:PHE:HA	1.74	0.52
1:B:249:MET:HG2	1:B:256:ILE:HB	1.91	0.52
1:D:397:ASN:OD1	1:D:400:PHE:HD1	1.93	0.52
2:F:550:CYS:HB2	2:F:551:PRO:CD	2.40	0.52
1:B:350:ASP:OD2	1:B:356:PHE:CE2	2.62	0.52
1:D:90:ASN:HB3	1:D:93:VAL:HG13	1.92	0.52
2:E:482:HIS:HD2	2:E:522:PHE:HA	1.73	0.52
2:H:482:HIS:CD2	2:H:522:PHE:HA	2.44	0.52
1:D:432:ASN:O	1:D:435:GLU:HB3	2.09	0.52
1:D:365:THR:HB	1:D:368:ASP:H	1.74	0.52
1:A:222:LEU:O	1:A:226:VAL:HG23	2.09	0.52
1:A:493:HIS:CE1	1:A:497:TYR:CE1	2.97	0.52
1:B:456:LEU:HD23	1:B:477:TRP:HH2	1.74	0.52
2:E:566:ILE:HA	2:E:599:THR:O	2.10	0.52
1:D:580:ASN:HD21	1:D:582:ARG:HH12	1.56	0.52
1:B:162:LEU:HD11	1:B:490:PRO:HB2	1.91	0.52
1:B:222:LEU:O	1:B:226:VAL:HG23	2.10	0.52
1:B:242:ALA:HA	1:B:245:ARG:HG2	1.92	0.52
1:D:249:MET:HG2	1:D:256:ILE:HB	1.92	0.51
1:A:397:ASN:OD1	1:A:400:PHE:CD1	2.63	0.51
1:D:206:ASP:OD1	1:D:398:GLU:HG2	2.10	0.51
1:D:276:THR:HG23	1:D:445:THR:OG1	2.09	0.51
1:D:290:ASN:HD21	1:D:292:ASP:HB2	1.74	0.51
1:A:578:ASN:OD1	1:A:579:MET:N	2.43	0.51
1:A:526:GLN:HE21	1:A:526:GLN:HA	1.75	0.51
2:F:483:THR:CG2	2:F:519:THR:CG2	2.80	0.51
1:B:469:PRO:O	1:B:473:TRP:CD1	2.64	0.51
1:B:209:VAL:HG21	1:B:565:PRO:HB3	1.92	0.51
1:A:245:ARG:O	1:A:249:MET:HG3	2.10	0.51
2:F:535:SER:C	2:F:537:GLY:H	2.14	0.51
1:D:582:ARG:O	1:D:583:PRO:C	2.48	0.51
1:A:320:LEU:HD13	1:A:380:GLN:HG2	1.93	0.51
1:C:276:THR:OG1	1:C:445:THR:HG23	2.10	0.51
1:A:90:ASN:HB3	1:A:93:VAL:HG13	1.92	0.51
2:F:482:HIS:CD2	2:F:483:THR:N	2.79	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:482:HIS:HD2	2:F:522:PHE:HA	1.75	0.51
2:E:498:TYR:O	2:E:499:VAL:CB	2.37	0.51
2:F:600:TRP:HE3	2:F:600:TRP:O	1.94	0.51
2:F:544:TYR:CE1	2:F:582:GLU:HB3	2.45	0.51
1:B:389:PRO:HG2	1:B:392:LEU:HD22	1.91	0.51
1:A:287:GLN:H	1:A:287:GLN:HE21	1.57	0.51
1:B:320:LEU:HB3	1:B:321:PRO:CD	2.41	0.51
1:D:276:THR:OG1	1:D:445:THR:HG23	2.10	0.51
1:D:116:LEU:O	1:D:120:LEU:HD12	2.10	0.51
1:B:20:THR:HB	1:B:23:GLU:HB2	1.94	0.51
1:D:142:LEU:HD22	1:D:147:GLY:HA2	1.93	0.51
1:A:582:ARG:O	1:A:583:PRO:C	2.48	0.50
1:B:49:ASN:HB3	1:B:58:ASN:HD22	1.76	0.50
1:C:217:TYR:CE1	1:C:578:ASN:ND2	2.74	0.50
1:D:543:ASP:O	1:D:545:SER:N	2.44	0.50
2:E:550:CYS:HB2	2:E:551:PRO:HD2	1.93	0.50
1:A:275:TRP:O	1:A:276:THR:C	2.49	0.50
1:A:91:LEU:H	1:A:91:LEU:HD12	1.75	0.50
1:C:249:MET:HG2	1:C:256:ILE:HB	1.94	0.50
1:B:454:TYR:OH	1:B:458:LYS:HD3	2.10	0.50
1:D:107:VAL:HG22	1:D:107:VAL:O	2.10	0.50
1:C:390:PHE:HA	1:C:393:ARG:HD2	1.94	0.50
1:A:107:VAL:O	1:A:107:VAL:HG22	2.12	0.50
1:D:209:VAL:HG21	1:D:565:PRO:HB3	1.93	0.50
1:B:290:ASN:HD21	1:B:292:ASP:HB2	1.76	0.50
1:C:290:ASN:HD21	1:C:292:ASP:HB2	1.77	0.50
2:F:504:GLN:HG2	2:F:505:VAL:N	2.26	0.50
1:A:574:VAL:HG23	1:A:575:GLY:N	2.26	0.50
1:C:397:ASN:OD1	1:C:400:PHE:CD1	2.65	0.50
1:D:526:GLN:HE21	1:D:526:GLN:HA	1.76	0.50
1:B:601:ASN:ND2	1:D:254:SER:O	2.44	0.49
2:G:570:THR:O	2:G:571:VAL:HG12	2.12	0.49
1:B:332:MET:O	1:B:332:MET:HG2	2.10	0.49
1:C:578:ASN:OD1	1:C:579:MET:N	2.46	0.49
1:D:177:ARG:HB3	1:D:178:PRO:HD3	1.94	0.49
2:E:577:CYS:O	2:E:578:ASN:C	2.51	0.49
1:C:52:THR:CG2	1:C:53:ASN:N	2.75	0.49
1:D:222:LEU:O	1:D:226:VAL:HG23	2.13	0.49
1:B:226:VAL:O	1:B:229:THR:HG22	2.12	0.49
1:B:522:GLN:NE2	1:B:523:PHE:CE2	2.80	0.49
1:B:418:LEU:O	1:B:421:ILE:HG22	2.13	0.49
1:B:284:PRO:HG3	1:B:436:ILE:HG22	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:553:SER:O	2:H:554:PHE:CD2	2.65	0.49
1:D:414:THR:HG23	1:D:417:HIS:H	1.77	0.49
1:D:92:THR:O	1:D:96:GLN:HG3	2.13	0.49
2:G:575:GLY:O	2:G:600:TRP:CH2	2.66	0.49
1:C:242:ALA:HA	1:C:245:ARG:HG2	1.94	0.49
1:B:574:VAL:HG23	1:B:575:GLY:N	2.28	0.49
1:A:543:ASP:O	1:A:545:SER:N	2.45	0.49
1:C:293:VAL:CG2	1:C:366:MET:HG3	2.43	0.49
1:D:287:GLN:H	1:D:287:GLN:HE21	1.59	0.49
1:A:414:THR:HG23	1:A:417:HIS:H	1.76	0.49
1:D:279:TYR:HB2	1:D:444:LEU:HD23	1.95	0.49
1:A:520:LEU:HD22	1:A:581:VAL:HA	1.95	0.49
1:B:199:TYR:O	1:B:202:TYR:HB3	2.13	0.49
2:E:535:SER:C	2:E:537:GLY:H	2.15	0.49
1:D:284:PRO:HG3	1:D:436:ILE:HG22	1.94	0.49
2:G:482:HIS:CD2	2:G:522:PHE:HA	2.48	0.49
1:B:560:LEU:HD21	1:B:564:GLU:HB2	1.95	0.49
1:A:187:LYS:HE3	1:A:199:TYR:CE1	2.48	0.49
1:B:226:VAL:CA	1:B:229:THR:HG22	2.42	0.49
1:A:318:VAL:HG12	1:A:551:GLY:HA3	1.94	0.49
2:F:482:HIS:CD2	2:F:522:PHE:HA	2.48	0.48
1:C:365:THR:HB	1:C:368:ASP:H	1.78	0.48
1:C:469:PRO:O	1:C:473:TRP:CD1	2.66	0.48
1:C:318:VAL:O	1:C:551:GLY:HA3	2.12	0.48
2:H:600:TRP:HE3	2:H:600:TRP:O	1.96	0.48
1:C:253:PRO:O	1:C:254:SER:HB2	2.13	0.48
1:D:397:ASN:OD1	1:D:400:PHE:CD1	2.66	0.48
1:A:338:ASN:O	1:A:340:GLN:N	2.46	0.48
1:A:20:THR:HB	1:A:23:GLU:HB2	1.95	0.48
1:B:432:ASN:O	1:B:435:GLU:HB3	2.13	0.48
2:H:535:SER:C	2:H:537:GLY:H	2.16	0.48
1:B:287:GLN:HE21	1:B:287:GLN:H	1.60	0.48
1:D:162:LEU:HD11	1:D:490:PRO:HB2	1.94	0.48
1:C:529:LEU:HD11	1:C:554:LEU:HB2	1.94	0.48
1:A:209:VAL:HG21	1:A:565:PRO:HB3	1.95	0.48
2:E:522:PHE:C	2:E:522:PHE:CD1	2.86	0.48
2:H:577:CYS:O	2:H:578:ASN:C	2.52	0.48
1:B:543:ASP:O	1:B:545:SER:N	2.46	0.48
1:A:261:CYS:HB3	1:A:487:VAL:N	2.28	0.48
1:A:92:THR:O	1:A:96:GLN:HG3	2.13	0.48
1:C:276:THR:HG23	1:C:445:THR:OG1	2.13	0.48
2:G:550:CYS:HB2	2:G:551:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:322:ASN:O	2:G:586:HIS:HE1	1.96	0.48
1:C:284:PRO:HG3	1:C:436:ILE:HG22	1.95	0.48
1:B:324:THR:O	1:B:327:PHE:HB3	2.14	0.48
1:D:166:GLU:OE2	1:D:497:TYR:OH	2.19	0.48
1:D:493:HIS:CE1	1:D:497:TYR:CE1	3.02	0.48
2:E:581:LEU:HD23	2:E:593:VAL:HG23	1.95	0.48
1:A:443:ALA:HB2	1:A:588:PHE:CE2	2.49	0.48
1:B:254:SER:O	1:D:601:ASN:ND2	2.47	0.48
1:B:353:LYS:HA	2:F:498:TYR:CD2	2.48	0.48
1:B:414:THR:HG23	1:B:417:HIS:H	1.77	0.48
1:C:320:LEU:HB3	1:C:321:PRO:CD	2.44	0.48
1:A:432:ASN:O	1:A:435:GLU:HB3	2.13	0.48
2:H:522:PHE:C	2:H:522:PHE:CD1	2.86	0.47
2:F:491:ALA:O	2:F:531:VAL:CG2	2.59	0.47
1:B:293:VAL:CG2	1:B:366:MET:HG3	2.44	0.47
1:D:275:TRP:O	1:D:276:THR:C	2.50	0.47
1:C:248:LEU:HB3	1:C:256:ILE:HD13	1.97	0.47
2:H:566:ILE:HA	2:H:599:THR:O	2.14	0.47
1:A:279:TYR:HB2	1:A:444:LEU:HD23	1.96	0.47
1:C:226:VAL:O	1:C:229:THR:HG22	2.14	0.47
1:B:274:PHE:CD2	1:B:449:THR:HB	2.49	0.47
2:G:522:PHE:CD1	2:G:522:PHE:C	2.87	0.47
2:H:578:ASN:N	2:H:578:ASN:HD22	1.90	0.47
1:A:242:ALA:HA	1:A:245:ARG:HG2	1.95	0.47
1:D:360:MET:HE3	1:D:375:GLU:HG3	1.96	0.47
1:B:269:ASP:OD2	1:B:272:GLY:N	2.34	0.47
1:C:287:GLN:H	1:C:287:GLN:HE21	1.62	0.47
2:G:482:HIS:CD2	2:G:483:THR:N	2.83	0.47
1:D:560:LEU:HD21	1:D:564:GLU:HB2	1.96	0.47
1:B:187:LYS:HE3	1:B:199:TYR:CZ	2.49	0.47
1:D:269:ASP:OD2	1:D:272:GLY:N	2.34	0.47
1:C:226:VAL:CA	1:C:229:THR:HG22	2.44	0.47
1:A:162:LEU:HD13	1:A:490:PRO:HB2	1.95	0.47
1:C:91:LEU:CD1	1:C:91:LEU:H	2.27	0.47
1:B:529:LEU:HG	1:B:550:ALA:HB1	1.96	0.47
1:C:522:GLN:NE2	1:C:523:PHE:CE2	2.83	0.47
1:D:483:GLU:HG2	1:D:608:THR:HG21	1.97	0.47
1:D:20:THR:HB	1:D:23:GLU:HB2	1.96	0.47
1:B:532:ALA:O	1:B:549:GLU:HG2	2.14	0.47
1:A:483:GLU:HG2	1:A:608:THR:HG21	1.95	0.47
1:C:338:ASN:O	1:C:340:GLN:N	2.47	0.47
1:D:338:ASN:O	1:D:340:GLN:N	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:432:ASN:O	1:C:435:GLU:HB3	2.14	0.47
1:A:398:GLU:OE2	1:A:514:ARG:HB3	2.15	0.47
1:A:489:GLU:HG2	1:A:489:GLU:O	2.14	0.47
1:B:545:SER:O	1:B:546:ASN:CB	2.61	0.47
1:A:226:VAL:O	1:A:229:THR:HG22	2.15	0.46
1:A:96:GLN:HG2	1:A:392:LEU:HD11	1.98	0.46
2:G:535:SER:C	2:G:537:GLY:H	2.18	0.46
2:F:570:THR:O	2:F:571:VAL:HG12	2.14	0.46
1:C:526:GLN:HE21	1:C:526:GLN:HA	1.80	0.46
1:B:81:GLN:NE2	1:B:101:GLN:HB2	2.30	0.46
1:C:81:GLN:NE2	1:C:101:GLN:HB2	2.30	0.46
1:A:274:PHE:CD2	1:A:449:THR:HB	2.51	0.46
1:D:532:ALA:O	1:D:549:GLU:HG2	2.14	0.46
1:B:526:GLN:HE21	1:B:526:GLN:HA	1.79	0.46
1:D:578:ASN:OD1	1:D:579:MET:N	2.48	0.46
1:D:261:CYS:HB3	1:D:487:VAL:N	2.30	0.46
1:A:375:GLU:O	1:A:378:HIS:HB2	2.16	0.46
1:B:51:ASN:ND2	1:B:343:VAL:CG2	2.64	0.46
1:C:51:ASN:HB3	1:C:342:ALA:HB1	1.97	0.46
1:B:81:GLN:CA	1:B:81:GLN:NE2	2.75	0.46
1:D:226:VAL:CA	1:D:229:THR:HG22	2.46	0.46
1:D:162:LEU:HD13	1:D:490:PRO:HB2	1.94	0.46
1:B:261:CYS:HB3	1:B:486:GLY:O	2.15	0.46
1:A:332:MET:O	1:A:332:MET:HG2	2.14	0.46
1:C:209:VAL:HG21	1:C:565:PRO:HB3	1.97	0.46
2:H:578:ASN:N	2:H:578:ASN:ND2	2.61	0.46
1:C:521:TYR:O	1:C:524:GLN:N	2.49	0.46
2:F:550:CYS:HB2	2:F:551:PRO:HD2	1.97	0.46
1:B:253:PRO:O	1:B:254:SER:HB2	2.16	0.46
1:B:398:GLU:OE2	1:B:514:ARG:HB3	2.15	0.46
2:E:578:ASN:ND2	2:E:578:ASN:N	2.61	0.46
1:D:166:GLU:OE1	1:D:493:HIS:HE1	1.99	0.46
1:B:248:LEU:HB3	1:B:256:ILE:HD13	1.96	0.46
1:D:249:MET:SD	1:D:258:PRO:HG3	2.56	0.46
1:A:318:VAL:O	1:A:551:GLY:HA3	2.15	0.46
2:E:528:TYR:HE1	2:E:543:ILE:HD12	1.81	0.46
1:C:199:TYR:O	1:C:202:TYR:HB3	2.16	0.46
1:A:335:ASP:HB2	1:A:361:CYS:SG	2.56	0.46
1:B:529:LEU:HD11	1:B:554:LEU:HB2	1.98	0.46
1:D:22:GLU:O	1:D:26:LYS:HG3	2.15	0.46
1:C:355:ASP:OD2	1:C:357:ARG:NH1	2.39	0.46
2:F:522:PHE:CD1	2:F:522:PHE:C	2.89	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:498:TYR:HD1	2:H:499:VAL:N	2.13	0.46
2:H:499:VAL:HG22	2:H:585:TRP:CG	2.51	0.46
1:A:259:ILE:HA	1:A:603:PHE:CD1	2.51	0.46
1:B:51:ASN:HB3	1:B:342:ALA:HB1	1.98	0.45
2:F:498:TYR:O	2:F:499:VAL:CB	2.40	0.45
1:A:226:VAL:CA	1:A:229:THR:HG22	2.46	0.45
1:D:327:PHE:CD1	1:D:327:PHE:C	2.89	0.45
1:B:146:PRO:O	1:B:147:GLY:C	2.55	0.45
2:E:528:TYR:CE1	2:E:543:ILE:HB	2.51	0.45
1:D:482:ARG:HE	1:D:488:VAL:HG12	1.81	0.45
1:C:274:PHE:CD2	1:C:449:THR:HB	2.51	0.45
1:B:374:HIS:CE1	1:B:406:GLU:HG2	2.51	0.45
1:C:146:PRO:O	1:C:147:GLY:C	2.54	0.45
1:A:253:PRO:O	1:A:254:SER:CB	2.65	0.45
1:D:269:ASP:OD2	1:D:269:ASP:C	2.55	0.45
1:C:144:LEU:HB2	1:C:168:TRP:CH2	2.51	0.45
1:D:520:LEU:HD22	1:D:581:VAL:HA	1.98	0.45
1:D:411:SER:O	1:D:414:THR:HG22	2.16	0.45
1:C:411:SER:O	1:C:414:THR:HG22	2.17	0.45
1:D:351:LEU:H	1:D:351:LEU:HD12	1.79	0.45
1:C:322:ASN:O	2:G:586:HIS:CE1	2.69	0.45
2:F:595:ALA:HB3	2:F:597:TYR:CE2	2.51	0.45
2:E:600:TRP:CE3	2:E:600:TRP:N	2.84	0.45
2:G:544:TYR:CE1	2:G:582:GLU:HB3	2.51	0.45
2:F:578:ASN:N	2:F:578:ASN:HD22	1.96	0.45
1:D:225:ASP:O	1:D:229:THR:HG22	2.17	0.45
1:C:478:TRP:HA	1:C:481:LYS:HB2	1.99	0.45
1:A:259:ILE:HA	1:A:603:PHE:HD1	1.81	0.45
1:B:338:ASN:O	1:B:340:GLN:N	2.50	0.45
1:C:20:THR:HB	1:C:23:GLU:HB2	1.99	0.45
1:C:81:GLN:CA	1:C:81:GLN:NE2	2.75	0.45
1:A:290:ASN:HD21	1:A:292:ASP:HB2	1.78	0.45
1:C:162:LEU:HD13	1:C:490:PRO:CB	2.46	0.45
1:B:397:ASN:OD1	1:B:400:PHE:CD1	2.68	0.45
2:F:528:TYR:HE1	2:F:543:ILE:HD12	1.82	0.45
1:A:166:GLU:OE1	1:A:493:HIS:HE1	2.00	0.45
1:A:165:TRP:CZ3	1:A:490:PRO:HD2	2.52	0.45
1:B:521:TYR:O	1:B:524:GLN:N	2.50	0.45
1:B:22:GLU:OE2	1:B:90:ASN:HB2	2.17	0.45
1:B:425:SER:OG	1:B:427:ASP:HB2	2.17	0.45
1:A:22:GLU:O	1:A:26:LYS:HG3	2.16	0.45
1:B:523:PHE:O	1:B:524:GLN:C	2.55	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:560:LEU:HD21	1:A:564:GLU:HB2	1.99	0.44
2:G:600:TRP:CE3	2:G:600:TRP:N	2.85	0.44
1:D:187:LYS:HE3	1:D:199:TYR:CE1	2.52	0.44
1:B:493:HIS:CE1	1:B:497:TYR:CE1	3.06	0.44
2:E:570:THR:O	2:E:571:VAL:HG12	2.16	0.44
1:A:454:TYR:OH	1:A:458:LYS:HD3	2.17	0.44
1:A:370:LEU:HD21	1:A:413:ALA:HB2	2.00	0.44
1:B:578:ASN:OD1	1:B:579:MET:N	2.51	0.44
1:D:574:VAL:HG23	1:D:575:GLY:N	2.33	0.44
1:B:206:ASP:OD1	1:B:398:GLU:HG2	2.18	0.44
1:C:532:ALA:O	1:C:549:GLU:HG2	2.18	0.44
1:A:155:SER:O	1:A:161:ARG:HD2	2.18	0.44
1:D:543:ASP:OD1	1:D:545:SER:OG	2.36	0.44
1:D:318:VAL:HG12	1:D:551:GLY:HA3	2.00	0.44
2:E:553:SER:O	2:E:554:PHE:CD2	2.71	0.44
2:H:504:GLN:HG2	2:H:505:VAL:N	2.33	0.44
1:C:259:ILE:HA	1:C:603:PHE:CD1	2.53	0.44
1:C:560:LEU:HD21	1:C:564:GLU:HB2	2.00	0.44
1:C:574:VAL:HG23	1:C:575:GLY:N	2.32	0.44
1:C:529:LEU:HG	1:C:550:ALA:HB1	1.99	0.44
1:A:96:GLN:NE2	1:A:389:PRO:HB2	2.33	0.44
1:C:275:TRP:O	1:C:276:THR:C	2.56	0.44
1:D:146:PRO:O	1:D:147:GLY:C	2.56	0.44
1:D:274:PHE:CD2	1:D:449:THR:HB	2.53	0.44
1:D:52:THR:CG2	1:D:53:ASN:N	2.81	0.44
1:B:166:GLU:OE1	1:B:493:HIS:HE1	2.00	0.44
1:D:293:VAL:CG2	1:D:366:MET:HG3	2.48	0.44
1:B:469:PRO:O	1:B:473:TRP:HD1	2.01	0.44
1:D:469:PRO:O	1:D:473:TRP:CD1	2.71	0.44
1:D:168:TRP:O	1:D:172:VAL:HG22	2.18	0.44
1:D:225:ASP:O	1:D:229:THR:CG2	2.65	0.44
1:A:482:ARG:HE	1:A:488:VAL:HG12	1.83	0.44
1:C:351:LEU:HD12	1:C:351:LEU:H	1.82	0.44
2:F:499:VAL:HG22	2:F:585:TRP:CG	2.53	0.44
1:A:51:ASN:ND2	1:A:343:VAL:CG2	2.65	0.44
1:B:276:THR:OG1	1:B:445:THR:HG23	2.17	0.44
1:A:274:PHE:HD2	1:A:449:THR:HB	1.83	0.44
1:D:320:LEU:HD13	1:D:380:GLN:HG2	2.00	0.44
1:D:489:GLU:HG3	1:D:491:VAL:O	2.18	0.44
1:A:491:VAL:HG13	1:A:492:PRO:HD2	1.99	0.44
2:E:499:VAL:HG22	2:E:585:TRP:CG	2.52	0.43
2:F:577:CYS:O	2:F:578:ASN:C	2.57	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:199:TYR:O	1:A:202:TYR:HB3	2.18	0.43
1:A:529:LEU:HD11	1:A:554:LEU:HB2	2.00	0.43
1:B:478:TRP:HA	1:B:481:LYS:HB2	2.00	0.43
1:B:19:SER:O	1:B:20:THR:C	2.56	0.43
1:D:259:ILE:HA	1:D:603:PHE:HD1	1.82	0.43
1:D:34:HIS:CD2	1:D:34:HIS:C	2.91	0.43
1:B:274:PHE:HD2	1:B:449:THR:HB	1.82	0.43
1:B:482:ARG:HE	1:B:488:VAL:HG12	1.82	0.43
1:C:482:ARG:HE	1:C:488:VAL:HG12	1.82	0.43
1:B:521:TYR:O	1:B:523:PHE:N	2.51	0.43
1:A:505:HIS:N	1:A:505:HIS:CD2	2.85	0.43
2:E:511:GLY:HA3	3:E:1512:NAG:H3	2.01	0.43
1:C:278:LEU:HD12	1:C:278:LEU:HA	1.86	0.43
1:A:177:ARG:HB3	1:A:178:PRO:HD3	2.00	0.43
2:G:550:CYS:HB2	2:G:551:PRO:HD2	2.01	0.43
1:A:311:ALA:O	1:A:314:PHE:HB3	2.18	0.43
1:C:187:LYS:HE3	1:C:199:TYR:CZ	2.53	0.43
1:A:491:VAL:CG1	1:A:492:PRO:HD2	2.49	0.43
1:C:122:THR:O	1:C:126:ILE:HG13	2.18	0.43
2:F:498:TYR:HD1	2:F:499:VAL:N	2.16	0.43
1:D:81:GLN:CA	1:D:81:GLN:NE2	2.80	0.43
2:H:553:SER:O	2:H:554:PHE:HD2	2.02	0.43
1:B:166:GLU:OE1	1:B:493:HIS:CE1	2.72	0.43
1:A:146:PRO:O	1:A:147:GLY:C	2.57	0.43
1:D:318:VAL:O	1:D:551:GLY:HA3	2.18	0.43
1:A:446:ILE:HG23	1:A:519:THR:HG21	2.00	0.43
1:C:501:ALA:HA	1:C:506:VAL:CG1	2.49	0.43
1:C:181:GLU:O	1:C:184:VAL:HG22	2.18	0.43
1:C:327:PHE:CD1	1:C:327:PHE:C	2.92	0.43
1:B:91:LEU:H	1:B:91:LEU:CD1	2.30	0.43
1:A:276:THR:OG1	1:A:445:THR:HG23	2.19	0.43
2:F:543:ILE:HG12	2:F:583:ALA:CB	2.47	0.43
1:B:181:GLU:O	1:B:184:VAL:HG22	2.18	0.43
2:E:504:GLN:HG2	2:E:505:VAL:N	2.32	0.43
2:G:543:ILE:HG12	2:G:583:ALA:CB	2.49	0.43
1:A:580:ASN:HD21	1:A:582:ARG:NH1	2.15	0.43
1:A:411:SER:O	1:A:414:THR:HG22	2.18	0.43
1:D:259:ILE:HA	1:D:603:PHE:CD1	2.53	0.43
1:C:206:ASP:OD1	1:C:398:GLU:HG2	2.19	0.43
1:B:351:LEU:H	1:B:351:LEU:HD12	1.84	0.43
1:C:279:TYR:HB2	1:C:444:LEU:HD23	2.00	0.43
1:B:47:SER:O	1:B:50:TYR:HB3	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:166:GLU:OE1	1:C:493:HIS:CE1	2.72	0.43
1:D:257:SER:HA	1:D:258:PRO:HD3	1.88	0.43
2:H:544:TYR:CE1	2:H:582:GLU:HB3	2.53	0.43
1:D:101:GLN:O	1:D:101:GLN:HG3	2.19	0.43
1:B:455:MET:HB3	1:B:455:MET:HE2	1.95	0.43
1:D:501:ALA:HA	1:D:506:VAL:CG1	2.48	0.43
1:D:162:LEU:HD13	1:D:490:PRO:CB	2.49	0.42
1:D:165:TRP:CZ3	1:D:490:PRO:HD2	2.54	0.42
1:D:335:ASP:HB2	1:D:361:CYS:SG	2.59	0.42
1:A:34:HIS:C	1:A:34:HIS:CD2	2.91	0.42
1:B:155:SER:O	1:B:161:ARG:HD2	2.19	0.42
1:D:229:THR:OG1	1:D:581:VAL:HB	2.19	0.42
1:B:351:LEU:HD13	1:B:355:ASP:OD2	2.18	0.42
2:E:498:TYR:HD1	2:E:499:VAL:N	2.17	0.42
1:A:52:THR:CG2	1:A:53:ASN:N	2.81	0.42
1:A:249:MET:SD	1:A:258:PRO:HG3	2.58	0.42
1:A:184:VAL:HG12	1:A:464:PHE:HE2	1.84	0.42
1:B:365:THR:HB	1:B:368:ASP:H	1.84	0.42
2:G:568:PHE:HD1	2:G:596:LEU:HD11	1.85	0.42
1:C:51:ASN:ND2	1:C:343:VAL:CG2	2.68	0.42
2:F:575:GLY:O	2:F:600:TRP:CH2	2.72	0.42
1:C:166:GLU:OE1	1:C:493:HIS:HE1	2.02	0.42
2:F:581:LEU:HD23	2:F:593:VAL:HG23	2.01	0.42
1:D:456:LEU:HD13	1:D:460:ARG:HD2	2.02	0.42
1:C:398:GLU:OE2	1:C:514:ARG:HB3	2.19	0.42
2:F:498:TYR:CD1	2:F:498:TYR:C	2.93	0.42
1:D:96:GLN:HG2	1:D:392:LEU:CD1	2.49	0.42
1:D:253:PRO:O	1:D:254:SER:CB	2.68	0.42
2:F:568:PHE:HD1	2:F:596:LEU:HD11	1.84	0.42
2:H:525:ARG:HB3	2:H:525:ARG:HE	1.60	0.42
1:D:454:TYR:OH	1:D:458:LYS:HD3	2.19	0.42
1:D:278:LEU:HD12	1:D:278:LEU:HA	1.97	0.42
1:A:162:LEU:HD13	1:A:490:PRO:CB	2.49	0.42
1:C:493:HIS:CE1	1:C:497:TYR:CE1	3.07	0.42
1:B:275:TRP:O	1:B:276:THR:C	2.57	0.42
2:E:535:SER:C	2:E:537:GLY:N	2.73	0.42
1:C:257:SER:HA	1:C:258:PRO:HD3	1.84	0.42
1:B:322:ASN:O	2:F:586:HIS:CE1	2.71	0.42
2:F:578:ASN:N	2:F:578:ASN:ND2	2.63	0.42
1:B:269:ASP:OD2	1:B:269:ASP:C	2.58	0.42
1:A:360:MET:HE3	1:A:375:GLU:HG3	2.02	0.42
1:C:259:ILE:HA	1:C:603:PHE:HD1	1.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:443:ALA:HB2	1:D:588:PHE:CE2	2.55	0.42
1:C:443:ALA:HB2	1:C:588:PHE:CE2	2.55	0.42
1:C:34:HIS:C	1:C:34:HIS:CD2	2.93	0.42
1:D:446:ILE:HG23	1:D:519:THR:HG21	2.00	0.42
2:H:498:TYR:CD1	2:H:499:VAL:N	2.88	0.42
1:D:166:GLU:OE1	1:D:493:HIS:CE1	2.72	0.42
1:B:162:LEU:HD13	1:B:490:PRO:CB	2.49	0.42
2:H:600:TRP:CE3	2:H:600:TRP:N	2.88	0.42
1:A:169:ARG:NH2	1:A:270:MET:O	2.52	0.42
1:C:332:MET:O	1:C:332:MET:HG2	2.20	0.42
1:B:327:PHE:CD1	1:B:327:PHE:C	2.92	0.42
1:D:499:ASP:N	1:D:500:PRO:HD2	2.35	0.42
1:B:225:ASP:O	1:B:229:THR:CG2	2.68	0.42
1:B:121:ASN:O	1:B:125:THR:HG23	2.20	0.42
1:A:407:ILE:HA	1:A:410:LEU:HD12	2.01	0.42
1:D:184:VAL:HG12	1:D:464:PHE:HE2	1.85	0.42
1:A:48:TRP:CE2	1:A:357:ARG:HD2	2.55	0.42
1:A:198:ASP:H	1:A:201:ASP:HB3	1.85	0.42
1:A:127:TYR:CD1	1:A:127:TYR:C	2.93	0.42
1:A:327:PHE:C	1:A:327:PHE:CD1	2.93	0.41
2:H:550:CYS:HB2	2:H:551:PRO:HD2	2.00	0.41
1:B:52:THR:HG22	1:B:53:ASN:N	2.35	0.41
1:C:269:ASP:C	1:C:269:ASP:OD2	2.58	0.41
2:F:511:GLY:HA3	3:F:1512:NAG:H3	2.02	0.41
1:D:198:ASP:HB2	1:D:464:PHE:O	2.21	0.41
1:C:168:TRP:O	1:C:172:VAL:HG22	2.20	0.41
1:B:520:LEU:HD22	1:B:581:VAL:HA	2.03	0.41
1:A:166:GLU:OE1	1:A:493:HIS:CE1	2.73	0.41
1:D:365:THR:HG22	1:D:367:ASP:H	1.86	0.41
1:B:559:ARG:HH11	1:B:559:ARG:HB2	1.85	0.41
1:C:324:THR:HG23	1:C:327:PHE:HB2	2.02	0.41
2:F:600:TRP:CE3	2:F:600:TRP:N	2.87	0.41
1:D:439:LEU:HD23	1:D:591:LEU:HB2	2.03	0.41
1:C:225:ASP:O	1:C:229:THR:HG22	2.21	0.41
1:C:524:GLN:CD	1:C:580:ASN:H	2.24	0.41
1:D:198:ASP:H	1:D:201:ASP:HB3	1.85	0.41
1:C:456:LEU:HD13	1:C:460:ARG:HD2	2.03	0.41
1:A:206:ASP:OD1	1:A:398:GLU:HG2	2.20	0.41
1:D:489:GLU:O	1:D:489:GLU:HG2	2.19	0.41
1:D:226:VAL:O	1:D:229:THR:HG22	2.20	0.41
1:C:505:HIS:N	1:C:505:HIS:CD2	2.87	0.41
1:D:418:LEU:HA	1:D:421:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:22:GLU:O	1:C:26:LYS:HG3	2.19	0.41
2:H:570:THR:O	2:H:571:VAL:HG12	2.20	0.41
2:H:511:GLY:HA3	3:H:1512:NAG:H3	2.02	0.41
1:B:443:ALA:HB2	1:B:588:PHE:CE2	2.56	0.41
2:G:577:CYS:O	2:G:578:ASN:C	2.59	0.41
1:A:101:GLN:HG3	1:A:101:GLN:O	2.21	0.41
2:F:531:VAL:O	2:F:532:LYS:C	2.58	0.41
1:D:96:GLN:NE2	1:D:389:PRO:HB2	2.35	0.41
1:C:469:PRO:O	1:C:473:TRP:HD1	2.04	0.41
1:C:425:SER:OG	1:C:427:ASP:HB2	2.20	0.41
1:D:461:TRP:CH2	1:D:513:ILE:HG13	2.55	0.41
1:C:47:SER:O	1:C:50:TYR:HB3	2.21	0.41
1:A:229:THR:OG1	1:A:581:VAL:HB	2.21	0.41
2:E:553:SER:HA	2:E:579:PHE:CE1	2.53	0.41
1:B:165:TRP:CZ3	1:B:490:PRO:HD2	2.55	0.41
1:B:225:ASP:O	1:B:229:THR:HG22	2.21	0.41
1:C:520:LEU:HD22	1:C:581:VAL:HA	2.03	0.41
1:A:293:VAL:CG2	1:A:366:MET:HG3	2.50	0.41
1:A:418:LEU:HA	1:A:421:ILE:HG22	2.03	0.41
1:A:455:MET:HB3	1:A:455:MET:HE2	1.89	0.41
1:A:526:GLN:O	1:A:530:CYS:SG	2.79	0.41
2:E:504:GLN:HE21	2:E:504:GLN:HB3	1.68	0.41
1:D:535:HIS:CD2	1:D:536:GLU:N	2.89	0.41
2:E:544:TYR:CE1	2:E:582:GLU:HB3	2.55	0.41
2:G:595:ALA:HB3	2:G:597:TYR:CE2	2.56	0.41
1:B:144:LEU:HB2	1:B:168:TRP:CH2	2.54	0.41
1:B:259:ILE:HA	1:B:603:PHE:CD1	2.55	0.41
1:A:570:LEU:HD23	1:A:570:LEU:HA	1.91	0.41
1:A:493:HIS:CE1	1:A:497:TYR:CZ	3.08	0.41
1:C:196:TYR:CD1	1:C:202:TYR:HA	2.55	0.41
2:E:491:ALA:O	2:E:531:VAL:CG2	2.66	0.41
1:C:22:GLU:OE2	1:C:90:ASN:HB2	2.21	0.41
1:D:82:MET:O	1:D:84:PRO:HD3	2.21	0.41
1:D:73:LEU:HD12	1:D:73:LEU:HA	1.90	0.41
1:B:34:HIS:C	1:B:34:HIS:CD2	2.94	0.41
1:D:332:MET:O	1:D:332:MET:HG2	2.22	0.41
1:A:574:VAL:CG2	1:A:575:GLY:N	2.84	0.40
1:D:398:GLU:OE2	1:D:514:ARG:HB3	2.20	0.40
1:D:252:TYR:CE1	1:D:266:LEU:HD22	2.56	0.40
1:A:148:LEU:O	1:A:151:ILE:N	2.53	0.40
1:D:104:GLY:O	1:D:107:VAL:CG1	2.68	0.40
1:A:217:TYR:CE1	1:A:578:ASN:ND2	2.87	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:522:GLN:NE2	1:A:523:PHE:CE2	2.89	0.40
1:B:279:TYR:HB2	1:B:444:LEU:HD23	2.03	0.40
1:A:439:LEU:HD23	1:A:591:LEU:HB2	2.04	0.40
1:A:278:LEU:HA	1:A:278:LEU:HD12	1.97	0.40
1:D:529:LEU:HD11	1:D:554:LEU:HB2	2.03	0.40
1:A:532:ALA:O	1:A:549:GLU:HG2	2.20	0.40
1:D:363:LYS:HB2	1:D:363:LYS:HE3	1.90	0.40
1:C:562:LYS:CG	1:C:562:LYS:O	2.69	0.40
1:A:196:TYR:CD1	1:A:202:TYR:HA	2.56	0.40
2:H:553:SER:HA	2:H:579:PHE:CE1	2.54	0.40
1:A:524:GLN:CG	1:A:583:PRO:HG2	2.47	0.40
1:C:248:LEU:HA	1:C:248:LEU:HD23	1.98	0.40
1:C:580:ASN:ND2	1:C:581:VAL:H	2.20	0.40
1:D:217:TYR:CE1	1:D:578:ASN:ND2	2.82	0.40
2:G:504:GLN:HB3	2:G:504:GLN:HE21	1.73	0.40
2:E:543:ILE:HG12	2:E:583:ALA:CB	2.51	0.40
1:C:274:PHE:HD2	1:C:449:THR:HB	1.85	0.40
1:B:259:ILE:HA	1:B:603:PHE:HD1	1.85	0.40
1:A:47:SER:O	1:A:50:TYR:HB3	2.22	0.40
1:C:613:TYR:CD1	1:C:613:TYR:O	2.74	0.40
1:B:21:ILE:CG1	1:B:87:GLU:HG2	2.51	0.40
1:C:225:ASP:O	1:C:229:THR:CG2	2.70	0.40
2:G:581:LEU:HD23	2:G:593:VAL:HG23	2.03	0.40
1:B:96:GLN:HG2	1:B:392:LEU:HD11	2.03	0.40
1:D:526:GLN:O	1:D:530:CYS:SG	2.80	0.40
1:B:555:PHE:O	1:B:559:ARG:HG2	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:71:ALA:O	2:G:518:ARG:NH2[3_554]	1.69	0.51
2:F:518:ARG:NH2	1:D:71:ALA:O[3_454]	2.04	0.16
2:F:572:GLU:OE2	1:D:24:GLN:OE1[3_454]	2.09	0.11
1:A:24:GLN:OE1	2:G:572:GLU:OE2[3_554]	2.13	0.07

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	585/597 (98%)	516 (88%)	55 (9%)	14 (2%)	9	53
1	B	585/597 (98%)	515 (88%)	57 (10%)	13 (2%)	10	55
1	C	585/597 (98%)	514 (88%)	57 (10%)	14 (2%)	9	53
1	D	585/597 (98%)	515 (88%)	56 (10%)	14 (2%)	9	53
2	E	106/136 (78%)	87 (82%)	13 (12%)	6 (6%)	3	24
2	F	106/136 (78%)	86 (81%)	13 (12%)	7 (7%)	2	18
2	G	106/136 (78%)	85 (80%)	14 (13%)	7 (7%)	2	18
2	H	106/136 (78%)	86 (81%)	14 (13%)	6 (6%)	3	24
All	All	2764/2932 (94%)	2404 (87%)	279 (10%)	81 (3%)	7	46

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	PRO
2	E	499	VAL
2	E	521	HIS
2	E	571	VAL
2	E	578	ASN
1	B	146	PRO
2	F	499	VAL
2	F	521	HIS
2	F	571	VAL
1	C	146	PRO
2	G	499	VAL
2	G	521	HIS
2	G	571	VAL
2	G	578	ASN
1	D	146	PRO
2	H	499	VAL
2	H	521	HIS
2	H	571	VAL
2	H	578	ASN
1	A	147	GLY
2	E	577	CYS
1	B	147	GLY
1	B	522	GLN
1	B	544	ILE

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Mol	Chain	Res	Type
2	F	578	ASN
1	C	147	GLY
1	D	147	GLY
1	A	56	GLU
1	A	284	PRO
1	A	294	THR
1	A	522	GLN
1	A	544	ILE
1	B	56	GLU
1	B	284	PRO
1	B	294	THR
1	C	56	GLU
1	C	284	PRO
1	C	294	THR
1	C	522	GLN
1	D	56	GLU
1	D	284	PRO
1	D	294	THR
1	D	544	ILE
2	H	577	CYS
2	H	601	SER
1	A	254	SER
1	A	264	ALA
1	A	335	ASP
2	E	601	SER
1	B	335	ASP
1	B	505	HIS
2	F	601	SER
1	C	335	ASP
1	C	505	HIS
2	G	601	SER
1	D	254	SER
1	D	335	ASP
1	D	522	GLN
1	D	608	THR
1	A	608	THR
1	B	291	ILE
1	B	504	PHE
2	F	577	CYS
1	C	277	ASN
1	C	291	ILE
1	C	504	PHE

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Mol	Chain	Res	Type
2	G	577	CYS
1	D	264	ALA
1	A	291	ILE
1	B	254	SER
2	F	551	PRO
1	C	254	SER
1	C	544	ILE
1	D	291	ILE
1	D	352	GLY
1	A	107	VAL
1	B	352	GLY
2	G	551	PRO
1	A	352	GLY
1	D	107	VAL
1	C	185	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	523/527 (99%)	442 (84%)	81 (16%)	4	19
1	B	523/527 (99%)	442 (84%)	81 (16%)	4	19
1	C	523/527 (99%)	444 (85%)	79 (15%)	4	21
1	D	523/527 (99%)	441 (84%)	82 (16%)	4	19
2	E	98/121 (81%)	74 (76%)	24 (24%)	1	3
2	F	98/121 (81%)	75 (76%)	23 (24%)	1	4
2	G	98/121 (81%)	74 (76%)	24 (24%)	1	3
2	H	98/121 (81%)	71 (72%)	27 (28%)	0	2
All	All	2484/2592 (96%)	2063 (83%)	421 (17%)	3	15

All (421) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	21	ILE

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Mol	Chain	Res	Type
1	A	29	LEU
1	A	39	LEU
1	A	43	SER
1	A	45	LEU
1	A	47	SER
1	A	51	ASN
1	A	52	THR
1	A	55	THR
1	A	62	MET
1	A	63	ASN
1	A	77	SER
1	A	78	THR
1	A	81	GLN
1	A	82	MET
1	A	87	GLU
1	A	89	GLN
1	A	95	LEU
1	A	97	LEU
1	A	100	LEU
1	A	131	LYS
1	A	137	ASN
1	A	145	GLU
1	A	160	GLU
1	A	171	GLU
1	A	176	LEU
1	A	183	TYR
1	A	186	LEU
1	A	190	MET
1	A	198	ASP
1	A	213	ASP
1	A	224	GLU
1	A	233	ILE
1	A	240	LEU
1	A	279	TYR
1	A	287	GLN
1	A	291	ILE
1	A	294	THR
1	A	299	ASP
1	A	309	LYS
1	A	313	LYS
1	A	324	THR
1	A	330	ASN

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Mol	Chain	Res	Type
1	A	333	LEU
1	A	341	LYS
1	A	345	HIS
1	A	351	LEU
1	A	365	THR
1	A	371	THR
1	A	380	GLN
1	A	381	TYR
1	A	400	PHE
1	A	401	HIS
1	A	407	ILE
1	A	423	LEU
1	A	427	ASP
1	A	429	GLN
1	A	444	LEU
1	A	455	MET
1	A	469	PRO
1	A	488	VAL
1	A	503	LEU
1	A	513	ILE
1	A	519	THR
1	A	526	GLN
1	A	529	LEU
1	A	545	SER
1	A	546	ASN
1	A	557	MET
1	A	558	LEU
1	A	559	ARG
1	A	560	LEU
1	A	562	LYS
1	A	563	SER
1	A	573	VAL
1	A	577	LYS
1	A	582	ARG
1	A	597	ASP
1	A	604	VAL
1	A	608	THR
2	E	482	HIS
2	E	483	THR
2	E	486	ASN
2	E	497	CYS
2	E	498	TYR

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Mol	Chain	Res	Type
2	E	504	GLN
2	E	509	LEU
2	E	515	VAL
2	E	519	THR
2	E	520	SER
2	E	522	PHE
2	E	524	ILE
2	E	525	ARG
2	E	531	VAL
2	E	538	ASP
2	E	545	LEU
2	E	553	SER
2	E	569	SER
2	E	571	VAL
2	E	578	ASN
2	E	588	THR
2	E	591	THR
2	E	593	VAL
2	E	600	TRP
1	B	19	SER
1	B	21	ILE
1	B	27	THR
1	B	29	LEU
1	B	31	LYS
1	B	39	LEU
1	B	43	SER
1	B	45	LEU
1	B	51	ASN
1	B	52	THR
1	B	55	THR
1	B	62	MET
1	B	63	ASN
1	B	77	SER
1	B	78	THR
1	B	81	GLN
1	B	87	GLU
1	B	89	GLN
1	B	95	LEU
1	B	97	LEU
1	B	100	LEU
1	B	120	LEU
1	B	131	LYS

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Mol	Chain	Res	Type
1	B	137	ASN
1	B	145	GLU
1	B	160	GLU
1	B	176	LEU
1	B	183	TYR
1	B	186	LEU
1	B	190	MET
1	B	198	ASP
1	B	213	ASP
1	B	224	GLU
1	B	233	ILE
1	B	240	LEU
1	B	287	GLN
1	B	291	ILE
1	B	294	THR
1	B	299	ASP
1	B	309	LYS
1	B	313	LYS
1	B	318	VAL
1	B	322	ASN
1	B	324	THR
1	B	327	PHE
1	B	330	ASN
1	B	333	LEU
1	B	341	LYS
1	B	351	LEU
1	B	371	THR
1	B	380	GLN
1	B	381	TYR
1	B	400	PHE
1	B	401	HIS
1	B	407	ILE
1	B	423	LEU
1	B	425	SER
1	B	427	ASP
1	B	429	GLN
1	B	433	GLU
1	B	444	LEU
1	B	455	MET
1	B	488	VAL
1	B	503	LEU
1	B	513	ILE

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Mol	Chain	Res	Type
1	B	519	THR
1	B	526	GLN
1	B	529	LEU
1	B	545	SER
1	B	546	ASN
1	B	557	MET
1	B	558	LEU
1	B	559	ARG
1	B	560	LEU
1	B	563	SER
1	B	573	VAL
1	B	577	LYS
1	B	582	ARG
1	B	597	ASP
1	B	604	VAL
1	B	608	THR
2	F	482	HIS
2	F	483	THR
2	F	486	ASN
2	F	497	CYS
2	F	498	TYR
2	F	504	GLN
2	F	509	LEU
2	F	515	VAL
2	F	519	THR
2	F	520	SER
2	F	522	PHE
2	F	524	ILE
2	F	525	ARG
2	F	531	VAL
2	F	533	SER
2	F	545	LEU
2	F	553	SER
2	F	569	SER
2	F	571	VAL
2	F	578	ASN
2	F	588	THR
2	F	591	THR
2	F	600	TRP
1	C	19	SER
1	C	21	ILE
1	C	27	THR

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Mol	Chain	Res	Type
1	C	29	LEU
1	C	31	LYS
1	C	39	LEU
1	C	43	SER
1	C	45	LEU
1	C	52	THR
1	C	55	THR
1	C	62	MET
1	C	63	ASN
1	C	77	SER
1	C	78	THR
1	C	81	GLN
1	C	87	GLU
1	C	89	GLN
1	C	93	VAL
1	C	95	LEU
1	C	97	LEU
1	C	100	LEU
1	C	117	ASN
1	C	120	LEU
1	C	131	LYS
1	C	137	ASN
1	C	145	GLU
1	C	160	GLU
1	C	176	LEU
1	C	186	LEU
1	C	190	MET
1	C	198	ASP
1	C	213	ASP
1	C	224	GLU
1	C	233	ILE
1	C	240	LEU
1	C	287	GLN
1	C	291	ILE
1	C	294	THR
1	C	299	ASP
1	C	309	LYS
1	C	313	LYS
1	C	318	VAL
1	C	322	ASN
1	C	324	THR
1	C	330	ASN

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Mol	Chain	Res	Type
1	C	333	LEU
1	C	341	LYS
1	C	351	LEU
1	C	371	THR
1	C	380	GLN
1	C	381	TYR
1	C	400	PHE
1	C	401	HIS
1	C	407	ILE
1	C	423	LEU
1	C	427	ASP
1	C	429	GLN
1	C	433	GLU
1	C	444	LEU
1	C	455	MET
1	C	488	VAL
1	C	503	LEU
1	C	513	ILE
1	C	519	THR
1	C	526	GLN
1	C	529	LEU
1	C	545	SER
1	C	546	ASN
1	C	557	MET
1	C	558	LEU
1	C	559	ARG
1	C	560	LEU
1	C	563	SER
1	C	573	VAL
1	C	577	LYS
1	C	582	ARG
1	C	597	ASP
1	C	604	VAL
1	C	608	THR
2	G	482	HIS
2	G	483	THR
2	G	486	ASN
2	G	497	CYS
2	G	498	TYR
2	G	504	GLN
2	G	509	LEU
2	G	515	VAL

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Mol	Chain	Res	Type
2	G	519	THR
2	G	520	SER
2	G	522	PHE
2	G	524	ILE
2	G	525	ARG
2	G	531	VAL
2	G	533	SER
2	G	538	ASP
2	G	545	LEU
2	G	553	SER
2	G	569	SER
2	G	571	VAL
2	G	578	ASN
2	G	588	THR
2	G	591	THR
2	G	600	TRP
1	D	19	SER
1	D	21	ILE
1	D	29	LEU
1	D	39	LEU
1	D	43	SER
1	D	45	LEU
1	D	51	ASN
1	D	52	THR
1	D	55	THR
1	D	56	GLU
1	D	62	MET
1	D	63	ASN
1	D	77	SER
1	D	78	THR
1	D	81	GLN
1	D	82	MET
1	D	87	GLU
1	D	89	GLN
1	D	91	LEU
1	D	95	LEU
1	D	97	LEU
1	D	100	LEU
1	D	131	LYS
1	D	137	ASN
1	D	145	GLU
1	D	160	GLU

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Mol	Chain	Res	Type
1	D	171	GLU
1	D	176	LEU
1	D	183	TYR
1	D	186	LEU
1	D	190	MET
1	D	198	ASP
1	D	213	ASP
1	D	224	GLU
1	D	233	ILE
1	D	240	LEU
1	D	279	TYR
1	D	287	GLN
1	D	291	ILE
1	D	294	THR
1	D	299	ASP
1	D	309	LYS
1	D	313	LYS
1	D	322	ASN
1	D	324	THR
1	D	330	ASN
1	D	333	LEU
1	D	341	LYS
1	D	345	HIS
1	D	351	LEU
1	D	365	THR
1	D	371	THR
1	D	380	GLN
1	D	381	TYR
1	D	400	PHE
1	D	401	HIS
1	D	407	ILE
1	D	423	LEU
1	D	427	ASP
1	D	429	GLN
1	D	433	GLU
1	D	444	LEU
1	D	455	MET
1	D	488	VAL
1	D	503	LEU
1	D	513	ILE
1	D	526	GLN
1	D	529	LEU

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Mol	Chain	Res	Type
1	D	545	SER
1	D	546	ASN
1	D	557	MET
1	D	558	LEU
1	D	559	ARG
1	D	560	LEU
1	D	562	LYS
1	D	563	SER
1	D	573	VAL
1	D	577	LYS
1	D	582	ARG
1	D	597	ASP
1	D	604	VAL
1	D	608	THR
2	H	482	HIS
2	H	483	THR
2	H	486	ASN
2	H	488	THR
2	H	497	CYS
2	H	498	TYR
2	H	504	GLN
2	H	509	LEU
2	H	512	ASN
2	H	515	VAL
2	H	519	THR
2	H	520	SER
2	H	522	PHE
2	H	524	ILE
2	H	525	ARG
2	H	531	VAL
2	H	533	SER
2	H	538	ASP
2	H	545	LEU
2	H	553	SER
2	H	569	SER
2	H	571	VAL
2	H	578	ASN
2	H	588	THR
2	H	591	THR
2	H	596	LEU
2	H	600	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	34	HIS
1	A	42	GLN
1	A	49	ASN
1	A	63	ASN
1	A	81	GLN
1	A	89	GLN
1	A	96	GLN
1	A	287	GLN
1	A	290	ASN
1	A	380	GLN
1	A	493	HIS
1	A	505	HIS
1	A	524	GLN
1	A	526	GLN
1	A	535	HIS
1	A	556	ASN
1	A	580	ASN
1	A	586	ASN
2	E	482	HIS
2	E	504	GLN
2	E	578	ASN
1	B	24	GLN
1	B	34	HIS
1	B	42	GLN
1	B	49	ASN
1	B	63	ASN
1	B	81	GLN
1	B	96	GLN
1	B	137	ASN
1	B	210	ASN
1	B	287	GLN
1	B	290	ASN
1	B	380	GLN
1	B	493	HIS
1	B	505	HIS
1	B	524	GLN
1	B	526	GLN
1	B	535	HIS
1	B	556	ASN
1	B	580	ASN
1	B	586	ASN

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Mol	Chain	Res	Type
2	F	482	HIS
2	F	504	GLN
2	F	578	ASN
2	F	586	HIS
1	C	24	GLN
1	C	34	HIS
1	C	42	GLN
1	C	49	ASN
1	C	63	ASN
1	C	81	GLN
1	C	96	GLN
1	C	137	ASN
1	C	287	GLN
1	C	290	ASN
1	C	380	GLN
1	C	493	HIS
1	C	505	HIS
1	C	524	GLN
1	C	526	GLN
1	C	535	HIS
1	C	556	ASN
1	C	580	ASN
1	C	586	ASN
2	G	482	HIS
2	G	504	GLN
2	G	578	ASN
2	G	586	HIS
1	D	24	GLN
1	D	34	HIS
1	D	42	GLN
1	D	49	ASN
1	D	63	ASN
1	D	81	GLN
1	D	89	GLN
1	D	96	GLN
1	D	137	ASN
1	D	287	GLN
1	D	290	ASN
1	D	380	GLN
1	D	493	HIS
1	D	505	HIS
1	D	524	GLN

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Mol	Chain	Res	Type
1	D	526	GLN
1	D	535	HIS
1	D	556	ASN
1	D	580	ASN
1	D	586	ASN
2	H	482	HIS
2	H	504	GLN
2	H	578	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

16 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	$\# Z > 2$
3	NAG	A	800	1	12,14,15	0.43	0	15,19,21	1.34	2 (13%)
3	NAG	A	801	1	12,14,15	0.85	0	15,19,21	1.73	4 (26%)
3	NAG	B	800	1	12,14,15	0.47	0	15,19,21	1.75	4 (26%)
3	NAG	B	801	1	12,14,15	0.96	1 (8%)	15,19,21	1.70	5 (33%)
3	NAG	C	800	1	12,14,15	0.45	0	15,19,21	1.68	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	801	1	12,14,15	0.84	0	15,19,21	1.62	4 (26%)
3	NAG	D	800	1	12,14,15	0.44	0	15,19,21	1.40	1 (6%)
3	NAG	D	801	1	12,14,15	0.82	0	15,19,21	1.63	3 (20%)
3	NAG	E	1486	2	12,14,15	0.83	1 (8%)	15,19,21	0.95	1 (6%)
3	NAG	E	1512	2	12,14,15	0.42	0	15,19,21	2.11	5 (33%)
3	NAG	F	1486	2	12,14,15	0.81	1 (8%)	15,19,21	1.01	1 (6%)
3	NAG	F	1512	2	12,14,15	0.42	0	15,19,21	2.12	4 (26%)
3	NAG	G	1486	2	12,14,15	0.79	1 (8%)	15,19,21	0.99	1 (6%)
3	NAG	G	1512	2	12,14,15	0.45	0	15,19,21	2.15	4 (26%)
3	NAG	H	1486	2	12,14,15	0.84	1 (8%)	15,19,21	0.99	1 (6%)
3	NAG	H	1512	2	12,14,15	0.47	0	15,19,21	2.21	5 (33%)

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	800	1	-	0/6/23/26	0/1/1/1
3	NAG	A	801	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	800	1	-	0/6/23/26	0/1/1/1
3	NAG	B	801	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	800	1	-	0/6/23/26	0/1/1/1
3	NAG	C	801	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	800	1	-	0/6/23/26	0/1/1/1
3	NAG	D	801	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	1486	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	1512	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	F	1486	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	F	1512	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	G	1486	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	G	1512	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	H	1486	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	H	1512	2	1/1/5/7	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1486	NAG	O5-C5	-2.58	1.40	1.45
3	F	1486	NAG	O5-C5	-2.52	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1486	NAG	O5-C5	-2.51	1.40	1.45
3	B	801	NAG	C2-N2	2.47	1.49	1.46
3	G	1486	NAG	O5-C5	-2.46	1.40	1.45

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1512	NAG	O5-C5-C4	6.52	118.92	110.65
3	G	1512	NAG	O5-C5-C4	6.47	118.86	110.65
3	E	1512	NAG	O5-C5-C4	6.23	118.56	110.65
3	H	1512	NAG	O5-C5-C4	6.17	118.48	110.65
3	B	800	NAG	O5-C5-C6	4.60	111.81	106.98
3	C	800	NAG	O5-C5-C6	4.40	111.59	106.98
3	A	801	NAG	C2-N2-C7	3.88	129.60	123.09
3	D	800	NAG	O5-C5-C6	3.83	111.00	106.98
3	B	801	NAG	C2-N2-C7	3.74	129.37	123.09
3	D	801	NAG	C2-N2-C7	3.52	129.00	123.09
3	C	801	NAG	C2-N2-C7	3.38	128.76	123.09
3	A	800	NAG	O5-C5-C6	3.34	110.49	106.98
3	F	1486	NAG	O5-C5-C4	-2.95	106.92	110.65
3	H	1512	NAG	O5-C5-C6	2.92	110.05	106.98
3	A	801	NAG	C3-C4-C5	-2.86	105.09	110.20
3	G	1486	NAG	O5-C5-C4	-2.85	107.03	110.65
3	G	1512	NAG	C2-N2-C7	2.82	127.83	123.09
3	D	801	NAG	C3-C4-C5	-2.75	105.29	110.20
3	H	1512	NAG	C2-N2-C7	2.73	127.67	123.09
3	C	801	NAG	C3-C4-C5	-2.70	105.38	110.20
3	H	1486	NAG	O5-C5-C4	-2.64	107.31	110.65
3	H	1512	NAG	C6-C5-C4	-2.63	106.64	113.00
3	E	1512	NAG	C6-C5-C4	-2.63	106.65	113.00
3	H	1512	NAG	C3-C4-C5	2.63	114.90	110.20
3	E	1486	NAG	O5-C5-C4	-2.57	107.39	110.65
3	A	801	NAG	O7-C7-C8	-2.51	117.15	122.04
3	F	1512	NAG	C2-N2-C7	2.50	127.28	123.09
3	E	1512	NAG	C2-N2-C7	2.49	127.27	123.09
3	B	800	NAG	O5-C5-C4	2.44	113.75	110.65
3	C	800	NAG	O5-C5-C4	2.43	113.74	110.65
3	F	1512	NAG	C6-C5-C4	-2.42	107.14	113.00
3	B	801	NAG	C3-C4-C5	-2.42	105.89	110.20
3	B	801	NAG	O7-C7-C8	-2.38	117.40	122.04
3	E	1512	NAG	O5-C5-C6	2.35	109.45	106.98
3	E	1512	NAG	C3-C4-C5	2.34	114.39	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1512	NAG	C6-C5-C4	-2.33	107.38	113.00
3	F	1512	NAG	C3-C4-C5	2.31	114.32	110.20
3	B	800	NAG	C6-C5-C4	-2.30	107.45	113.00
3	B	801	NAG	O7-C7-N2	2.30	126.70	121.90
3	G	1512	NAG	C3-C4-C5	2.27	114.25	110.20
3	B	801	NAG	O3-C3-C2	2.26	113.82	109.09
3	A	800	NAG	O5-C5-C4	2.17	113.41	110.65
3	C	800	NAG	C6-C5-C4	-2.16	107.79	113.00
3	C	801	NAG	O7-C7-N2	2.14	126.36	121.90
3	B	800	NAG	C2-N2-C7	2.10	126.61	123.09
3	C	801	NAG	O7-C7-C8	-2.08	117.99	122.04
3	A	801	NAG	O7-C7-N2	2.02	126.12	121.90
3	D	801	NAG	O3-C3-C2	2.01	113.31	109.09
3	C	800	NAG	C2-N2-C7	2.00	126.45	123.09

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	1512	NAG	C1
3	E	1512	NAG	C1
3	A	801	NAG	C1
3	F	1486	NAG	C1
3	C	801	NAG	C1
3	H	1486	NAG	C1
3	H	1512	NAG	C1
3	D	801	NAG	C1
3	E	1486	NAG	C1
3	G	1486	NAG	C1
3	B	801	NAG	C1
3	F	1512	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	593/597 (99%)	0.58	40 (6%) 17 4	43, 46, 48, 52	0
1	B	593/597 (99%)	1.39	140 (23%) 1 1	43, 46, 48, 51	0
1	C	593/597 (99%)	0.45	47 (7%) 13 4	43, 46, 48, 52	0
1	D	593/597 (99%)	0.45	45 (7%) 14 4	43, 46, 48, 52	0
2	E	110/136 (80%)	1.94	43 (39%) 1 0	27, 46, 48, 54	0
2	F	110/136 (80%)	1.57	32 (29%) 1 1	27, 46, 48, 54	0
2	G	110/136 (80%)	3.39	103 (93%) 0 0	27, 46, 48, 54	0
2	H	110/136 (80%)	0.30	0 100 100	27, 46, 48, 54	0
All	All	2812/2932 (95%)	0.89	450 (16%) 3 1	27, 46, 48, 54	0

All (450) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	577	LYS	10.2
1	B	133	CYS	8.5
2	G	567	CYS	8.2
1	B	354	GLY	7.3
1	B	56	GLU	6.9
1	B	57	GLU	6.9
1	D	532	ALA	6.8
1	B	336	PRO	6.7
1	B	342	ALA	6.7
1	C	580	ASN	6.7
1	B	136	ASP	6.6
2	G	483	THR	6.5
1	B	613	TYR	6.4
2	G	482	HIS	6.3
1	B	341	LYS	6.2
2	G	484	ASP	6.1

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Mol	Chain	Res	Type	RSRZ
2	G	516	CYS	6.1
1	B	319	GLY	6.0
1	B	340	GLN	5.7
1	D	578	ASN	5.6
2	E	593	VAL	5.6
1	C	536	GLU	5.6
2	G	581	LEU	5.5
2	F	522	PHE	5.5
2	E	522	PHE	5.5
1	B	83	TYR	5.5
2	G	568	PHE	5.4
1	B	325	GLN	5.3
2	G	598	VAL	5.3
1	B	65	ALA	5.3
2	G	599	THR	5.2
2	F	523	SER	5.2
2	G	600	TRP	5.2
1	B	207	TYR	5.1
1	D	560	LEU	5.1
1	D	576	ALA	5.0
1	D	559	ARG	5.0
1	B	255	TYR	5.0
1	B	430	GLU	4.9
1	C	579	MET	4.9
2	G	505	VAL	4.9
2	F	594	GLY	4.9
1	B	127	TYR	4.8
1	D	567	THR	4.8
2	G	596	LEU	4.8
2	E	521	HIS	4.7
2	G	548	GLY	4.7
2	G	524	ILE	4.7
1	B	385	TYR	4.7
2	F	595	ALA	4.6
2	E	602	GLU	4.5
1	B	359	LEU	4.5
2	G	601	SER	4.5
1	B	366	MET	4.4
1	C	577	LYS	4.4
1	A	424	LEU	4.3
2	G	550	CYS	4.3
2	G	526	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	560	LEU	4.3
1	D	582	ARG	4.3
1	B	417	HIS	4.3
2	G	543	ILE	4.3
1	D	539	LEU	4.3
2	E	491	ALA	4.3
2	F	596	LEU	4.2
2	G	488	THR	4.2
1	D	540	HIS	4.2
1	C	595	LEU	4.1
2	G	587	TYR	4.1
1	B	388	GLN	4.1
1	B	138	PRO	4.1
1	C	493	HIS	4.1
1	B	362	THR	4.1
1	B	447	VAL	4.0
2	F	526	TYR	4.0
2	G	578	ASN	4.0
1	D	501	ALA	4.0
2	E	492	SER	4.0
1	C	511	SER	4.0
1	D	566	TRP	4.0
2	G	489	ALA	4.0
2	G	495	GLY	4.0
2	G	593	VAL	4.0
2	G	527	ILE	4.0
1	B	439	LEU	3.9
2	E	567	CYS	3.9
2	G	487	PHE	3.9
2	E	524	ILE	3.9
2	G	566	ILE	3.9
2	G	504	GLN	3.9
1	C	578	ASN	3.9
2	G	554	PHE	3.9
2	G	497	CYS	3.9
2	G	520	SER	3.9
2	G	577	CYS	3.9
2	E	595	ALA	3.9
2	G	528	TYR	3.8
2	F	521	HIS	3.8
1	B	386	ALA	3.8
2	G	549	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	369	PHE	3.8
2	G	602	GLU	3.8
2	G	574	PRO	3.8
1	B	168	TRP	3.7
1	B	217	TYR	3.7
1	B	240	LEU	3.7
2	G	551	PRO	3.7
1	B	356	PHE	3.7
2	G	552	PHE	3.7
2	E	493	PHE	3.7
1	B	288	LYS	3.7
2	E	532	LYS	3.7
2	E	581	LEU	3.6
2	G	519	THR	3.6
1	B	427	ASP	3.6
1	B	166	GLU	3.6
2	E	592	ILE	3.6
1	D	549	GLU	3.6
1	B	131	LYS	3.6
1	B	162	LEU	3.6
1	B	110	GLU	3.6
2	G	544	TYR	3.6
1	B	424	LEU	3.5
2	G	586	HIS	3.5
1	B	415	PRO	3.5
2	E	516	CYS	3.5
2	G	493	PHE	3.5
2	E	573	VAL	3.5
1	A	57	GLU	3.5
1	B	173	GLY	3.5
2	G	502	PRO	3.5
1	B	268	GLY	3.4
2	F	602	GLU	3.4
2	G	590	TYR	3.4
1	B	119	ILE	3.4
2	G	491	ALA	3.4
1	C	492	PRO	3.4
1	B	297	MET	3.4
2	G	534	GLY	3.4
1	C	543	ASP	3.4
2	G	595	ALA	3.4
1	B	428	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
2	G	545	LEU	3.4
2	G	575	GLY	3.3
1	B	420	SER	3.3
2	G	594	GLY	3.3
1	B	282	THR	3.3
2	G	511	GLY	3.3
1	C	568	LEU	3.3
2	G	499	VAL	3.3
2	E	515	VAL	3.3
2	E	504	GLN	3.3
1	B	353	LYS	3.3
2	G	506	ASN	3.3
2	G	525	ARG	3.3
2	G	515	VAL	3.3
2	E	534	GLY	3.3
1	C	565	PRO	3.3
1	B	460	ARG	3.2
2	G	523	SER	3.2
2	G	582	GLU	3.2
2	G	507	ILE	3.2
1	C	588	PHE	3.2
1	B	156	LEU	3.2
1	B	614	ALA	3.2
1	C	599	ASN	3.2
2	E	574	PRO	3.2
1	C	512	PHE	3.2
2	F	528	TYR	3.2
2	G	498	TYR	3.2
2	G	580	PRO	3.2
1	B	426	PRO	3.2
1	B	429	GLN	3.2
2	F	593	VAL	3.2
2	G	485	ILE	3.2
1	A	21	ILE	3.2
1	B	450	LEU	3.2
1	D	136	ASP	3.1
1	B	266	LEU	3.1
1	B	527	GLU	3.1
1	B	204	ARG	3.1
1	D	542	CYS	3.1
1	B	300	GLN	3.1
1	C	486	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	23	GLU	3.1
1	B	299	ASP	3.1
1	B	53	ASN	3.1
1	B	219	ARG	3.0
2	G	490	THR	3.0
1	B	86	GLN	3.0
1	D	570	LEU	3.0
2	G	576	SER	3.0
1	B	239	HIS	3.0
2	G	592	ILE	3.0
2	G	597	TYR	3.0
1	B	52	THR	3.0
2	G	517	VAL	3.0
1	A	195	HIS	3.0
1	D	579	MET	3.0
2	E	525	ARG	3.0
1	B	271	TRP	3.0
2	E	528	TYR	3.0
2	G	536	PRO	3.0
1	C	544	ILE	3.0
1	B	66	GLY	3.0
1	B	243	TYR	3.0
2	E	482	HIS	3.0
1	A	261	CYS	3.0
2	E	483	THR	3.0
1	B	252	TYR	3.0
2	G	572	GLU	3.0
1	A	270	MET	2.9
1	A	52	THR	2.9
2	F	567	CYS	2.9
2	F	525	ARG	2.9
1	D	550	ALA	2.9
1	B	258	PRO	2.9
1	C	501	ALA	2.9
1	B	418	LEU	2.9
1	B	379	ILE	2.9
2	E	533	SER	2.9
2	E	549	THR	2.9
1	B	210	ASN	2.9
2	G	522	PHE	2.9
1	D	498	CYS	2.9
2	E	530	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
2	G	588	THR	2.9
1	B	170	SER	2.9
2	G	513	THR	2.9
2	E	583	ALA	2.9
2	F	568	PHE	2.9
1	C	523	PHE	2.9
2	G	500	CYS	2.8
2	G	530	ARG	2.8
2	G	573	VAL	2.8
1	B	267	LEU	2.8
2	G	533	SER	2.8
2	G	508	SER	2.8
1	A	284	PRO	2.8
1	C	503	LEU	2.8
2	E	517	VAL	2.8
1	B	446	ILE	2.8
1	A	139	GLN	2.8
1	B	333	LEU	2.8
2	F	482	HIS	2.8
1	A	101	GLN	2.8
1	A	83	TYR	2.8
2	G	591	THR	2.8
1	B	176	LEU	2.8
1	C	581	VAL	2.8
1	B	337	GLY	2.8
1	A	22	GLU	2.8
1	B	301	ALA	2.7
2	G	584	THR	2.7
1	B	174	LYS	2.7
1	C	547	SER	2.7
1	B	608	THR	2.7
1	D	548	THR	2.7
2	G	579	PHE	2.7
1	D	541	LYS	2.7
1	D	568	LEU	2.7
2	G	494	GLY	2.7
1	C	494	ASP	2.7
1	B	529	LEU	2.6
1	B	241	HIS	2.6
1	B	253	PRO	2.6
1	B	389	PRO	2.6
1	B	281	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	510	TYR	2.6
2	E	518	ARG	2.6
2	G	547	SER	2.6
1	B	42	GLN	2.6
1	D	493	HIS	2.6
2	G	585	TRP	2.6
2	F	502	PRO	2.6
2	E	496	SER	2.6
2	G	521	HIS	2.6
1	C	574	VAL	2.6
1	D	558	LEU	2.6
2	E	582	GLU	2.6
1	B	448	GLY	2.6
1	B	414	THR	2.5
2	E	488	THR	2.5
1	A	332	MET	2.5
1	B	169	ARG	2.5
1	D	544	ILE	2.5
1	B	376	MET	2.5
2	G	583	ALA	2.5
1	A	540	HIS	2.5
2	E	545	LEU	2.5
2	F	493	PHE	2.5
1	B	108	LEU	2.5
1	B	68	LYS	2.5
1	C	546	ASN	2.5
1	B	332	MET	2.5
1	B	419	LYS	2.5
1	B	367	ASP	2.5
2	E	494	GLY	2.5
1	B	329	GLU	2.5
1	B	604	VAL	2.5
1	B	290	ASN	2.5
2	G	546	LYS	2.5
2	F	530	ARG	2.5
1	B	320	LEU	2.5
1	B	456	LEU	2.5
1	A	58	ASN	2.5
2	G	531	VAL	2.5
2	G	503	HIS	2.5
1	A	176	LEU	2.4
2	G	542	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	600	LYS	2.4
1	B	338	ASN	2.4
1	B	404	VAL	2.4
1	D	601	ASN	2.4
2	F	534	GLY	2.4
2	F	543	ILE	2.4
2	G	518	ARG	2.4
2	G	486	ASN	2.4
2	F	576	SER	2.4
2	G	496	SER	2.4
1	B	295	ASP	2.4
2	G	512	ASN	2.4
1	D	484	ILE	2.4
2	E	531	VAL	2.4
2	G	529	ASN	2.4
1	C	558	LEU	2.4
1	A	373	HIS	2.4
1	D	545	SER	2.4
1	B	321	PRO	2.4
1	A	456	LEU	2.4
1	B	254	SER	2.4
1	C	542	CYS	2.4
1	C	521	TYR	2.3
1	D	565	PRO	2.3
1	C	557	MET	2.3
2	G	514	SER	2.3
1	C	491	VAL	2.3
2	G	541	TRP	2.3
1	B	21	ILE	2.3
1	D	527	GLU	2.3
1	D	502	SER	2.3
2	G	571	VAL	2.3
1	A	224	GLU	2.3
2	E	507	ILE	2.3
1	C	600	LYS	2.3
2	G	532	LYS	2.3
1	B	469	PRO	2.3
1	B	573	VAL	2.3
1	C	497	TYR	2.3
1	B	28	PHE	2.3
1	B	132	VAL	2.3
2	F	591	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	436	ILE	2.3
1	A	415	PRO	2.3
1	B	438	PHE	2.3
1	A	465	LYS	2.3
1	B	343	VAL	2.3
1	D	428	PHE	2.3
1	A	255	TYR	2.3
1	B	470	LYS	2.3
1	A	336	PRO	2.2
1	D	490	PRO	2.2
1	A	215	TYR	2.2
1	B	134	ASN	2.2
1	C	540	HIS	2.2
2	F	517	VAL	2.2
2	E	543	ILE	2.2
2	G	537	GLY	2.2
1	B	383	MET	2.2
2	F	581	LEU	2.2
2	F	585	TRP	2.2
2	E	519	THR	2.2
1	C	548	THR	2.2
1	D	516	TYR	2.2
2	F	486	ASN	2.2
1	A	396	ALA	2.2
1	B	91	LEU	2.2
1	D	562	LYS	2.2
2	G	570	THR	2.2
1	C	539	LEU	2.2
2	F	598	VAL	2.2
1	B	532	ALA	2.2
1	C	575	GLY	2.2
2	F	590	TYR	2.2
1	A	263	PRO	2.2
1	D	561	GLY	2.2
1	A	100	LEU	2.2
1	D	587	TYR	2.2
1	B	64	ASN	2.2
1	B	234	LYS	2.2
2	E	505	VAL	2.2
2	E	579	PHE	2.2
2	F	548	GLY	2.2
2	G	589	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	391	LEU	2.2
1	D	547	SER	2.2
1	A	613	TYR	2.2
1	B	197	GLU	2.1
1	B	215	TYR	2.1
1	B	259	ILE	2.1
1	B	572	ASN	2.1
1	D	557	MET	2.1
1	A	314	PHE	2.1
1	D	424	LEU	2.1
1	B	344	CYS	2.1
2	F	507	ILE	2.1
1	A	136	ASP	2.1
1	A	236	LEU	2.1
1	B	183	TYR	2.1
1	D	495	GLU	2.1
2	G	569	SER	2.1
2	G	510	ASN	2.1
1	C	545	SER	2.1
1	C	156	LEU	2.1
2	E	600	TRP	2.1
1	C	499	ASP	2.1
1	B	273	ARG	2.1
1	B	588	PHE	2.1
1	C	552	GLN	2.1
1	B	165	TRP	2.1
1	B	444	LEU	2.1
2	G	501	LYS	2.1
1	B	550	ALA	2.1
2	F	536	PRO	2.1
1	A	381	TYR	2.1
2	E	568	PHE	2.1
1	A	259	ILE	2.1
1	A	262	LEU	2.1
1	C	483	GLU	2.1
1	C	591	LEU	2.1
2	F	586	HIS	2.1
1	D	496	THR	2.1
1	A	301	ALA	2.0
1	A	428	PHE	2.0
1	B	137	ASN	2.0
1	C	564	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	120	LEU	2.0
1	B	296	ALA	2.0
1	C	509	ASP	2.0
2	E	552	PHE	2.0
1	B	177	ARG	2.0
1	D	597	ASP	2.0
1	A	455	MET	2.0
1	A	464	PHE	2.0
1	B	87	GLU	2.0
2	F	600	TRP	2.0
1	D	538	PRO	2.0
1	A	82	MET	2.0
1	C	550	ALA	2.0
1	B	595	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	D	800	14/15	0.25	1.46	76,81,85,85	0
3	NAG	C	800	14/15	0.29	0.44	76,81,84,85	0
3	NAG	D	801	14/15	0.32	0.38	65,70,74,75	0
3	NAG	C	801	14/15	0.30	-0.21	65,70,74,75	0
3	NAG	H	1486	14/15	0.30	-0.22	86,104,108,109	0
3	NAG	H	1512	14/15	0.32	-0.27	94,105,108,109	0
3	NAG	B	801	14/15	0.36	-0.61	65,70,74,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	801	14/15	0.26	-0.63	65,70,74,75	0
3	NAG	F	1486	14/15	0.41	-0.79	86,104,108,109	0
3	NAG	A	800	14/15	0.22	-0.84	76,81,85,85	0
3	NAG	E	1512	14/15	0.23	-0.86	94,105,108,109	0
3	NAG	B	800	14/15	0.20	-0.87	76,81,85,85	0
3	NAG	E	1486	14/15	0.24	-1.83	86,104,108,109	0
3	NAG	G	1486	14/15	0.22	-2.66	86,104,108,109	0
3	NAG	G	1512	14/15	0.28	-3.59	94,105,108,109	0
3	NAG	F	1512	14/15	0.22	-4.20	94,105,108,109	0

6.5 Other polymers ⓘ

There are no such residues in this entry.