



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:26 AM UTC

PDB ID : 3WLW / pdb_00003wlw
Title : Molecular Architecture of the ErbB2 Extracellular Domain Homodimer
Authors : Hu, S.; Lou, Z.Y.; Guo, Y.J.
Deposited on : 2013-11-15
Resolution : 3.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

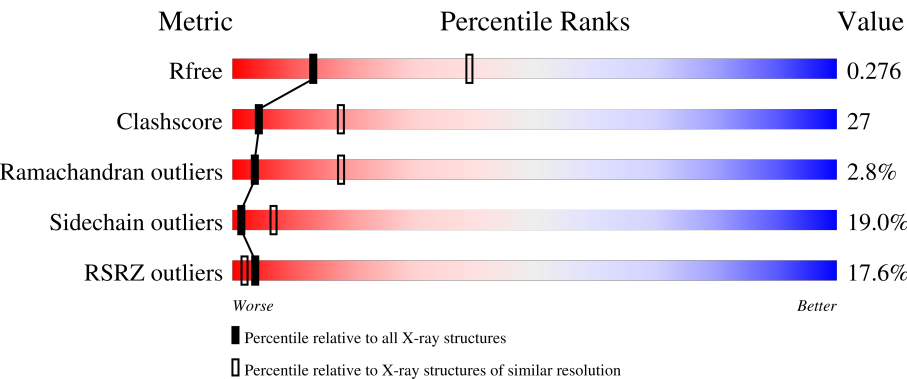
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.09 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}	180053	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	564	10% 56%32%9% . .
1	B	564	8% 52%34%12% . .
2	C	217	41% 43%45%11% .
2	H	217	14% 51%37%10% .
3	D	217	45% 35%39%20%6%

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Mol	Chain	Length	Quality of chain
3	L	217	
4	E	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	E	1	-	-	X	-
5	NAG	B	1001	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15155 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 Receptor tyrosine-protein kinase erbB-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4277	2656	769	805	47			
1	B	555	Total	C	N	O	S	0	0	0
			4277	2656	769	805	47			

- Molecule 2 is a protein called Antibody H Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1624	1021	269	327	7			
2	C	217	Total	C	N	O	S	0	0	0
			1624	1021	269	327	7			

- Molecule 3 is a protein called Antibody L Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	217	Total	C	N	O	S	0	0	0
			1616	1001	269	340	6			
3	D	217	Total	C	N	O	S	0	0	0
			1616	1001	269	340	6			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

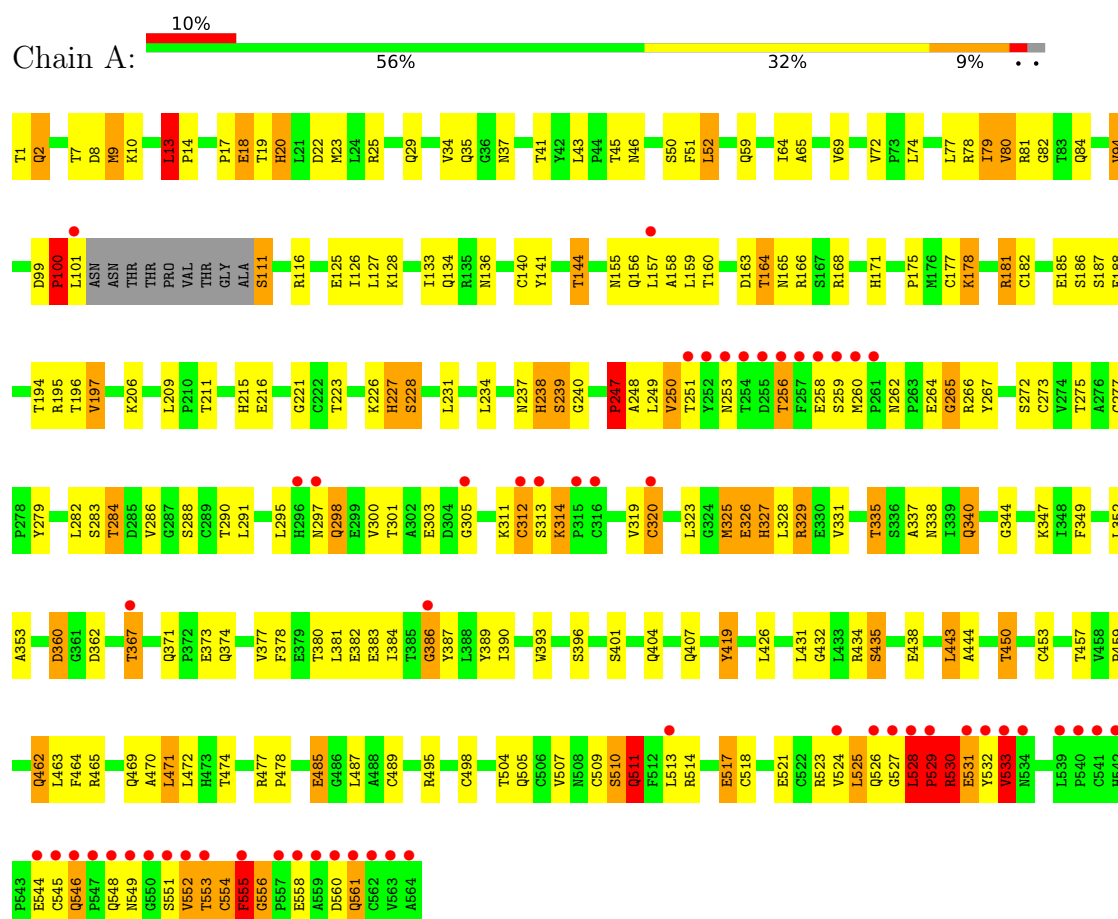
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	27	Total	O	0	0
			27	27		
6	B	14	Total	O	0	0
			14	14		
6	H	2	Total	O	0	0
			2	2		
6	L	5	Total	O	0	0
			5	5		
6	C	12	Total	O	0	0
			12	12		
6	D	19	Total	O	0	0
			19	19		

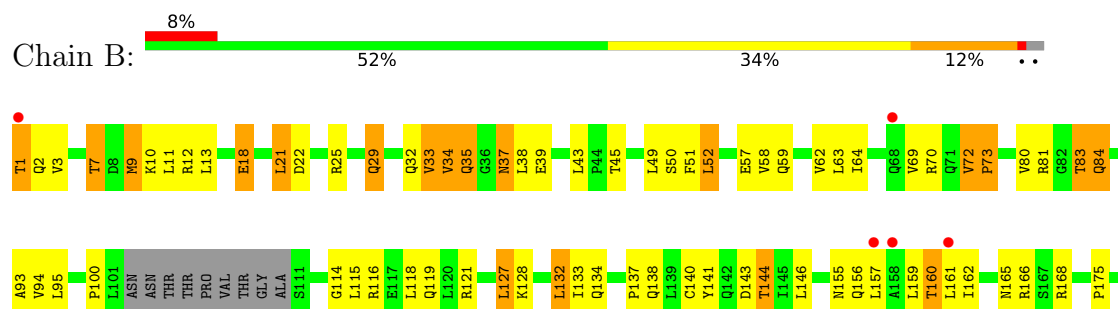
3 Residue-property plots

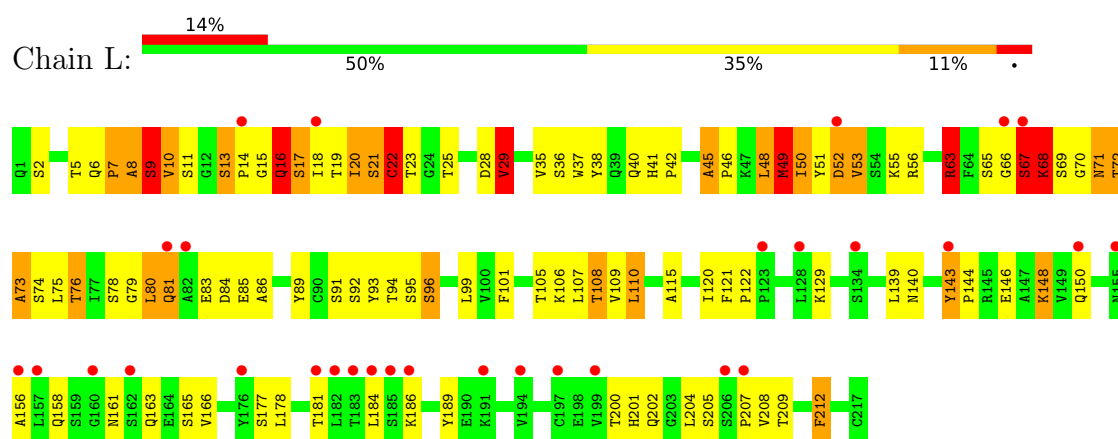
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Receptor tyrosine-protein kinase erbB-2

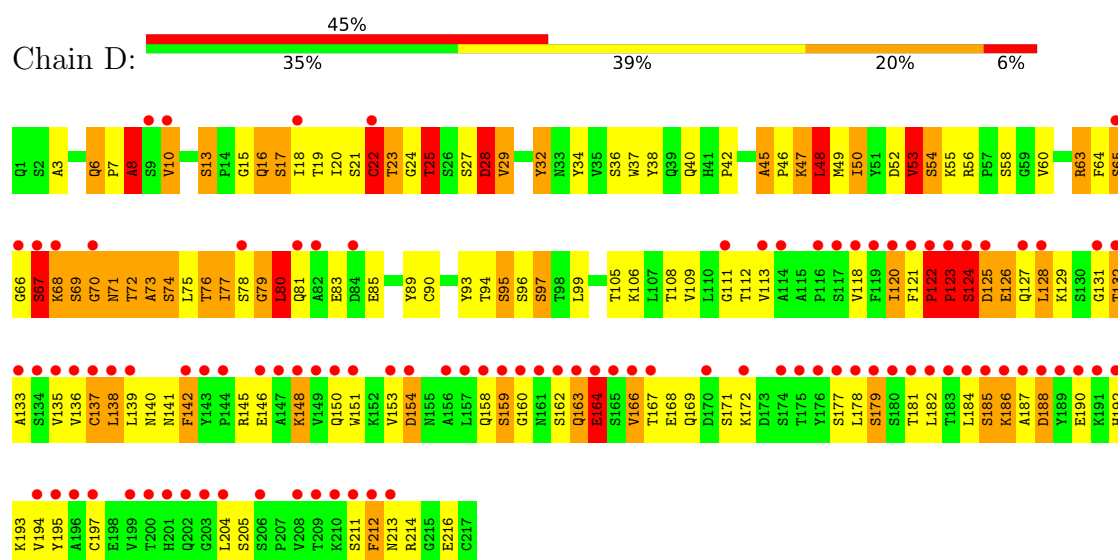


• Molecule 1: Receptor tyrosine-protein kinase erbB-2

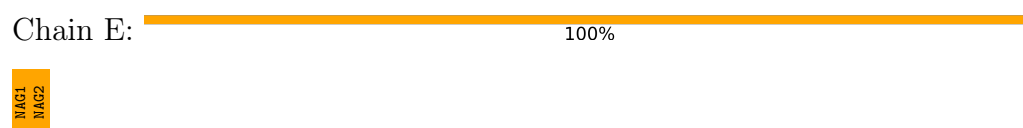




• Molecule 3: Antibody L Chain



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.72Å 104.19Å 116.71Å 106.89° 99.65° 111.12°	Depositor
Resolution (Å)	32.26 – 3.09 32.26 – 3.09	Depositor EDS
% Data completeness (in resolution range)	97.2 (32.26-3.09) 92.2 (32.26-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.232 , 0.269 0.242 , 0.276	Depositor DCC
R_{free} test set	3059 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15155	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.76	3/4374 (0.1%)	1.33	55/5950 (0.9%)
1	B	0.77	3/4374 (0.1%)	1.27	49/5950 (0.8%)
2	C	0.62	0/1664	1.18	16/2268 (0.7%)
2	H	0.64	1/1664 (0.1%)	1.31	24/2268 (1.1%)
3	D	0.84	2/1649 (0.1%)	1.60	45/2241 (2.0%)
3	L	0.78	1/1649 (0.1%)	1.50	33/2241 (1.5%)
All	All	0.75	10/15374 (0.1%)	1.35	222/20918 (1.1%)

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	3
1	B	0	1
2	C	0	2
2	H	0	1
3	D	0	6
3	L	0	4
All	All	0	17

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	GLY	C-N	15.57	1.53	1.33
1	B	539	LEU	C-N	15.16	1.53	1.33
1	A	247	PRO	C-N	11.40	1.49	1.33
3	L	46	PRO	CA-C	-6.84	1.44	1.52
1	B	543	PRO	C-N	6.27	1.42	1.33
1	B	557	PRO	N-CD	5.70	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	122	PRO	CA-C	5.55	1.57	1.52
3	D	74	SER	CA-C	-5.49	1.48	1.53
1	A	529	PRO	N-CD	5.35	1.55	1.47
2	H	130	PRO	N-CD	5.25	1.55	1.47

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	132	SER	N-CA-C	-19.48	88.63	113.17
3	L	53	VAL	N-CA-C	-18.18	94.78	112.96
1	A	326	GLU	CB-CA-C	-17.00	86.43	110.06
2	H	90	ASP	N-CA-C	-14.46	92.63	112.30
3	L	29	VAL	N-CA-C	-14.18	98.78	112.96
1	A	510	SER	CB-CA-C	-13.69	90.22	111.17
1	A	511	GLN	N-CA-CB	13.49	123.27	109.51
1	A	197	VAL	N-CA-CB	-13.13	95.09	112.16
1	B	531	GLU	N-CA-C	12.37	125.53	110.19
3	L	48	LEU	N-CA-CB	-12.31	89.81	109.87
3	D	126	GLU	N-CA-C	-12.18	98.08	113.43
1	B	530	ARG	N-CA-C	12.17	128.22	111.92
3	D	7	PRO	CB-CA-C	-12.14	91.42	110.49
3	D	7	PRO	N-CA-C	12.11	135.34	114.75
1	B	269	PHE	CB-CA-C	11.89	134.09	110.42
3	L	68	LYS	N-CA-C	11.73	126.61	107.73
1	B	428	ILE	N-CA-C	11.43	124.28	109.30
2	H	62	GLN	N-CA-CB	-11.32	91.07	110.32
3	D	28	ASP	N-CA-C	11.24	127.18	112.12
1	A	511	GLN	N-CA-C	-11.18	95.63	108.49
3	D	160	GLY	N-CA-C	-10.86	100.13	112.29
3	D	23	THR	N-CA-C	-10.62	91.75	109.80
2	H	94	TYR	N-CA-C	10.58	126.33	111.52
2	C	94	TYR	N-CA-C	10.49	125.45	111.28
1	B	512	PHE	N-CA-C	10.41	123.22	110.41
3	D	53	VAL	N-CA-CB	10.36	128.32	111.23
1	A	546	GLN	N-CA-CB	-10.08	92.42	110.37
3	D	67	SER	CB-CA-C	-10.02	92.79	110.03
3	D	79	GLY	N-CA-C	-9.81	93.70	111.25
3	L	53	VAL	N-CA-CB	9.78	132.31	112.75
3	D	205	SER	N-CA-C	9.61	124.26	112.54
1	A	386	GLY	N-CA-C	-9.56	99.47	112.57
1	A	546	GLN	N-CA-C	9.51	130.83	109.81
3	L	15	GLY	N-CA-C	-9.50	100.83	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	TYR	N-CA-C	9.49	122.77	110.53
1	A	240	GLY	N-CA-C	-9.44	90.81	113.18
1	A	531	GLU	N-CA-C	9.37	120.25	108.45
3	D	22	CYS	N-CA-C	9.01	125.34	111.56
1	B	178	LYS	N-CA-C	8.98	121.98	111.02
3	D	3	ALA	N-CA-C	8.89	122.77	110.24
1	A	196	THR	N-CA-C	8.86	123.64	113.01
2	C	88	SER	N-CA-C	-8.79	94.95	108.31
3	D	81	GLN	N-CA-C	-8.66	97.67	110.23
1	A	387	TYR	N-CA-CB	-8.63	98.10	110.44
3	L	49	MET	N-CA-C	-8.62	94.58	108.55
2	C	62	GLN	CB-CA-C	-8.51	97.19	110.04
3	L	52	ASP	CA-C-N	-8.51	112.23	121.84
3	L	52	ASP	C-N-CA	-8.51	112.23	121.84
1	B	428	ILE	CB-CA-C	-8.38	98.48	111.71
1	B	100	PRO	N-CA-C	8.34	129.65	112.47
1	A	313	SER	N-CA-C	8.26	121.86	111.69
1	A	177	CYS	CB-CA-C	8.20	122.56	110.26
3	D	25	THR	N-CA-C	8.18	123.04	110.36
1	B	250	VAL	CA-C-N	8.14	133.73	120.94
1	B	250	VAL	C-N-CA	8.14	133.73	120.94
1	A	431	LEU	N-CA-C	8.13	123.75	112.45
1	B	494	ALA	CB-CA-C	-8.11	98.48	110.16
1	B	37	ASN	N-CA-C	8.10	122.33	107.99
1	A	556	GLY	CA-C-N	8.10	129.96	119.84
1	A	556	GLY	C-N-CA	8.10	129.96	119.84
1	B	7	THR	CB-CA-C	-8.03	94.41	110.30
3	D	28	ASP	CB-CA-C	-7.95	98.07	111.26
3	L	9	SER	CB-CA-C	-7.91	94.67	110.42
3	D	32	TYR	N-CA-C	7.91	124.72	114.75
1	B	527	GLY	N-CA-C	7.90	119.53	111.56
3	D	125	ASP	CB-CA-C	-7.86	94.78	110.42
3	D	140	ASN	N-CA-C	7.83	120.57	111.02
2	H	132	SER	N-CA-CB	7.79	122.03	110.49
3	L	84	ASP	N-CA-C	-7.79	100.88	111.87
1	A	111	SER	CA-C-N	-7.74	110.17	119.84
1	A	111	SER	C-N-CA	-7.74	110.17	119.84
1	B	72	VAL	CA-C-N	7.72	129.50	119.84
1	B	72	VAL	C-N-CA	7.72	129.50	119.84
1	A	100	PRO	CB-CA-C	-7.61	99.01	111.56
1	A	177	CYS	N-CA-C	-7.57	98.47	109.59
1	A	432	GLY	N-CA-C	7.56	125.87	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	195	THR	N-CA-CB	-7.46	97.87	110.49
1	B	528	LEU	CA-C-N	-7.46	110.51	119.84
1	B	528	LEU	C-N-CA	-7.46	110.51	119.84
3	L	45	ALA	CA-C-N	7.45	127.45	119.78
3	L	45	ALA	C-N-CA	7.45	127.45	119.78
1	A	545	CYS	N-CA-CB	-7.43	97.94	110.49
2	H	148	ASP	N-CA-C	7.39	121.44	111.24
2	H	62	GLN	N-CA-C	7.36	121.35	112.38
1	A	291	LEU	N-CA-C	-7.35	104.83	114.31
1	B	162	ILE	N-CA-C	7.30	118.63	108.12
2	C	190	SER	N-CA-C	-7.30	104.26	113.02
3	D	69	SER	N-CA-C	-7.28	99.68	110.23
1	A	314	LYS	N-CA-C	-7.26	96.13	109.06
2	H	60	TYR	CB-CA-C	-7.25	94.23	109.38
2	H	61	ALA	N-CA-C	-7.17	99.67	110.28
1	A	544	GLU	CB-CA-C	-7.17	100.35	111.74
3	L	143	TYR	N-CA-C	-7.10	97.47	108.55
3	L	17	SER	N-CA-C	-7.09	91.14	111.00
2	H	149	TYR	N-CA-C	7.08	119.88	109.69
3	D	8	ALA	CB-CA-C	-7.02	101.76	111.73
3	L	70	GLY	N-CA-C	-7.00	102.02	111.54
1	A	303	GLU	N-CA-C	-6.98	103.67	111.28
1	A	313	SER	CB-CA-C	-6.97	97.95	110.70
3	L	140	ASN	N-CA-C	6.96	118.65	111.14
1	A	100	PRO	N-CA-C	6.92	126.73	112.47
3	D	54	SER	N-CA-C	6.92	118.94	109.11
3	D	164	GLU	N-CA-C	6.88	119.28	107.93
3	D	55	LYS	N-CA-C	6.83	119.61	108.55
3	D	69	SER	CB-CA-C	6.82	121.04	109.72
2	C	129	ALA	CA-C-N	6.74	128.26	119.84
2	C	129	ALA	C-N-CA	6.74	128.26	119.84
1	B	29	GLN	N-CA-C	6.71	125.09	110.80
1	B	494	ALA	N-CA-C	6.66	119.88	109.96
3	D	204	LEU	N-CA-C	-6.61	101.23	110.35
1	B	10	LYS	CB-CA-C	-6.58	108.99	116.63
2	H	142	LEU	N-CA-C	6.53	119.12	108.08
1	B	397	LEU	CA-C-N	6.53	127.49	120.83
1	B	397	LEU	C-N-CA	6.53	127.49	120.83
1	B	525	LEU	CB-CA-C	6.52	119.59	109.03
3	D	211	SER	N-CA-C	6.46	120.02	109.24
3	D	142	PHE	N-CA-C	6.43	116.95	107.88
1	A	510	SER	N-CA-C	-6.40	106.18	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	48	LEU	N-CA-C	6.37	119.00	109.25
1	B	269	PHE	N-CA-C	-6.32	97.34	110.80
2	C	89	ASP	N-CA-C	-6.29	93.39	111.00
2	H	61	ALA	CB-CA-C	-6.28	98.92	109.65
1	B	385	THR	N-CA-C	-6.25	99.02	108.96
1	A	548	GLN	N-CA-C	6.12	118.79	110.35
2	H	60	TYR	N-CA-C	6.10	119.14	109.50
1	B	314	LYS	N-CA-C	-6.09	103.12	110.13
2	C	191	SER	O-C-N	6.08	128.57	122.12
3	D	123	PRO	CA-N-CD	-6.08	103.49	112.00
3	D	10	VAL	N-CA-C	6.07	117.54	110.62
3	D	118	VAL	N-CA-C	6.05	115.06	106.53
1	B	429	SER	N-CA-C	6.05	119.13	111.69
1	A	533	VAL	N-CA-C	6.01	116.59	108.17
3	D	190	GLU	N-CA-C	6.01	119.08	111.69
1	A	544	GLU	N-CA-C	6.00	120.95	108.53
1	A	277	CYS	CA-C-N	5.95	126.29	119.92
1	A	277	CYS	C-N-CA	5.95	126.29	119.92
2	C	88	SER	CA-C-N	5.95	132.41	121.70
2	C	88	SER	C-N-CA	5.95	132.41	121.70
3	D	74	SER	N-CA-C	5.95	117.69	107.28
3	D	45	ALA	O-C-N	5.94	128.15	121.32
1	A	419	TYR	N-CA-C	5.92	118.47	107.99
1	B	539	LEU	CA-C-N	-5.92	113.69	119.78
1	B	539	LEU	C-N-CA	-5.92	113.69	119.78
2	H	61	ALA	N-CA-CB	-5.89	101.32	109.97
2	H	141	ALA	N-CA-C	5.88	123.33	110.80
1	A	101	LEU	N-CA-CB	5.88	120.49	110.50
3	D	48	LEU	N-CA-CB	-5.86	101.62	110.35
3	D	29	VAL	N-CA-C	-5.86	97.16	109.34
3	L	16	GLN	CA-C-N	5.83	132.20	121.70
3	L	16	GLN	C-N-CA	5.83	132.20	121.70
1	B	178	LYS	CB-CA-C	-5.81	101.69	110.92
1	A	325	MET	CB-CA-C	5.76	125.47	111.65
1	A	43	LEU	CA-C-N	5.74	125.65	119.85
1	A	43	LEU	C-N-CA	5.74	125.65	119.85
3	D	160	GLY	CA-C-O	-5.72	118.28	122.23
1	A	326	GLU	N-CA-C	-5.68	101.78	110.30
1	B	455	VAL	N-CA-C	-5.67	105.20	110.53
1	A	20	HIS	N-CA-C	5.64	117.88	111.11
1	A	530	ARG	N-CA-C	5.62	122.78	110.80
2	H	195	THR	N-CA-C	-5.61	105.53	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	9	SER	CA-C-O	5.59	128.50	120.51
3	L	67	SER	CB-CA-C	-5.58	98.84	109.66
3	L	72	THR	CA-C-N	5.55	131.69	121.70
3	L	72	THR	C-N-CA	5.55	131.69	121.70
1	B	328	LEU	N-CA-C	-5.55	105.49	114.09
1	B	127	LEU	N-CA-C	5.53	117.74	111.11
1	B	512	PHE	N-CA-CB	-5.52	102.81	110.38
1	A	136	ASN	CA-C-N	5.52	126.73	119.84
1	A	136	ASN	C-N-CA	5.52	126.73	119.84
1	B	533	VAL	N-CA-C	5.51	116.04	107.28
3	D	13	SER	CA-C-N	5.49	126.70	119.84
3	D	13	SER	C-N-CA	5.49	126.70	119.84
1	B	502	GLY	CA-C-N	5.48	125.17	119.64
1	B	502	GLY	C-N-CA	5.48	125.17	119.64
1	B	556	GLY	CA-C-N	-5.47	113.00	119.84
1	B	556	GLY	C-N-CA	-5.47	113.00	119.84
1	B	100	PRO	CB-CA-C	-5.47	102.53	111.56
2	H	129	ALA	CA-C-N	-5.47	113.00	119.84
2	H	129	ALA	C-N-CA	-5.47	113.00	119.84
3	L	22	CYS	CA-C-N	5.46	131.52	121.70
3	L	22	CYS	C-N-CA	5.46	131.52	121.70
3	D	34	TYR	N-CA-C	-5.45	102.02	109.71
1	B	426	LEU	N-CA-C	5.44	118.86	110.42
2	C	95	TYR	N-CA-C	5.39	118.10	110.50
3	D	65	SER	N-CA-C	5.38	116.20	107.32
1	A	72	VAL	CA-C-N	5.36	126.54	119.84
1	A	72	VAL	C-N-CA	5.36	126.54	119.84
1	B	137	PRO	CA-C-O	-5.36	115.31	121.36
3	L	21	SER	N-CA-C	5.35	118.87	111.71
3	D	72	THR	CA-C-N	5.34	131.31	121.70
3	D	72	THR	C-N-CA	5.34	131.31	121.70
1	B	305	GLY	N-CA-C	5.33	120.32	114.40
1	A	431	LEU	CB-CA-C	-5.33	100.03	110.11
1	A	13	LEU	CA-C-N	5.31	126.47	119.84
1	A	13	LEU	C-N-CA	5.31	126.47	119.84
2	C	129	ALA	N-CA-C	5.30	118.75	109.48
3	L	21	SER	CA-C-N	-5.28	111.45	121.54
3	L	21	SER	C-N-CA	-5.28	111.45	121.54
1	B	1	THR	CB-CA-C	5.28	120.71	109.10
2	H	122	GLY	CA-C-N	5.27	126.09	120.13
2	H	122	GLY	C-N-CA	5.27	126.09	120.13
2	C	120	THR	N-CA-C	5.26	117.32	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	HIS	CA-C-N	-5.25	114.38	119.78
1	A	171	HIS	C-N-CA	-5.25	114.38	119.78
2	H	99	GLU	N-CA-C	5.23	117.05	108.52
1	A	195	ARG	N-CA-C	5.22	121.92	110.80
2	C	180	TYR	N-CA-C	5.17	117.20	110.53
1	B	198	CYS	N-CA-C	5.17	118.13	110.48
2	H	205	LYS	CA-C-N	-5.16	114.39	120.12
2	H	205	LYS	C-N-CA	-5.16	114.39	120.12
3	L	143	TYR	CA-C-O	-5.14	115.77	120.50
1	A	195	ARG	CB-CA-C	-5.13	100.21	110.42
3	L	81	GLN	N-CA-C	-5.11	100.55	108.31
1	B	328	LEU	N-CA-CB	5.10	118.97	111.01
3	D	70	GLY	N-CA-C	-5.10	105.23	112.37
3	L	9	SER	CA-C-N	5.09	131.14	121.97
3	L	9	SER	C-N-CA	5.09	131.14	121.97
1	B	331	VAL	N-CA-C	5.08	115.62	108.36
3	D	53	VAL	N-CA-C	-5.05	98.83	109.34
2	C	170	PHE	N-CA-C	5.05	117.62	110.40
2	H	102	GLY	N-CA-C	-5.03	107.15	114.90
3	D	80	LEU	N-CA-C	-5.03	97.82	107.57

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	SER	Peptide
1	A	247	PRO	Mainchain
1	A	77	LEU	Peptide
1	B	529	PRO	Peptide
2	C	190	SER	Peptide
2	C	88	SER	Peptide
3	D	121	PHE	Mainchain
3	D	159	SER	Peptide
3	D	22	CYS	Peptide
3	D	63	ARG	Peptide
3	D	67	SER	Peptide
3	D	8	ALA	Peptide
2	H	152	GLU	Peptide
3	L	16	GLN	Peptide
3	L	22	CYS	Peptide
3	L	63	ARG	Peptide
3	L	67	SER	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	4277	0	4106	148	0
1	B	4277	0	4108	226	3
2	C	1624	0	1567	111	2
2	H	1624	0	1567	82	1
3	D	1616	0	1548	149	0
3	L	1616	0	1548	93	0
4	E	28	0	25	8	0
5	B	14	0	13	10	0
6	A	27	0	0	4	0
6	B	14	0	0	1	0
6	C	12	0	0	6	0
6	D	19	0	0	4	0
6	H	2	0	0	0	0
6	L	5	0	0	1	0
All	All	15155	0	14482	789	3

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 27.

All (789) 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:B:546:GLN:CG	1:B:548:GLN:HG3	1.37	1.53
3:D:123:PRO:HB2	3:D:127:GLN:CD	1.29	1.52
1:A:237:ASN:HD21	4:E:1:NAG:C1	1.21	1.47
3:D:123:PRO:CB	3:D:127:GLN:NE2	1.79	1.44
1:B:250:VAL:CB	1:B:260:MET:O	1.69	1.39
1:B:546:GLN:HG2	1:B:548:GLN:CG	1.52	1.36
2:H:131:SER:OG	2:H:133:LYS:HB3	1.23	1.33
3:D:123:PRO:HB2	3:D:127:GLN:NE2	1.01	1.32
2:H:131:SER:OG	2:H:133:LYS:CB	1.77	1.31
1:A:553:THR:HG22	6:A:1114:HOH:O	1.36	1.24
1:B:250:VAL:HG12	1:B:261:PRO:CA	1.67	1.23
1:B:250:VAL:HB	1:B:260:MET:O	1.12	1.23
1:A:238:HIS:HB2	1:A:273:CYS:SG	1.79	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:131:SER:OG	2:H:133:LYS:CA	1.88	1.21
2:H:131:SER:OG	2:H:133:LYS:N	1.73	1.21
3:D:23:THR:CG2	3:D:72:THR:HG22	1.69	1.20
1:B:549:ASN:O	1:B:550:GLY:O	1.60	1.20
3:D:22:CYS:CB	3:D:73:ALA:HB1	1.71	1.19
1:B:250:VAL:CG1	1:B:261:PRO:HA	1.76	1.16
2:C:128:LEU:HD22	3:D:122:PRO:O	1.43	1.15
3:L:94:THR:HG22	3:L:96:SER:H	1.12	1.15
3:D:22:CYS:HB2	3:D:73:ALA:CB	1.74	1.15
1:A:553:THR:CG2	6:A:1114:HOH:O	1.90	1.13
1:B:237:ASN:CG	5:B:1001:NAG:C1	2.19	1.12
1:A:528:LEU:O	1:A:530:ARG:N	1.83	1.11
3:D:123:PRO:CB	3:D:127:GLN:CD	2.19	1.10
1:B:546:GLN:O	1:B:548:GLN:N	1.86	1.08
1:B:250:VAL:CG1	1:B:260:MET:O	2.02	1.08
1:A:326:GLU:O	1:A:327:HIS:HB3	1.54	1.07
1:B:545:CYS:SG	1:B:562:CYS:SG	1.31	1.07
3:D:23:THR:HG22	3:D:72:THR:HG22	1.35	1.06
1:A:528:LEU:C	1:A:530:ARG:H	1.63	1.05
1:A:528:LEU:HB2	1:A:529:PRO:HD3	1.37	1.05
1:B:247:PRO:HB2	1:B:265:GLY:HA2	1.32	1.04
2:C:128:LEU:CD2	3:D:122:PRO:O	2.05	1.04
2:C:130:PRO:HG2	2:C:193:LEU:HD11	1.38	1.04
3:D:131:GLY:HA2	3:D:186:LYS:HB2	1.40	1.04
1:B:542:HIS:CE1	1:B:543:PRO:HD2	1.92	1.04
1:B:546:GLN:CG	1:B:548:GLN:CG	2.23	1.03
3:L:9:SER:C	3:L:11:SER:H	1.66	1.03
2:C:130:PRO:HG3	2:C:142:LEU:HB3	1.38	1.02
3:D:24:GLY:O	3:D:71:ASN:HB3	1.63	0.99
1:B:553:THR:HG22	1:B:554:CYS:H	1.24	0.99
1:B:546:GLN:C	1:B:548:GLN:H	1.69	0.98
3:D:67:SER:O	3:D:68:LYS:HB2	1.58	0.98
1:B:545:CYS:O	1:B:546:GLN:HB2	1.61	0.98
2:C:189:PRO:HB3	2:C:191:SER:HB3	1.42	0.98
1:B:237:ASN:ND2	5:B:1001:NAG:O5	1.94	0.97
3:L:9:SER:O	3:L:11:SER:N	1.96	0.97
1:A:384:ILE:HG22	1:A:386:GLY:O	1.65	0.95
3:D:94:THR:HG22	3:D:96:SER:H	1.28	0.95
1:B:546:GLN:HE21	1:B:548:GLN:CB	1.79	0.95
1:B:541:CYS:O	1:B:542:HIS:O	1.84	0.95
1:B:553:THR:HG22	1:B:554:CYS:N	1.82	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:23:THR:CG2	3:D:72:THR:CG2	2.46	0.94
3:D:123:PRO:CA	3:D:127:GLN:NE2	2.31	0.94
1:A:554:CYS:SG	1:A:555:PHE:N	2.35	0.94
2:H:131:SER:HG	2:H:133:LYS:HB3	1.12	0.94
1:A:528:LEU:HB2	1:A:529:PRO:CD	1.98	0.93
3:D:16:GLN:HA	3:D:17:SER:HB3	1.51	0.93
3:L:72:THR:HA	3:L:73:ALA:HB3	1.48	0.93
1:B:250:VAL:HG12	1:B:261:PRO:HA	0.94	0.92
3:D:23:THR:CB	3:D:72:THR:HG22	1.98	0.92
1:A:237:ASN:HD21	4:E:1:NAG:C2	1.82	0.91
3:D:69:SER:O	3:D:72:THR:O	1.87	0.91
3:L:9:SER:OG	3:L:10:VAL:N	1.98	0.91
1:B:237:ASN:HD21	5:B:1001:NAG:C1	1.56	0.91
3:L:35:VAL:O	3:L:52:ASP:O	1.91	0.89
1:B:545:CYS:CB	1:B:562:CYS:SG	2.61	0.88
3:D:72:THR:HA	3:D:73:ALA:HB3	1.56	0.87
1:B:545:CYS:O	1:B:546:GLN:CB	2.22	0.87
2:H:131:SER:HG	2:H:133:LYS:CB	1.73	0.87
2:C:51:ILE:HG12	2:C:58:THR:HG22	1.54	0.86
1:B:327:HIS:O	1:B:327:HIS:CD2	2.28	0.86
3:D:16:GLN:CA	3:D:17:SER:HB3	2.05	0.86
1:B:546:GLN:HE21	1:B:548:GLN:CD	1.83	0.86
1:A:510:SER:O	1:A:511:GLN:OE1	1.94	0.86
2:C:203:ASN:HD21	2:C:205:LYS:HG3	1.40	0.86
1:B:546:GLN:NE2	1:B:548:GLN:HB2	1.89	0.86
3:D:123:PRO:C	3:D:127:GLN:HE21	1.84	0.86
1:B:528:LEU:HB2	1:B:529:PRO:HD3	1.56	0.85
3:L:13:SER:HA	3:L:110:LEU:HB2	1.56	0.85
4:E:1:NAG:O3	4:E:2:NAG:O5	1.93	0.85
1:A:238:HIS:HB2	1:A:273:CYS:CB	2.06	0.85
3:L:72:THR:HA	3:L:73:ALA:CB	2.07	0.84
1:B:250:VAL:HA	1:B:262:ASN:H	1.42	0.83
1:B:553:THR:O	1:B:554:CYS:O	1.95	0.83
1:A:532:TYR:HB3	1:A:554:CYS:SG	2.17	0.83
3:D:23:THR:HB	3:D:72:THR:CG2	2.08	0.83
2:C:142:LEU:HD22	2:C:193:LEU:HD12	1.60	0.83
2:H:131:SER:CB	2:H:133:LYS:HB3	2.09	0.83
1:B:546:GLN:NE2	1:B:548:GLN:CB	2.41	0.82
1:B:83:THR:HG22	1:B:84:GLN:HG3	1.61	0.82
1:B:546:GLN:HG3	1:B:548:GLN:HG3	1.58	0.82
3:D:72:THR:HA	3:D:73:ALA:CB	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:29:VAL:HG21	3:L:73:ALA:HB2	1.59	0.82
1:B:250:VAL:HB	1:B:260:MET:C	2.05	0.82
1:A:144:THR:HG21	1:A:182:CYS:H	1.44	0.81
3:D:123:PRO:HB2	3:D:127:GLN:HE21	1.41	0.81
1:B:250:VAL:HG12	1:B:260:MET:O	1.76	0.81
2:C:139:THR:O	6:C:308:HOH:O	1.98	0.81
1:B:272:SER:HB3	5:B:1001:NAG:O7	1.81	0.81
1:A:524:VAL:HG11	1:A:533:VAL:HG22	1.61	0.81
1:B:553:THR:CG2	1:B:554:CYS:H	1.82	0.81
2:H:131:SER:CB	2:H:133:LYS:H	1.94	0.81
2:H:60:TYR:HE1	2:H:70:MET:HG3	1.45	0.80
1:B:140:CYS:HA	1:B:166:ARG:HH21	1.45	0.80
3:L:40:GLN:O	3:L:86:ALA:HB1	1.81	0.80
1:B:523:ARG:HG2	1:B:527:GLY:HA3	1.62	0.80
2:C:51:ILE:HG13	2:C:70:MET:HB2	1.62	0.80
3:D:123:PRO:C	3:D:127:GLN:NE2	2.40	0.79
3:D:23:THR:HB	3:D:72:THR:HG22	1.62	0.79
2:C:142:LEU:CD2	2:C:193:LEU:HD12	2.12	0.79
1:B:428:ILE:O	1:B:428:ILE:HG13	1.81	0.79
1:B:541:CYS:C	1:B:542:HIS:O	2.23	0.79
3:D:120:ILE:HD12	3:D:212:PHE:HB3	1.62	0.79
1:A:253:ASN:ND2	1:A:256:THR:OG1	2.13	0.79
3:L:23:THR:HB	3:L:72:THR:OG1	1.82	0.79
3:L:9:SER:C	3:L:11:SER:N	2.33	0.78
1:B:545:CYS:SG	1:B:562:CYS:CB	2.72	0.78
1:B:546:GLN:HE21	1:B:548:GLN:CG	1.96	0.78
2:C:128:LEU:HD23	3:D:123:PRO:HA	1.64	0.78
2:H:89:ASP:CG	2:H:89:ASP:O	2.24	0.77
2:H:91:THR:HG23	2:H:114:THR:HA	1.68	0.76
1:A:362:ASP:HB3	1:A:367:THR:HG23	1.66	0.76
3:L:20:ILE:HD12	3:L:20:ILE:H	1.50	0.76
2:C:193:LEU:HA	2:C:198:TYR:HE2	1.50	0.76
3:D:123:PRO:CB	3:D:127:GLN:HE22	1.94	0.75
1:A:18:GLU:N	1:A:18:GLU:OE1	2.18	0.75
1:A:238:HIS:CB	1:A:273:CYS:SG	2.69	0.75
2:H:190:SER:HA	2:H:193:LEU:HD13	1.67	0.75
1:B:546:GLN:HG3	1:B:548:GLN:HE21	1.49	0.75
3:L:20:ILE:HD12	3:L:20:ILE:N	2.02	0.75
1:B:237:ASN:HD21	5:B:1001:NAG:H61	1.52	0.75
2:C:142:LEU:HD22	2:C:193:LEU:CD1	2.16	0.75
1:B:250:VAL:CA	1:B:260:MET:O	2.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:133:LYS:HZ1	3:D:212:PHE:HB2	1.52	0.74
2:H:48:MET:HG2	2:H:64:LEU:HD21	1.68	0.74
1:A:250:VAL:HG21	1:A:259:SER:HB3	1.70	0.73
3:L:94:THR:HG22	3:L:96:SER:N	1.97	0.73
2:C:158:TRP:HZ3	2:C:198:TYR:HB3	1.50	0.73
1:B:81:ARG:HG2	1:B:127:LEU:HD12	1.70	0.73
1:A:326:GLU:O	1:A:327:HIS:CB	2.34	0.73
1:B:438:GLU:OE2	1:B:465:ARG:NH1	2.22	0.73
1:B:542:HIS:NE2	1:B:543:PRO:HD2	2.03	0.72
3:L:5:THR:O	3:L:22:CYS:C	2.33	0.72
1:B:541:CYS:O	1:B:542:HIS:C	2.32	0.72
1:B:546:GLN:HG3	1:B:548:GLN:NE2	2.04	0.72
3:D:124:SER:C	3:D:126:GLU:H	1.98	0.72
1:A:528:LEU:HD23	1:A:528:LEU:N	2.05	0.72
1:A:256:THR:HB	1:A:258:GLU:HG3	1.71	0.71
1:B:530:ARG:O	1:B:530:ARG:HG3	1.88	0.71
1:A:453:CYS:SG	1:A:477:ARG:NH1	2.63	0.71
3:L:83:GLU:HA	3:L:85:GLU:HG3	1.73	0.71
2:C:194:GLY:HA3	2:C:217:PRO:HG2	1.72	0.71
1:B:22:ASP:OD1	1:B:25:ARG:NH1	2.23	0.71
3:L:14:PRO:HD3	3:L:110:LEU:H	1.56	0.71
3:D:123:PRO:O	3:D:124:SER:OG	2.07	0.71
1:A:140:CYS:HA	1:A:166:ARG:HH21	1.54	0.71
3:L:41:HIS:HB3	3:L:42:PRO:HD2	1.71	0.71
3:L:16:GLN:HB2	3:L:17:SER:OG	1.91	0.71
1:B:237:ASN:HD21	5:B:1001:NAG:C6	2.04	0.70
1:B:546:GLN:HG2	1:B:548:GLN:CB	2.21	0.70
2:H:38:ARG:HB3	2:H:48:MET:HE2	1.73	0.70
3:D:50:ILE:HG21	3:D:56:ARG:HG2	1.73	0.70
1:A:529:PRO:O	1:A:530:ARG:O	2.10	0.69
1:B:546:GLN:NE2	1:B:548:GLN:CD	2.50	0.69
3:L:22:CYS:HB3	3:L:23:THR:HA	1.74	0.69
2:H:16:GLU:O	2:H:86:LEU:HB2	1.92	0.69
3:L:5:THR:O	3:L:22:CYS:O	2.11	0.69
1:A:279:TYR:OH	1:A:438:GLU:OE2	2.11	0.69
1:B:250:VAL:CG1	1:B:260:MET:C	2.64	0.69
1:B:524:VAL:HG11	1:B:533:VAL:HG22	1.76	0.68
1:A:347:LYS:HE2	1:A:349:PHE:CZ	2.28	0.68
1:B:237:ASN:OD1	5:B:1001:NAG:C1	2.42	0.68
3:D:133:ALA:N	3:D:184:LEU:O	2.26	0.68
1:B:237:ASN:HD21	5:B:1001:NAG:C5	2.05	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:131:SER:O	2:H:135:THR:HG23	1.94	0.68
3:L:67:SER:O	3:L:68:LYS:HB2	1.92	0.68
1:B:33:VAL:HG13	1:B:57:GLU:HB2	1.76	0.68
2:H:51:ILE:HG12	2:H:58:THR:HG22	1.75	0.67
1:B:542:HIS:CG	1:B:543:PRO:CD	2.77	0.67
1:A:249:LEU:HD11	1:A:267:TYR:CZ	2.28	0.67
2:C:151:PRO:HD2	2:C:206:PRO:HB3	1.77	0.67
3:D:111:GLY:O	6:D:314:HOH:O	2.12	0.67
1:A:528:LEU:C	1:A:530:ARG:N	2.33	0.67
1:B:494:ALA:HB3	1:B:508:ASN:HB3	1.76	0.67
2:H:64:LEU:HB3	2:H:68:VAL:HG22	1.76	0.66
1:B:263:PRO:O	1:B:264:GLU:HG2	1.96	0.66
2:H:150:PHE:HD2	2:H:179:LEU:HD23	1.60	0.66
3:D:52:ASP:O	3:D:53:VAL:HG22	1.96	0.66
3:D:18:ILE:HG22	3:D:19:THR:H	1.59	0.66
3:L:143:TYR:O	3:L:201:HIS:NE2	2.29	0.66
3:D:67:SER:O	3:D:68:LYS:CB	2.41	0.66
1:B:374:GLN:O	1:B:377:VAL:HG13	1.94	0.66
2:C:91:THR:HG23	2:C:114:THR:HA	1.77	0.66
3:D:150:GLN:O	6:D:307:HOH:O	2.13	0.66
1:B:247:PRO:CB	1:B:265:GLY:HA2	2.19	0.66
3:D:8:ALA:HA	3:D:105:THR:HA	1.78	0.66
2:H:51:ILE:HD11	2:H:70:MET:C	2.22	0.65
3:D:94:THR:HG22	3:D:96:SER:N	2.07	0.65
2:C:183:SER:OG	2:C:184:SER:N	2.29	0.65
3:D:16:GLN:HA	3:D:17:SER:CB	2.26	0.65
1:A:407:GLN:HA	1:A:435:SER:O	1.97	0.65
3:D:23:THR:HG21	3:D:72:THR:CG2	2.25	0.65
1:B:284:THR:HG22	1:B:287:GLY:H	1.62	0.65
1:A:266:ARG:HG2	1:A:266:ARG:HH11	1.62	0.65
2:H:130:PRO:O	2:H:131:SER:HB3	1.96	0.65
3:D:139:LEU:HD22	3:D:178:LEU:HB3	1.79	0.65
1:A:22:ASP:OD1	1:A:25:ARG:NH1	2.29	0.65
2:C:139:THR:HA	2:C:190:SER:H	1.60	0.65
1:B:284:THR:HG22	1:B:288:SER:H	1.62	0.64
1:B:144:THR:HG21	1:B:182:CYS:H	1.62	0.64
2:H:125:VAL:HG21	2:H:211:VAL:HG11	1.79	0.64
3:D:139:LEU:HB3	3:D:142:PHE:CE2	2.33	0.64
1:A:51:PHE:CE1	1:A:52:LEU:HD13	2.32	0.64
1:A:404:GLN:OE1	1:A:434:ARG:NH1	2.30	0.64
3:L:8:ALA:HA	3:L:106:LYS:H	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:HD13	1:B:161:LEU:HD23	1.80	0.64
1:B:542:HIS:HB2	1:B:557:PRO:O	1.97	0.64
3:D:25:THR:N	3:D:28:ASP:OD2	2.28	0.64
1:B:325:MET:O	1:B:329:ARG:HB3	1.98	0.63
3:D:23:THR:HB	3:D:72:THR:HG23	1.80	0.63
3:D:139:LEU:HB3	3:D:142:PHE:HE2	1.61	0.63
1:B:324:GLY:HA2	1:B:329:ARG:HA	1.81	0.63
1:B:542:HIS:CD2	1:B:543:PRO:HD2	2.32	0.63
2:C:51:ILE:HG21	2:C:72:THR:HG23	1.81	0.63
3:D:17:SER:HB3	3:D:78:SER:O	1.98	0.63
1:A:459:PRO:HB2	1:A:462:GLN:HG3	1.81	0.63
3:D:23:THR:CB	3:D:72:THR:CG2	2.67	0.63
1:B:237:ASN:ND2	5:B:1001:NAG:H61	2.14	0.62
1:B:250:VAL:HG12	1:B:260:MET:C	2.23	0.62
1:B:546:GLN:NE2	1:B:548:GLN:CG	2.61	0.62
1:A:265:GLY:O	1:A:266:ARG:HD3	1.99	0.62
3:D:22:CYS:HB2	3:D:73:ALA:HB1	0.81	0.62
3:D:132:THR:HA	3:D:185:SER:HA	1.82	0.62
2:C:135:THR:HA	6:C:308:HOH:O	1.98	0.62
3:D:24:GLY:O	3:D:71:ASN:CB	2.44	0.62
1:B:327:HIS:O	1:B:327:HIS:CG	2.48	0.62
1:B:383:GLU:OE1	1:B:410:ARG:NE	2.27	0.62
1:A:238:HIS:HB2	1:A:273:CYS:HB2	1.80	0.62
1:B:250:VAL:HA	1:B:262:ASN:N	2.13	0.62
1:B:335:THR:N	1:B:338:ASN:OD1	2.29	0.62
2:H:6:GLN:H	2:H:109:GLN:HE22	1.47	0.62
1:B:478:PRO:HB2	1:B:481:GLU:HB2	1.81	0.62
3:D:182:LEU:HG	3:D:184:LEU:HG	1.82	0.62
3:L:7:PRO:HG2	3:L:105:THR:HG21	1.82	0.62
3:D:16:GLN:CB	3:D:17:SER:HB3	2.30	0.62
1:A:335:THR:HG23	1:A:337:ALA:H	1.65	0.61
1:B:7:THR:O	1:B:39:GLU:OE1	2.18	0.61
1:B:144:THR:CG2	1:B:182:CYS:H	2.13	0.61
2:C:194:GLY:CA	2:C:217:PRO:HD2	2.30	0.61
1:A:175:PRO:O	3:D:32:TYR:OH	2.13	0.61
3:D:8:ALA:H	3:D:105:THR:HG22	1.65	0.61
1:A:141:TYR:OH	1:A:185:GLU:HG2	2.00	0.61
3:D:123:PRO:HB2	3:D:127:GLN:CG	2.25	0.61
3:L:143:TYR:O	3:L:201:HIS:CE1	2.54	0.60
2:C:189:PRO:HB2	2:C:192:SER:H	1.66	0.60
3:L:9:SER:C	3:L:10:VAL:HG12	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:VAL:HG22	1:A:133:ILE:HG23	1.83	0.60
1:A:298:GLN:HG2	1:A:312:CYS:SG	2.41	0.60
3:L:71:ASN:OD1	3:L:71:ASN:N	2.32	0.60
2:H:171:PRO:HG2	3:L:166:VAL:H	1.66	0.60
3:D:108:THR:OG1	3:D:169:GLN:NE2	2.33	0.60
1:B:546:GLN:HG2	1:B:548:GLN:HG3	0.64	0.60
1:B:542:HIS:ND1	1:B:543:PRO:HD2	2.16	0.60
1:B:552:VAL:O	1:B:552:VAL:HG13	2.01	0.60
2:C:188:VAL:HG11	2:C:198:TYR:HE1	1.66	0.60
3:D:15:GLY:O	3:D:16:GLN:HB3	2.02	0.60
1:B:284:THR:HG23	1:B:286:VAL:HG13	1.83	0.59
1:B:542:HIS:CD2	1:B:543:PRO:CD	2.86	0.59
3:D:19:THR:HG22	3:D:76:THR:HB	1.85	0.59
3:D:135:VAL:HB	3:D:182:LEU:HD23	1.85	0.59
1:B:300:VAL:HG12	1:B:301:THR:H	1.67	0.59
2:H:60:TYR:CE1	2:H:70:MET:HG3	2.32	0.59
1:A:144:THR:CG2	1:A:182:CYS:H	2.13	0.58
2:C:193:LEU:HA	2:C:198:TYR:CE2	2.35	0.58
3:L:19:THR:HG22	3:L:76:THR:HB	1.83	0.58
3:D:42:PRO:HG3	3:D:168:GLU:HG3	1.84	0.58
1:B:7:THR:OG1	1:B:39:GLU:OE1	2.19	0.58
1:B:546:GLN:C	1:B:548:GLN:N	2.40	0.58
1:A:237:ASN:CG	4:E:1:NAG:C1	2.74	0.58
2:C:18:LEU:HB2	2:C:86:LEU:HD21	1.86	0.58
1:A:523:ARG:HB2	1:A:531:GLU:HB2	1.85	0.58
1:B:51:PHE:CE1	1:B:52:LEU:HD13	2.38	0.58
1:B:209:LEU:HB3	1:B:211:THR:HG22	1.85	0.58
2:C:36:TRP:CE2	2:C:81:MET:HB2	2.39	0.58
3:D:128:LEU:HA	3:D:132:THR:O	2.03	0.58
1:A:141:TYR:O	1:A:144:THR:HG22	2.04	0.57
1:A:237:ASN:ND2	4:E:1:NAG:C7	2.67	0.57
1:B:274:VAL:HG12	1:B:276:ALA:H	1.69	0.57
3:L:16:GLN:HA	3:L:78:SER:O	2.05	0.57
3:L:35:VAL:HB	3:L:53:VAL:HG12	1.86	0.57
2:H:89:ASP:O	2:H:89:ASP:OD2	2.23	0.57
1:A:238:HIS:HA	1:A:273:CYS:HB2	1.84	0.57
1:B:58:VAL:HG11	1:B:62:VAL:HG22	1.86	0.57
3:D:17:SER:CB	3:D:78:SER:O	2.52	0.57
1:B:549:ASN:C	1:B:550:GLY:O	2.46	0.57
2:C:125:VAL:HG11	2:C:211:VAL:HG11	1.87	0.57
2:C:193:LEU:O	2:C:195:THR:CB	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:MET:O	1:B:12:ARG:HB2	2.05	0.56
2:H:149:TYR:CE1	2:H:180:TYR:HB2	2.40	0.56
3:D:72:THR:CA	3:D:73:ALA:HB3	2.32	0.56
1:A:352:LEU:HD12	1:A:384:ILE:HD11	1.87	0.56
3:D:123:PRO:HD2	3:D:124:SER:H	1.70	0.56
1:A:284:THR:HG22	1:A:288:SER:H	1.70	0.56
1:B:248:ALA:O	1:B:262:ASN:HB3	2.06	0.56
2:H:51:ILE:HG22	2:H:52:SER:N	2.20	0.56
3:D:145:ARG:NH2	3:D:166:VAL:HG11	2.20	0.56
1:B:194:THR:OG1	1:B:204:ARG:NH1	2.36	0.56
1:B:544:GLU:O	1:B:545:CYS:HB2	2.05	0.56
1:B:262:ASN:C	1:B:264:GLU:H	2.12	0.56
3:L:8:ALA:HA	3:L:105:THR:HB	1.88	0.56
2:H:150:PHE:CD2	2:H:179:LEU:HD23	2.40	0.56
3:L:22:CYS:HB3	3:L:23:THR:CA	2.35	0.56
2:C:193:LEU:O	2:C:195:THR:N	2.38	0.56
1:B:64:ILE:HD13	1:B:72:VAL:HG21	1.87	0.56
3:D:16:GLN:O	3:D:16:GLN:HG3	2.03	0.56
1:B:141:TYR:O	1:B:144:THR:HG22	2.07	0.55
1:B:215:HIS:CD2	1:B:227:HIS:HB3	2.41	0.55
2:H:6:GLN:H	2:H:109:GLN:NE2	2.03	0.55
2:H:131:SER:HG	2:H:133:LYS:CA	1.99	0.55
3:D:54:SER:HB3	3:D:66:GLY:O	2.07	0.55
3:D:124:SER:O	3:D:127:GLN:N	2.38	0.55
3:L:78:SER:OG	3:L:79:GLY:N	2.29	0.55
1:B:494:ALA:O	1:B:495:ARG:HB2	2.06	0.55
2:H:18:LEU:HD11	2:H:20:ILE:HG13	1.88	0.55
2:C:157:SER:HB3	2:C:201:ASN:HB2	1.89	0.55
3:D:16:GLN:HB2	3:D:17:SER:HB3	1.88	0.55
3:L:22:CYS:H	3:L:37:TRP:HH2	1.54	0.55
1:B:35:GLN:HG2	1:B:59:GLN:NE2	2.22	0.55
2:C:61:ALA:O	2:C:62:GLN:HB2	2.06	0.55
3:D:49:MET:HE3	3:D:60:VAL:HG13	1.88	0.55
3:D:70:GLY:HA2	3:D:72:THR:N	2.22	0.55
1:B:559:ALA:HA	1:B:562:CYS:SG	2.47	0.55
3:L:6:GLN:HB2	3:L:7:PRO:HD2	1.88	0.55
3:D:50:ILE:HD13	3:D:53:VAL:O	2.06	0.55
1:A:1:THR:OG1	1:A:2:GLN:N	2.39	0.55
1:B:489:CYS:SG	1:B:498:CYS:N	2.80	0.55
3:D:124:SER:C	3:D:126:GLU:N	2.65	0.55
2:C:166:GLY:HA3	2:C:187:THR:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ALA:HB2	1:B:355:LEU:HG	1.88	0.55
1:B:503:PRO:HD2	1:B:504:THR:HG22	1.89	0.55
1:B:546:GLN:CG	1:B:548:GLN:CD	2.79	0.55
1:B:63:LEU:HD13	1:B:93:ALA:HB3	1.89	0.54
1:A:248:ALA:O	1:A:262:ASN:ND2	2.37	0.54
1:A:553:THR:HG23	6:A:1114:HOH:O	1.78	0.54
2:C:124:SER:HB3	2:C:126:PHE:CE2	2.42	0.54
2:C:159:ASN:OD1	2:C:199:ILE:N	2.41	0.54
3:D:70:GLY:HA2	3:D:72:THR:H	1.72	0.54
2:C:158:TRP:CZ3	2:C:198:TYR:HB3	2.39	0.54
1:B:249:LEU:O	1:B:262:ASN:N	2.40	0.54
3:D:123:PRO:CA	3:D:127:GLN:HE22	2.10	0.54
1:B:542:HIS:ND1	1:B:543:PRO:CD	2.71	0.54
1:B:557:PRO:HD2	1:B:561:GLN:NE2	2.22	0.54
3:L:50:ILE:HG22	3:L:56:ARG:HA	1.89	0.54
2:C:204:HIS:CE1	2:C:206:PRO:HB2	2.43	0.54
1:B:385:THR:O	1:B:385:THR:OG1	2.26	0.54
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.43	0.54
1:B:542:HIS:CG	1:B:543:PRO:N	2.75	0.54
2:C:4:LEU:O	2:C:108:GLY:HA2	2.08	0.53
2:C:128:LEU:HD23	3:D:122:PRO:O	2.06	0.53
1:B:268:THR:C	1:B:269:PHE:O	2.48	0.53
2:H:18:LEU:HD23	2:H:86:LEU:HD11	1.89	0.53
2:C:45:LEU:HG	3:D:89:TYR:CZ	2.44	0.53
2:C:189:PRO:CB	2:C:191:SER:HB3	2.26	0.53
1:A:554:CYS:SG	1:A:556:GLY:N	2.82	0.53
3:L:23:THR:CB	3:L:72:THR:OG1	2.55	0.53
1:A:450:THR:O	1:A:477:ARG:HB2	2.07	0.53
1:A:253:ASN:HD22	1:A:256:THR:HG1	1.51	0.53
1:B:95:LEU:HD23	1:B:134:GLN:HB3	1.90	0.53
1:B:250:VAL:CG1	1:B:261:PRO:CA	2.57	0.53
1:B:183:TRP:N	1:B:189:ASP:O	2.31	0.53
2:C:159:ASN:N	2:C:199:ILE:O	2.35	0.52
3:D:6:GLN:HB2	3:D:105:THR:CG2	2.39	0.52
1:A:443:LEU:HD23	1:A:469:GLN:HA	1.91	0.52
1:B:143:ASP:OD1	1:B:143:ASP:N	2.40	0.52
2:H:157:SER:OG	2:H:161:GLY:N	2.41	0.52
1:B:248:ALA:O	1:B:265:GLY:HA3	2.10	0.52
1:B:555:PHE:HB2	1:B:562:CYS:HA	1.90	0.52
3:L:21:SER:O	3:L:22:CYS:C	2.50	0.52
1:B:35:GLN:HG2	1:B:59:GLN:HE21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:LEU:HD11	1:B:287:GLY:HA2	1.92	0.52
3:L:200:THR:HG23	3:L:207:PRO:HD3	1.92	0.52
1:A:14:PRO:O	1:A:17:PRO:HD3	2.09	0.52
1:B:262:ASN:O	1:B:264:GLU:N	2.38	0.52
2:C:39:GLN:OE1	3:D:40:GLN:NE2	2.37	0.52
1:B:29:GLN:HA	1:B:51:PHE:HB2	1.92	0.52
1:B:128:LYS:HA	1:B:155:ASN:OD1	2.10	0.52
2:H:95:TYR:CE1	3:L:45:ALA:HB2	2.44	0.52
2:H:167:VAL:O	2:H:168:HIS:ND1	2.43	0.52
3:L:148:LYS:HB3	3:L:200:THR:HB	1.91	0.52
1:B:542:HIS:CE1	1:B:543:PRO:CD	2.81	0.52
1:B:542:HIS:ND1	1:B:543:PRO:N	2.57	0.52
2:C:36:TRP:HB3	2:C:48:MET:HE3	1.91	0.52
2:C:142:LEU:HD13	6:C:306:HOH:O	2.09	0.52
2:C:193:LEU:O	2:C:195:THR:HB	2.10	0.52
3:D:47:LYS:HG3	3:D:48:LEU:N	2.24	0.52
3:D:164:GLU:OE1	3:D:178:LEU:HD21	2.10	0.52
2:H:2:VAL:HB	2:H:106:TYR:CE2	2.45	0.52
1:B:223:THR:O	1:B:223:THR:OG1	2.25	0.51
2:H:67:ARG:NH1	2:H:83:LEU:HD21	2.25	0.51
3:L:53:VAL:O	3:L:66:GLY:O	2.28	0.51
3:L:115:ALA:HB1	3:L:204:LEU:HG	1.92	0.51
2:C:185:VAL:HG21	3:D:138:LEU:HD22	1.91	0.51
3:D:145:ARG:HH21	3:D:166:VAL:HG11	1.76	0.51
1:A:533:VAL:HB	6:A:1111:HOH:O	2.10	0.51
2:H:81:MET:HE1	2:H:83:LEU:HB2	1.92	0.51
3:D:37:TRP:HB2	3:D:50:ILE:H	1.75	0.51
1:A:444:ALA:HB3	1:A:471:LEU:HD23	1.93	0.51
3:L:49:MET:O	3:L:49:MET:HG2	2.09	0.51
1:B:140:CYS:HA	1:B:166:ARG:NH2	2.22	0.51
1:B:528:LEU:HB2	1:B:529:PRO:CD	2.35	0.51
2:H:131:SER:HG	2:H:133:LYS:C	2.19	0.51
1:B:209:LEU:HB2	1:B:212:ASP:OD2	2.10	0.51
2:H:121:LYS:HG3	2:H:122:GLY:H	1.76	0.51
3:D:53:VAL:HG23	3:D:54:SER:N	2.26	0.50
3:D:71:ASN:N	3:D:71:ASN:OD1	2.40	0.50
3:D:123:PRO:HG2	3:D:127:GLN:HB3	1.93	0.50
2:C:64:LEU:HB3	2:C:68:VAL:HG22	1.93	0.50
2:C:123:PRO:HA	2:C:149:TYR:HB3	1.92	0.50
1:A:8:ASP:OD1	1:A:10:LYS:NZ	2.44	0.50
1:A:23:MET:HG3	1:A:419:TYR:OH	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:HG22	1:A:426:LEU:HD21	1.93	0.50
1:B:543:PRO:O	1:B:544:GLU:HB2	2.12	0.50
1:B:542:HIS:CG	1:B:543:PRO:HD2	2.43	0.50
3:L:83:GLU:HB3	6:L:301:HOH:O	2.12	0.50
2:C:73:ASP:OD1	2:C:75:SER:OG	2.28	0.50
3:D:17:SER:C	3:D:18:ILE:HG12	2.36	0.50
2:H:61:ALA:HB3	2:H:64:LEU:HB2	1.93	0.50
2:H:158:TRP:CH2	2:H:200:CYS:HB3	2.46	0.50
3:L:9:SER:O	3:L:10:VAL:HG12	2.10	0.50
3:D:135:VAL:HG12	3:D:151:TRP:CH2	2.46	0.50
1:A:529:PRO:C	1:A:530:ARG:HG3	2.37	0.50
1:A:560:ASP:HB3	1:A:561:GLN:OE1	2.11	0.50
2:H:131:SER:C	2:H:133:LYS:N	2.58	0.50
2:H:205:LYS:HA	2:H:208:ASN:H	1.76	0.50
3:L:72:THR:CA	3:L:73:ALA:HB3	2.33	0.50
1:A:344:GLY:HA2	1:A:380:THR:OG1	2.11	0.50
1:B:2:GLN:HG3	1:B:3:VAL:HG23	1.94	0.50
1:A:238:HIS:C	1:A:238:HIS:CD2	2.90	0.50
1:B:29:GLN:O	1:B:29:GLN:HG3	2.07	0.50
1:B:290:THR:HB	1:B:292:VAL:H	1.77	0.50
3:L:9:SER:O	3:L:10:VAL:CG1	2.60	0.50
3:D:153:VAL:HG13	3:D:195:TYR:CE1	2.47	0.50
1:A:323:LEU:HD23	1:A:328:LEU:HD13	1.93	0.49
3:D:136:VAL:HG13	3:D:181:THR:HG22	1.93	0.49
1:A:524:VAL:HG12	1:A:532:TYR:HA	1.94	0.49
2:H:18:LEU:HB3	2:H:86:LEU:HD21	1.93	0.49
2:H:167:VAL:C	2:H:168:HIS:HD1	2.21	0.49
1:A:19:THR:HB	1:A:472:LEU:HD13	1.93	0.49
1:B:265:GLY:C	1:B:266:ARG:HG2	2.37	0.49
1:B:545:CYS:SG	1:B:564:ALA:HB3	2.53	0.49
3:L:10:VAL:HG23	3:L:18:ILE:HG22	1.94	0.49
1:B:284:THR:CG2	1:B:286:VAL:HG13	2.42	0.49
1:B:546:GLN:CD	1:B:548:GLN:HB2	2.38	0.49
2:C:36:TRP:CZ2	2:C:81:MET:HB2	2.48	0.49
2:H:171:PRO:HD2	3:L:165:SER:HB3	1.93	0.49
1:A:64:ILE:O	1:A:94:VAL:HA	2.13	0.49
1:A:237:ASN:ND2	4:E:1:NAG:C2	2.58	0.49
1:A:419:TYR:CE1	1:A:443:LEU:HD12	2.48	0.49
3:D:154:ASP:HB2	3:D:192:HIS:ND1	2.28	0.49
1:A:221:GLY:C	1:A:231:LEU:HG	2.37	0.49
2:H:131:SER:C	2:H:133:LYS:H	2.03	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:188:VAL:HG11	2:C:198:TYR:CE1	2.46	0.49
1:B:146:LEU:HB2	1:B:181:ARG:CZ	2.43	0.49
1:A:319:VAL:HG21	1:A:349:PHE:HE1	1.78	0.48
2:H:4:LEU:HD22	2:H:22:CYS:SG	2.53	0.48
3:D:192:HIS:O	3:D:214:ARG:NH1	2.46	0.48
1:A:144:THR:O	1:A:181:ARG:HB3	2.13	0.48
1:A:237:ASN:ND2	4:E:1:NAG:N2	2.61	0.48
1:B:253:ASN:HB2	1:B:260:MET:HE3	1.95	0.48
1:B:372:PRO:HB3	1:B:397:LEU:HD11	1.95	0.48
2:C:23:LYS:HG3	2:C:78:THR:OG1	2.13	0.48
1:B:194:THR:HG1	1:B:204:ARG:HH11	1.58	0.48
1:B:278:PRO:HG2	1:B:281:TYR:CD1	2.48	0.48
1:B:446:ILE:HG13	1:B:471:LEU:HD21	1.95	0.48
1:B:551:SER:O	1:B:552:VAL:C	2.55	0.48
2:C:33:TRP:HB2	2:C:99:GLU:OE2	2.13	0.48
2:C:36:TRP:CZ3	2:C:96:CYS:HB3	2.48	0.48
1:B:250:VAL:HA	1:B:260:MET:O	2.13	0.48
1:B:250:VAL:CA	1:B:262:ASN:H	2.22	0.48
2:C:2:VAL:HG21	2:C:106:TYR:CZ	2.49	0.48
1:B:353:ALA:HA	1:B:389:TYR:O	2.14	0.48
1:B:551:SER:O	1:B:552:VAL:O	2.32	0.48
3:D:135:VAL:HG23	3:D:184:LEU:HD12	1.96	0.48
1:A:335:THR:HG22	1:A:338:ASN:ND2	2.29	0.48
1:A:128:LYS:HA	1:A:155:ASN:OD1	2.14	0.48
2:H:131:SER:OG	2:H:133:LYS:C	2.52	0.48
2:C:159:ASN:ND2	6:C:311:HOH:O	2.47	0.48
3:D:163:GLN:HG3	3:D:164:GLU:H	1.79	0.48
1:A:325:MET:O	1:A:329:ARG:N	2.47	0.47
1:A:528:LEU:HD23	1:A:528:LEU:H	1.77	0.47
1:B:18:GLU:HG3	1:B:474:THR:HG21	1.96	0.47
3:D:138:LEU:C	3:D:139:LEU:HD12	2.39	0.47
1:A:514:ARG:HD2	1:A:531:GLU:OE1	2.14	0.47
1:B:7:THR:C	1:B:39:GLU:OE1	2.57	0.47
1:B:1:THR:HG23	1:B:468:HIS:NE2	2.30	0.47
3:D:50:ILE:HG22	3:D:56:ARG:HA	1.95	0.47
3:D:53:VAL:HG23	3:D:54:SER:H	1.78	0.47
1:A:99:ASP:HA	1:A:100:PRO:HD3	1.73	0.47
1:A:300:VAL:HG12	1:A:301:THR:N	2.29	0.47
3:D:188:ASP:HB3	6:D:301:HOH:O	2.14	0.47
2:H:44:GLY:HA2	3:L:89:TYR:OH	2.14	0.47
2:H:127:PRO:HB3	2:H:215:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:SER:HB3	2:C:126:PHE:CZ	2.50	0.47
1:A:9:MET:HE1	1:A:20:HIS:HE1	1.79	0.47
1:A:489:CYS:SG	1:A:498:CYS:N	2.88	0.47
1:B:523:ARG:HD2	1:B:531:GLU:OE2	2.14	0.47
2:C:143:GLY:HA2	2:C:158:TRP:CZ2	2.49	0.47
3:D:45:ALA:HA	3:D:46:PRO:HD3	1.53	0.47
1:A:116:ARG:NH2	1:A:168:ARG:HH12	2.12	0.47
1:B:546:GLN:CD	1:B:548:GLN:CG	2.85	0.47
2:C:19:LYS:HG2	2:C:82:GLU:HB2	1.96	0.47
3:D:137:CYS:HB2	3:D:151:TRP:CZ2	2.49	0.47
1:B:524:VAL:HG12	1:B:532:TYR:HA	1.97	0.47
2:C:35:GLY:HA3	2:C:104:PHE:HE2	1.79	0.47
3:D:94:THR:C	3:D:96:SER:H	2.23	0.47
3:L:9:SER:C	3:L:10:VAL:CG1	2.87	0.46
3:D:23:THR:HG22	3:D:72:THR:CG2	2.22	0.46
3:D:123:PRO:CD	3:D:124:SER:H	2.27	0.46
1:A:140:CYS:HB2	1:A:168:ARG:HH21	1.80	0.46
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.63	0.46
1:B:119:GLN:OE1	1:B:121:ARG:NH2	2.49	0.46
1:B:144:THR:O	1:B:181:ARG:HB3	2.14	0.46
2:H:73:ASP:OD2	2:H:76:THR:HG23	2.16	0.46
3:L:23:THR:CG2	3:L:72:THR:OG1	2.63	0.46
2:C:88:SER:HB2	2:C:89:ASP:HB3	1.97	0.46
3:D:6:GLN:HB3	3:D:21:SER:O	2.15	0.46
3:L:91:SER:HB3	3:L:101:PHE:CD1	2.50	0.46
2:C:90:ASP:O	2:C:91:THR:C	2.58	0.46
2:C:168:HIS:HB3	6:D:316:HOH:O	2.15	0.46
3:D:17:SER:O	3:D:18:ILE:HG12	2.15	0.46
1:B:556:GLY:HA3	1:B:561:GLN:HG2	1.97	0.46
3:D:68:LYS:HG2	3:D:69:SER:H	1.80	0.46
1:A:168:ARG:HB2	2:C:31:SER:HB3	1.97	0.46
1:B:11:LEU:HD23	1:B:11:LEU:HA	1.76	0.46
2:H:51:ILE:CG1	2:H:70:MET:HB2	2.45	0.46
2:C:91:THR:HA	2:C:113:VAL:O	2.15	0.46
2:C:130:PRO:CG	2:C:193:LEU:HD11	2.26	0.46
3:D:131:GLY:C	3:D:186:LYS:H	2.24	0.46
1:A:29:GLN:HA	1:A:51:PHE:HB2	1.98	0.46
1:B:480:ASP:C	1:B:482:CYS:H	2.23	0.46
3:L:80:LEU:HD11	3:L:107:LEU:HD21	1.98	0.46
2:C:163:LEU:HD22	6:C:311:HOH:O	2.15	0.46
1:B:466:ASN:O	1:B:469:GLN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:130:PRO:HA	2:H:134:SER:OG	2.15	0.46
1:B:18:GLU:CD	1:B:18:GLU:H	2.23	0.46
3:L:41:HIS:HB3	3:L:42:PRO:CD	2.44	0.46
2:C:105:ASP:C	3:D:48:LEU:HD22	2.41	0.46
3:D:20:ILE:HG22	3:D:21:SER:N	2.29	0.46
3:D:8:ALA:HA	3:D:105:THR:CA	2.45	0.46
3:D:148:LYS:HA	3:D:148:LYS:HE3	1.97	0.46
3:L:8:ALA:HA	3:L:105:THR:CA	2.46	0.45
3:D:6:GLN:HE21	3:D:105:THR:HG23	1.81	0.45
3:D:64:PHE:CE1	3:D:77:ILE:HG12	2.51	0.45
3:D:78:SER:OG	3:D:79:GLY:N	2.48	0.45
1:A:404:GLN:O	1:A:435:SER:OG	2.34	0.45
3:L:72:THR:CA	3:L:73:ALA:CB	2.83	0.45
3:D:80:LEU:HA	3:D:80:LEU:HD13	1.54	0.45
2:H:54:TYR:HD2	2:H:55:ASN:HD22	1.64	0.45
3:D:18:ILE:HG22	3:D:19:THR:N	2.27	0.45
3:D:213:ASN:HB2	3:D:216:GLU:CD	2.41	0.45
1:A:517:GLU:HG3	1:A:518:CYS:N	2.27	0.45
1:B:226:LYS:HE2	1:B:226:LYS:HB3	1.64	0.45
2:H:18:LEU:HD12	2:H:19:LYS:N	2.31	0.45
2:C:121:LYS:NZ	6:C:305:HOH:O	2.50	0.45
2:C:150:PHE:CD2	2:C:179:LEU:HD23	2.52	0.45
3:D:123:PRO:O	3:D:127:GLN:NE2	2.49	0.45
1:B:146:LEU:N	1:B:191:GLN:OE1	2.40	0.45
1:A:393:TRP:HB2	1:A:426:LEU:HD22	1.98	0.45
1:B:59:GLN:O	1:B:83:THR:HB	2.17	0.45
1:B:239:SER:HA	5:B:1001:NAG:H83	1.97	0.45
1:B:274:VAL:HG12	1:B:276:ALA:N	2.32	0.45
1:A:238:HIS:O	1:A:239:SER:HB2	2.17	0.45
1:A:528:LEU:N	1:A:528:LEU:CD2	2.73	0.45
1:A:554:CYS:O	1:A:555:PHE:CD1	2.70	0.45
1:B:38:LEU:HA	1:B:38:LEU:HD12	1.77	0.45
1:B:326:GLU:O	1:B:327:HIS:ND1	2.50	0.45
2:H:36:TRP:CZ3	2:H:96:CYS:HB3	2.51	0.45
2:H:152:GLU:O	2:H:206:PRO:HG2	2.16	0.45
2:C:36:TRP:CD1	2:C:70:MET:HE2	2.52	0.45
2:C:173:VAL:O	2:C:180:TYR:HA	2.17	0.45
3:D:124:SER:O	3:D:126:GLU:N	2.50	0.45
1:A:13:LEU:HA	1:A:14:PRO:HD3	1.83	0.45
1:A:155:ASN:HD22	1:A:158:ALA:HB2	1.81	0.45
1:B:7:THR:O	1:B:37:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:17:SER:O	3:L:18:ILE:HG12	2.17	0.45
2:C:16:GLU:O	2:C:86:LEU:HB2	2.17	0.45
3:D:164:GLU:HA	3:D:179:SER:O	2.17	0.45
2:H:3:GLN:O	2:H:24:GLY:HA2	2.17	0.44
2:H:51:ILE:HG22	2:H:52:SER:O	2.16	0.44
1:A:140:CYS:HA	1:A:166:ARG:NH2	2.27	0.44
1:A:175:PRO:HB3	3:D:95:SER:HA	1.99	0.44
1:A:438:GLU:OE2	1:A:465:ARG:NH1	2.48	0.44
2:H:35:GLY:HA3	2:H:104:PHE:CE1	2.52	0.44
2:H:51:ILE:HD11	2:H:70:MET:O	2.16	0.44
2:C:188:VAL:HG21	2:C:198:TYR:CE1	2.52	0.44
3:L:63:ARG:HG2	3:L:78:SER:HB3	1.98	0.44
1:B:21:LEU:HD12	1:B:43:LEU:HD22	2.00	0.44
1:B:118:LEU:HD23	1:B:118:LEU:HA	1.69	0.44
1:B:186:SER:HB3	1:B:189:ASP:OD2	2.17	0.44
1:A:297:ASN:OD1	1:A:311:LYS:HG2	2.17	0.44
2:C:129:ALA:HA	2:C:130:PRO:HD3	1.54	0.44
2:C:194:GLY:HA3	2:C:217:PRO:CG	2.45	0.44
1:A:238:HIS:CD2	1:A:238:HIS:O	2.70	0.44
1:B:293:CYS:HA	1:B:294:PRO:HD3	1.87	0.44
3:L:13:SER:CA	3:L:110:LEU:HB2	2.40	0.44
2:C:33:TRP:O	2:C:34:ILE:HD12	2.17	0.44
3:D:22:CYS:CB	3:D:73:ALA:CB	2.61	0.44
1:B:480:ASP:C	1:B:482:CYS:N	2.76	0.44
2:C:185:VAL:HG11	3:D:138:LEU:HD22	2.00	0.44
3:D:185:SER:C	3:D:187:ALA:H	2.25	0.44
1:A:360:ASP:OD1	1:A:360:ASP:N	2.47	0.44
1:B:116:ARG:HA	1:B:138:GLN:O	2.17	0.44
1:B:480:ASP:N	1:B:480:ASP:OD1	2.51	0.44
3:L:40:GLN:C	3:L:86:ALA:HB1	2.41	0.44
3:L:80:LEU:O	3:L:81:GLN:C	2.61	0.44
3:D:83:GLU:HG3	3:D:171:SER:HB2	2.00	0.44
1:A:41:THR:HA	1:A:65:ALA:O	2.17	0.44
1:B:553:THR:CG2	1:B:554:CYS:N	2.48	0.44
2:H:216:GLU:H	2:H:216:GLU:HG2	1.61	0.44
3:L:8:ALA:HA	3:L:105:THR:HA	1.99	0.44
1:A:319:VAL:HG22	1:A:320:CYS:N	2.33	0.43
1:A:353:ALA:HA	1:A:389:TYR:O	2.17	0.43
1:A:371:GLN:C	1:A:373:GLU:H	2.26	0.43
1:B:119:GLN:HA	1:B:183:TRP:HB3	2.00	0.43
2:C:90:ASP:O	2:C:94:TYR:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:PHE:HE2	2:C:178:GLY:O	2.01	0.43
2:C:204:HIS:O	2:C:207:SER:N	2.50	0.43
1:B:249:LEU:C	1:B:262:ASN:HB3	2.43	0.43
1:B:404:GLN:OE1	1:B:434:ARG:NH1	2.51	0.43
3:L:16:GLN:HB2	3:L:17:SER:HG	1.82	0.43
3:D:172:LYS:HA	3:D:172:LYS:HD2	1.93	0.43
1:A:186:SER:OG	1:A:187:SER:N	2.50	0.43
1:A:238:HIS:CB	1:A:273:CYS:HB2	2.48	0.43
2:H:12:LYS:O	2:H:115:VAL:HA	2.18	0.43
2:H:158:TRP:CZ3	2:H:200:CYS:HB3	2.53	0.43
1:A:7:THR:O	1:A:37:ASN:HB2	2.18	0.43
1:A:401:SER:O	1:A:404:GLN:N	2.49	0.43
1:A:438:GLU:HB2	1:A:465:ARG:NH1	2.34	0.43
1:B:116:ARG:NH2	1:B:168:ARG:HH12	2.17	0.43
3:L:28:ASP:O	3:L:92:SER:OG	2.36	0.43
2:C:3:GLN:HB2	2:C:25:SER:OG	2.18	0.43
3:D:6:GLN:HB2	3:D:105:THR:HG23	2.00	0.43
4:E:2:NAG:C1	4:E:2:NAG:C8	2.96	0.43
1:A:215:HIS:CD2	1:A:227:HIS:HB3	2.53	0.43
1:A:374:GLN:O	1:A:377:VAL:HG13	2.18	0.43
1:B:219:ALA:HB2	1:B:234:LEU:HA	2.01	0.43
3:L:7:PRO:O	3:L:8:ALA:HB3	2.17	0.43
1:A:477:ARG:HA	1:A:478:PRO:HD3	1.83	0.43
1:B:70:ARG:HA	1:B:114:GLY:O	2.18	0.43
3:L:107:LEU:HD12	3:L:108:THR:N	2.32	0.43
2:C:6:GLN:H	2:C:109:GLN:CD	2.26	0.43
2:C:148:ASP:HA	2:C:179:LEU:HB2	2.00	0.43
1:B:34:VAL:O	1:B:34:VAL:HG22	2.18	0.43
1:B:43:LEU:HD13	1:B:49:LEU:HD21	2.00	0.43
1:B:555:PHE:HB3	1:B:561:GLN:O	2.18	0.43
3:L:5:THR:O	3:L:23:THR:N	2.52	0.43
2:C:6:GLN:O	2:C:109:GLN:NE2	2.52	0.43
2:C:143:GLY:HA2	2:C:158:TRP:CH2	2.53	0.43
1:A:527:GLY:HA2	1:A:528:LEU:HD23	2.01	0.43
1:B:361:GLY:HA2	1:B:369:PRO:HG3	2.00	0.43
1:B:442:GLY:O	1:B:469:GLN:HG2	2.18	0.43
3:L:91:SER:HB3	3:L:101:PHE:CE1	2.54	0.43
3:D:164:GLU:HG2	3:D:178:LEU:HD21	2.01	0.43
1:A:347:LYS:HD2	1:A:383:GLU:OE2	2.19	0.43
1:B:301:THR:HG23	1:B:306:THR:O	2.18	0.43
2:C:199:ILE:HG12	2:C:214:LYS:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:209:THR:O	2:C:211:VAL:HG23	2.19	0.43
1:B:546:GLN:CD	1:B:553:THR:HG23	2.44	0.43
2:H:51:ILE:HG22	2:H:52:SER:C	2.43	0.43
3:L:14:PRO:HD3	3:L:110:LEU:N	2.29	0.43
1:A:249:LEU:HD11	1:A:267:TYR:CE2	2.54	0.42
1:A:464:PHE:CE2	1:A:470:ALA:HA	2.54	0.42
1:B:226:LYS:HG2	1:B:229:ASP:OD2	2.19	0.42
1:B:366:ASN:ND2	6:B:1113:HOH:O	2.45	0.42
2:H:124:SER:HB3	2:H:126:PHE:CZ	2.54	0.42
2:H:150:PHE:CD1	2:H:151:PRO:HA	2.54	0.42
3:L:66:GLY:HA3	3:L:75:LEU:HA	2.00	0.42
1:A:178:LYS:H	1:A:178:LYS:HG3	1.32	0.42
2:H:33:TRP:HB2	2:H:99:GLU:OE2	2.20	0.42
3:L:68:LYS:HB3	3:L:73:ALA:H	1.84	0.42
3:D:153:VAL:HG13	3:D:195:TYR:HE1	1.84	0.42
1:B:175:PRO:HD3	3:L:93:TYR:OH	2.20	0.42
1:B:453:CYS:SG	1:B:477:ARG:HG2	2.58	0.42
1:B:546:GLN:CG	1:B:548:GLN:NE2	2.77	0.42
3:L:184:LEU:HD13	3:L:189:TYR:HD1	1.85	0.42
1:B:115:LEU:HD21	1:B:118:LEU:HD23	2.00	0.42
2:C:140:ALA:HB2	2:C:190:SER:HB3	2.01	0.42
2:C:194:GLY:N	2:C:217:PRO:HD2	2.33	0.42
3:D:151:TRP:CZ3	3:D:197:CYS:HB2	2.54	0.42
1:A:81:ARG:HG2	1:A:127:LEU:HD12	2.00	0.42
2:C:67:ARG:NH1	2:C:90:ASP:OD2	2.53	0.42
2:C:120:THR:OG1	2:C:151:PRO:HD3	2.19	0.42
2:C:186:VAL:HG22	2:C:188:VAL:HG13	2.00	0.42
3:D:154:ASP:OD1	3:D:193:LYS:N	2.53	0.42
1:A:164:THR:HG22	1:A:166:ARG:HH12	1.84	0.42
1:B:423:LEU:HB2	1:B:446:ILE:HG23	2.00	0.42
3:L:121:PHE:HA	3:L:122:PRO:HD2	1.84	0.42
2:C:132:SER:HA	2:C:135:THR:HG23	2.02	0.42
2:C:143:GLY:HA3	2:C:184:SER:O	2.19	0.42
1:A:157:LEU:HD23	1:A:157:LEU:HA	1.84	0.42
1:A:226:LYS:C	1:A:228:SER:H	2.27	0.42
3:L:8:ALA:HA	3:L:106:LYS:N	2.33	0.42
3:D:131:GLY:CA	3:D:186:LYS:HB2	2.30	0.42
2:H:6:GLN:HE21	2:H:6:GLN:HB3	1.73	0.42
1:B:250:VAL:HG12	1:B:261:PRO:N	2.26	0.42
1:B:321:TYR:CD2	1:B:326:GLU:HB3	2.54	0.42
1:B:509:CYS:SG	1:B:511:GLN:O	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:64:LEU:HB3	2:H:68:VAL:CG2	2.47	0.42
1:A:175:PRO:HG2	3:D:97:SER:OG	2.20	0.41
1:B:72:VAL:HA	1:B:73:PRO:HD2	1.90	0.41
3:L:8:ALA:N	3:L:105:THR:HG22	2.34	0.41
3:L:51:TYR:CE2	3:L:55:LYS:HD2	2.55	0.41
1:B:407:GLN:O	1:B:437:ARG:HG2	2.20	0.41
1:B:532:TYR:CZ	1:B:539:LEU:HB2	2.55	0.41
3:L:38:TYR:N	3:L:89:TYR:O	2.53	0.41
3:L:122:PRO:HB3	3:L:212:PHE:CE1	2.55	0.41
2:C:47:TRP:CG	3:D:99:LEU:HB3	2.55	0.41
2:C:193:LEU:HG	2:C:194:GLY:H	1.84	0.41
3:D:37:TRP:CD2	3:D:75:LEU:HB2	2.55	0.41
1:B:207:GLY:HA3	1:B:212:ASP:CG	2.45	0.41
1:B:262:ASN:C	1:B:264:GLU:N	2.77	0.41
2:H:183:SER:OG	2:H:184:SER:N	2.54	0.41
3:L:7:PRO:O	3:L:8:ALA:CB	2.69	0.41
2:C:64:LEU:O	2:C:67:ARG:HB2	2.20	0.41
2:C:140:ALA:HB2	2:C:190:SER:CB	2.50	0.41
1:A:163:ASP:OD1	1:A:164:THR:N	2.54	0.41
1:A:266:ARG:HH11	1:A:266:ARG:CG	2.31	0.41
1:A:463:LEU:N	1:A:463:LEU:HD12	2.36	0.41
3:D:178:LEU:HD23	3:D:179:SER:N	2.35	0.41
1:A:384:ILE:CG2	1:A:386:GLY:O	2.51	0.41
1:B:426:LEU:N	1:B:449:ASN:OD1	2.29	0.41
1:B:553:THR:C	1:B:554:CYS:O	2.59	0.41
1:A:510:SER:O	1:A:511:GLN:CD	2.61	0.41
1:A:525:LEU:HB2	1:A:526:GLN:HG3	2.01	0.41
1:B:445:LEU:HD12	1:B:472:LEU:O	2.20	0.41
2:H:18:LEU:HB3	2:H:86:LEU:CD2	2.51	0.41
2:H:88:SER:HB2	2:H:89:ASP:H	1.44	0.41
2:H:186:VAL:HG22	2:H:187:THR:H	1.86	0.41
3:L:156:ALA:O	3:L:158:GLN:HG2	2.20	0.41
3:L:166:VAL:HG23	3:L:177:SER:O	2.21	0.41
3:D:75:LEU:HD12	3:D:76:THR:H	1.84	0.41
1:A:79:ILE:HB	1:A:125:GLU:HB3	2.02	0.41
1:A:164:THR:O	1:A:165:ASN:C	2.64	0.41
1:A:209:LEU:HB2	1:A:211:THR:HG22	2.02	0.41
1:B:513:LEU:HD22	1:B:515:GLY:O	2.20	0.41
1:B:546:GLN:HG2	1:B:546:GLN:O	2.19	0.41
3:L:79:GLY:C	3:L:81:GLN:H	2.27	0.41
3:L:139:LEU:HD13	3:L:178:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:23:THR:HG21	3:D:72:THR:HG21	2.02	0.41
3:D:139:LEU:O	3:D:177:SER:HA	2.20	0.41
1:B:323:LEU:HB2	1:B:351:SER:O	2.20	0.41
2:H:34:ILE:HA	2:H:34:ILE:HD12	1.86	0.41
3:L:8:ALA:CA	3:L:105:THR:HB	2.51	0.41
3:L:10:VAL:HG13	3:L:107:LEU:HD13	2.03	0.41
3:L:80:LEU:HD13	3:L:80:LEU:HA	1.77	0.41
2:C:18:LEU:HD22	2:C:113:VAL:HG11	2.03	0.41
2:C:142:LEU:HD22	2:C:193:LEU:HD11	1.98	0.41
2:C:155:THR:HB	2:C:203:ASN:HB3	2.03	0.41
2:C:166:GLY:HA3	2:C:187:THR:O	2.21	0.41
3:D:49:MET:HA	3:D:50:ILE:HA	1.86	0.41
1:A:340:GLN:H	1:A:340:GLN:HG2	1.43	0.41
1:A:352:LEU:HD12	1:A:384:ILE:CD1	2.50	0.41
1:A:378:PHE:O	1:A:381:LEU:HB3	2.21	0.41
2:H:131:SER:OG	2:H:134:SER:N	2.54	0.41
1:A:319:VAL:HG21	1:A:349:PHE:CE1	2.56	0.40
1:A:551:SER:O	1:A:552:VAL:C	2.64	0.40
1:B:492:LEU:HD11	1:B:520:GLU:OE1	2.22	0.40
2:C:105:ASP:O	3:D:48:LEU:HD22	2.21	0.40
1:B:467:PRO:C	1:B:469:GLN:H	2.30	0.40
2:C:1:GLU:O	2:C:26:GLY:HA3	2.22	0.40
1:A:175:PRO:HD3	3:D:93:TYR:OH	2.22	0.40
1:A:443:LEU:HB3	1:A:470:ALA:O	2.21	0.40
1:B:397:LEU:H	1:B:397:LEU:HG	1.76	0.40
2:C:151:PRO:HD2	2:C:206:PRO:CB	2.49	0.40
1:A:80:VAL:HG22	1:A:126:ILE:HG12	2.03	0.40
1:A:155:ASN:ND2	1:A:158:ALA:HB2	2.36	0.40
1:B:194:THR:HG1	1:B:204:ARG:NH1	2.18	0.40
2:H:98:ARG:O	2:H:104:PHE:HA	2.22	0.40
2:H:100:GLY:N	2:H:103:ALA:O	2.43	0.40
3:D:67:SER:O	3:D:74:SER:HB2	2.22	0.40
1:A:82:GLY:HA3	1:A:128:LYS:O	2.22	0.40
1:B:51:PHE:CD1	1:B:52:LEU:HD13	2.56	0.40
2:H:131:SER:HG	2:H:134:SER:N	2.20	0.40
3:L:8:ALA:O	3:L:9:SER:CB	2.69	0.40
2:C:39:GLN:O	2:C:93:VAL:HG23	2.22	0.40
3:D:38:TYR:HD1	3:D:48:LEU:HA	1.87	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:THR:O	2:C:191:SER:O[1_654]	1.78	0.42
1:B:160:THR:C	2:C:191:SER:O[1_654]	2.02	0.18
1:B:532:TYR:OH	2:H:195:THR:O[1_566]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/564 (98%)	453 (82%)	86 (16%)	12 (2%)	5	21
1	B	551/564 (98%)	445 (81%)	90 (16%)	16 (3%)	3	17
2	C	215/217 (99%)	176 (82%)	35 (16%)	4 (2%)	6	24
2	H	215/217 (99%)	192 (89%)	18 (8%)	5 (2%)	5	21
3	D	215/217 (99%)	164 (76%)	41 (19%)	10 (5%)	2	10
3	L	215/217 (99%)	165 (77%)	43 (20%)	7 (3%)	3	15
All	All	1962/1996 (98%)	1595 (81%)	313 (16%)	54 (3%)	4	18

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	528	LEU
1	A	530	ARG
1	A	555	PHE
1	B	262	ASN
1	B	528	LEU
1	B	545	CYS
1	B	546	GLN
1	B	548	GLN
1	B	550	GLY
1	B	552	VAL
1	B	553	THR
1	B	554	CYS
1	B	555	PHE

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Mol	Chain	Res	Type
2	H	151	PRO
3	L	9	SER
3	L	10	VAL
3	L	73	ALA
2	C	130	PRO
2	C	194	GLY
3	D	53	VAL
3	D	68	LYS
3	D	123	PRO
3	D	124	SER
1	A	327	HIS
1	A	529	PRO
1	B	542	HIS
1	B	544	GLU
1	B	547	PRO
2	H	131	SER
3	L	7	PRO
2	C	195	THR
3	D	16	GLN
3	D	17	SER
3	D	73	ALA
3	D	125	ASP
1	A	239	SER
1	A	554	CYS
3	L	8	ALA
3	L	95	SER
2	C	193	LEU
3	D	95	SER
1	A	552	VAL
1	A	305	GLY
1	A	485	GLU
1	B	263	PRO
3	D	122	PRO
1	A	100	PRO
1	B	264	GLU
2	H	130	PRO
2	H	205	LYS
1	B	73	PRO
2	H	152	GLU
1	A	247	PRO
3	L	144	PRO

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	478/485 (99%)	387 (81%)	91 (19%)	1	7
1	B	478/485 (99%)	395 (83%)	83 (17%)	2	8
2	C	180/181 (99%)	148 (82%)	32 (18%)	2	8
2	H	180/181 (99%)	152 (84%)	28 (16%)	2	11
3	D	185/186 (100%)	134 (72%)	51 (28%)	0	1
3	L	185/186 (100%)	149 (80%)	36 (20%)	1	6
All	All	1686/1704 (99%)	1365 (81%)	321 (19%)	1	7

All (321) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	9	MET
1	A	13	LEU
1	A	18	GLU
1	A	34	VAL
1	A	35	GLN
1	A	45	THR
1	A	46	ASN
1	A	50	SER
1	A	52	LEU
1	A	59	GLN
1	A	69	VAL
1	A	74	LEU
1	A	78	ARG
1	A	79	ILE
1	A	80	VAL
1	A	84	GLN
1	A	94	VAL
1	A	134	GLN
1	A	144	THR
1	A	156	GLN
1	A	159	LEU

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Mol	Chain	Res	Type
1	A	160	THR
1	A	164	THR
1	A	178	LYS
1	A	181	ARG
1	A	188	GLU
1	A	194	THR
1	A	197	VAL
1	A	206	LYS
1	A	216	GLU
1	A	223	THR
1	A	227	HIS
1	A	228	SER
1	A	234	LEU
1	A	238	HIS
1	A	247	PRO
1	A	250	VAL
1	A	251	THR
1	A	256	THR
1	A	260	MET
1	A	264	GLU
1	A	272	SER
1	A	275	THR
1	A	282	LEU
1	A	283	SER
1	A	284	THR
1	A	286	VAL
1	A	290	THR
1	A	295	LEU
1	A	298	GLN
1	A	312	CYS
1	A	314	LYS
1	A	320	CYS
1	A	329	ARG
1	A	331	VAL
1	A	335	THR
1	A	340	GLN
1	A	360	ASP
1	A	367	THR
1	A	382	GLU
1	A	396	SER
1	A	435	SER
1	A	443	LEU

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Mol	Chain	Res	Type
1	A	450	THR
1	A	457	THR
1	A	462	GLN
1	A	471	LEU
1	A	474	THR
1	A	485	GLU
1	A	487	LEU
1	A	495	ARG
1	A	504	THR
1	A	505	GLN
1	A	507	VAL
1	A	509	CYS
1	A	511	GLN
1	A	513	LEU
1	A	517	GLU
1	A	521	GLU
1	A	525	LEU
1	A	528	LEU
1	A	529	PRO
1	A	530	ARG
1	A	533	VAL
1	A	546	GLN
1	A	549	ASN
1	A	553	THR
1	A	555	PHE
1	A	558	GLU
1	A	561	GLN
1	B	9	MET
1	B	13	LEU
1	B	18	GLU
1	B	21	LEU
1	B	32	GLN
1	B	33	VAL
1	B	34	VAL
1	B	35	GLN
1	B	45	THR
1	B	50	SER
1	B	52	LEU
1	B	69	VAL
1	B	80	VAL
1	B	83	THR
1	B	84	GLN

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Mol	Chain	Res	Type
1	B	94	VAL
1	B	132	LEU
1	B	133	ILE
1	B	144	THR
1	B	156	GLN
1	B	159	LEU
1	B	160	THR
1	B	165	ASN
1	B	181	ARG
1	B	195	ARG
1	B	197	VAL
1	B	206	LYS
1	B	213	CYS
1	B	216	GLU
1	B	223	THR
1	B	227	HIS
1	B	228	SER
1	B	234	LEU
1	B	256	THR
1	B	259	SER
1	B	272	SER
1	B	275	THR
1	B	282	LEU
1	B	284	THR
1	B	286	VAL
1	B	290	THR
1	B	295	LEU
1	B	300	VAL
1	B	312	CYS
1	B	314	LYS
1	B	316	CYS
1	B	318	ARG
1	B	320	CYS
1	B	331	VAL
1	B	367	THR
1	B	373	GLU
1	B	380	THR
1	B	382	GLU
1	B	396	SER
1	B	397	LEU
1	B	401	SER
1	B	409	ILE

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Mol	Chain	Res	Type
1	B	420	SER
1	B	422	THR
1	B	450	THR
1	B	465	ARG
1	B	471	LEU
1	B	481	GLU
1	B	485	GLU
1	B	491	GLN
1	B	492	LEU
1	B	504	THR
1	B	505	GLN
1	B	507	VAL
1	B	508	ASN
1	B	511	GLN
1	B	513	LEU
1	B	525	LEU
1	B	526	GLN
1	B	528	LEU
1	B	533	VAL
1	B	545	CYS
1	B	549	ASN
1	B	551	SER
1	B	554	CYS
1	B	555	PHE
1	B	558	GLU
1	B	561	GLN
2	H	10	GLU
2	H	11	VAL
2	H	18	LEU
2	H	34	ILE
2	H	43	GLN
2	H	50	TRP
2	H	51	ILE
2	H	64	LEU
2	H	68	VAL
2	H	70	MET
2	H	86	LEU
2	H	87	ARG
2	H	88	SER
2	H	91	THR
2	H	113	VAL
2	H	130	PRO

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Mol	Chain	Res	Type
2	H	132	SER
2	H	134	SER
2	H	135	THR
2	H	147	LYS
2	H	152	GLU
2	H	154	VAL
2	H	155	THR
2	H	163	LEU
2	H	173	VAL
2	H	182	LEU
2	H	190	SER
2	H	216	GLU
3	L	2	SER
3	L	13	SER
3	L	20	ILE
3	L	25	THR
3	L	29	VAL
3	L	36	SER
3	L	48	LEU
3	L	49	MET
3	L	50	ILE
3	L	63	ARG
3	L	65	SER
3	L	68	LYS
3	L	69	SER
3	L	71	ASN
3	L	74	SER
3	L	76	THR
3	L	80	LEU
3	L	96	SER
3	L	99	LEU
3	L	108	THR
3	L	109	VAL
3	L	110	LEU
3	L	120	ILE
3	L	129	LYS
3	L	146	GLU
3	L	148	LYS
3	L	150	GLN
3	L	161	ASN
3	L	163	GLN
3	L	181	THR

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Mol	Chain	Res	Type
3	L	186	LYS
3	L	202	GLN
3	L	205	SER
3	L	208	VAL
3	L	209	THR
3	L	212	PHE
2	C	2	VAL
2	C	11	VAL
2	C	19	LYS
2	C	21	SER
2	C	34	ILE
2	C	39	GLN
2	C	43	GLN
2	C	50	TRP
2	C	51	ILE
2	C	55	ASN
2	C	68	VAL
2	C	69	THR
2	C	83	LEU
2	C	86	LEU
2	C	87	ARG
2	C	88	SER
2	C	112	LEU
2	C	114	THR
2	C	117	SER
2	C	120	THR
2	C	142	LEU
2	C	145	LEU
2	C	152	GLU
2	C	159	ASN
2	C	173	VAL
2	C	179	LEU
2	C	182	LEU
2	C	184	SER
2	C	188	VAL
2	C	195	THR
2	C	212	ASP
2	C	215	VAL
3	D	6	GLN
3	D	10	VAL
3	D	13	SER
3	D	22	CYS

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Mol	Chain	Res	Type
3	D	25	THR
3	D	27	SER
3	D	28	ASP
3	D	29	VAL
3	D	36	SER
3	D	47	LYS
3	D	48	LEU
3	D	50	ILE
3	D	58	SER
3	D	63	ARG
3	D	65	SER
3	D	71	ASN
3	D	76	THR
3	D	77	ILE
3	D	80	LEU
3	D	85	GLU
3	D	90	CYS
3	D	97	SER
3	D	106	LYS
3	D	109	VAL
3	D	112	THR
3	D	113	VAL
3	D	120	ILE
3	D	123	PRO
3	D	124	SER
3	D	128	LEU
3	D	129	LYS
3	D	132	THR
3	D	137	CYS
3	D	138	LEU
3	D	141	ASN
3	D	146	GLU
3	D	148	LYS
3	D	154	ASP
3	D	158	GLN
3	D	159	SER
3	D	162	SER
3	D	163	GLN
3	D	164	GLU
3	D	166	VAL
3	D	167	THR
3	D	179	SER

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Mol	Chain	Res	Type
3	D	185	SER
3	D	186	LYS
3	D	188	ASP
3	D	194	VAL
3	D	212	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	237	ASN
1	A	238	HIS
1	A	253	ASN
1	A	327	HIS
1	A	497	HIS
1	A	542	HIS
1	B	20	HIS
1	B	35	GLN
1	B	138	GLN
1	B	237	ASN
1	B	298	GLN
1	B	415	HIS
1	B	451	HIS
1	B	491	GLN
1	B	546	GLN
1	B	548	GLN
3	L	33	ASN
2	C	57	ASN
2	C	175	GLN
2	C	203	ASN
3	D	39	GLN
3	D	127	GLN
3	D	155	ASN
3	D	169	GLN
3	D	202	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 ⓘ

2 monosaccharides 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	E	1	4,1	14,14,15	0.38	0	17,19,21	0.72	1 (5%)
4	NAG	E	2	4	14,14,15	0.48	0	17,19,21	1.84	3 (17%)

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	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	NAG	C1-O5-C5	6.15	120.42	112.19
4	E	2	NAG	C4-C3-C2	3.06	115.50	111.02
4	E	2	NAG	O5-C1-C2	2.04	114.44	111.29
4	E	1	NAG	C3-C4-C5	2.02	113.89	110.23

There are no chirality outliers.

All (7) torsion outliers are listed below:

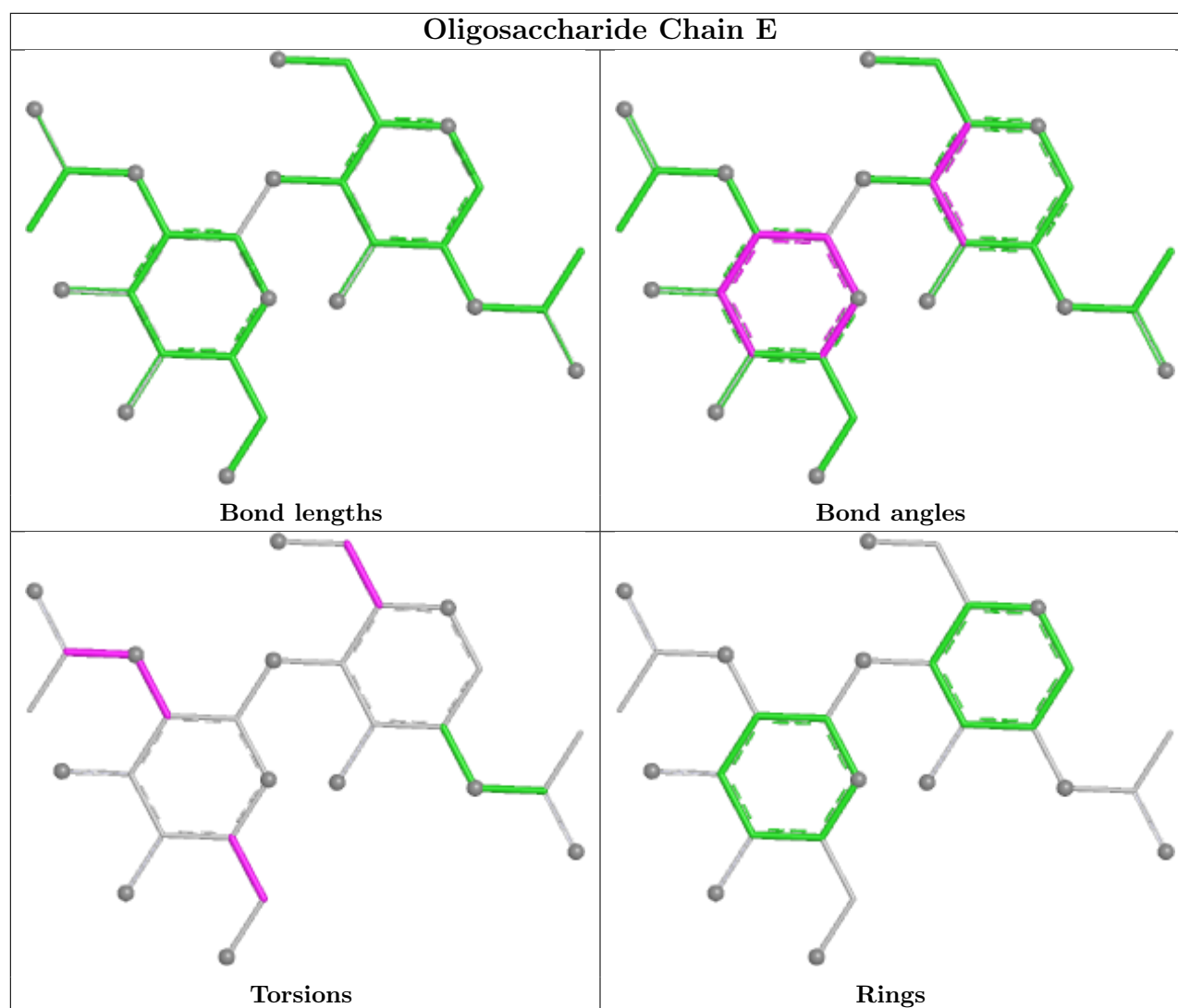
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C3-C2-N2-C7
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	E	2	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	2	0
4	E	1	NAG	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
5	NAG	B	1001	1	14,14,15	0.37	0	17,19,21	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1001	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1001	NAG	C8-C7-N2-C2
5	B	1001	NAG	O7-C7-N2-C2
5	B	1001	NAG	C4-C5-C6-O6
5	B	1001	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1001	NAG	10	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	555/564 (98%)	0.56	56 (10%) 12 6	28, 52, 125, 178	0
1	B	555/564 (98%)	0.49	47 (8%) 16 9	31, 54, 122, 152	0
2	C	217/217 (100%)	1.91	88 (40%) 0 0	39, 86, 170, 180	0
2	H	217/217 (100%)	0.77	30 (13%) 6 4	38, 70, 129, 178	0
3	D	217/217 (100%)	2.33	98 (45%) 0 0	45, 114, 187, 203	0
3	L	217/217 (100%)	1.12	30 (13%) 6 4	36, 102, 163, 185	0
All	All	1978/1996 (99%)	0.97	349 (17%) 4 2	28, 63, 166, 203	0

All (349) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	138	GLY	11.4
3	D	180	SER	10.7
3	D	147	ALA	8.9
3	D	161	ASN	8.7
2	C	142	LEU	7.8
2	C	190	SER	7.8
2	C	128	LEU	7.5
3	D	201	HIS	7.4
2	C	168	HIS	7.4
2	C	125	VAL	7.3
1	A	540	PRO	7.2
2	C	178	GLY	7.0
2	C	141	ALA	6.9
3	D	137	CYS	6.8
3	D	181	THR	6.8
2	C	217	PRO	6.7
3	D	122	PRO	6.4
1	A	559	ALA	6.3
2	C	192	SER	6.3

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Mol	Chain	Res	Type	RSRZ
3	D	139	LEU	6.2
2	C	127	PRO	6.1
2	C	197	THR	6.1
3	D	135	VAL	6.1
3	D	151	TRP	5.9
3	D	160	GLY	5.9
3	D	119	PHE	5.8
3	D	118	VAL	5.7
3	D	195	TYR	5.6
2	C	185	VAL	5.6
2	C	137	GLY	5.6
3	D	148	LYS	5.6
2	C	126	PHE	5.5
2	C	179	LEU	5.5
3	D	149	VAL	5.5
3	L	156	ALA	5.5
1	A	254	THR	5.4
3	D	199	VAL	5.4
3	D	162	SER	5.4
1	A	547	PRO	5.3
3	D	202	GLN	5.3
1	A	564	ALA	5.3
2	C	173	VAL	5.2
3	D	189	TYR	5.2
2	C	133	LYS	5.2
3	D	124	SER	5.1
3	D	187	ALA	5.1
2	C	215	VAL	5.1
1	B	564	ALA	5.1
3	D	185	SER	5.1
2	C	202	VAL	5.1
2	C	139	THR	5.1
3	D	136	VAL	5.1
2	C	165	SER	5.0
3	D	156	ALA	5.0
2	C	163	LEU	5.0
3	D	144	PRO	5.0
1	A	252	TYR	5.0
1	A	256	THR	4.9
1	A	550	GLY	4.9
1	A	563	VAL	4.9
1	A	513	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
2	C	183	SER	4.8
3	D	200	THR	4.8
2	C	140	ALA	4.7
2	C	150	PHE	4.7
3	D	138	LEU	4.7
3	D	159	SER	4.7
1	A	544	GLU	4.7
3	D	163	GLN	4.7
3	D	157	LEU	4.6
3	D	204	LEU	4.6
2	C	180	TYR	4.6
1	B	252	TYR	4.6
1	A	253	ASN	4.5
2	C	211	VAL	4.5
1	A	553	THR	4.5
2	C	130	PRO	4.4
1	A	533	VAL	4.4
3	D	120	ILE	4.4
2	C	186	VAL	4.4
2	C	135	THR	4.4
3	L	18	ILE	4.4
3	D	158	GLN	4.4
3	D	132	THR	4.4
3	D	188	ASP	4.3
3	D	116	PRO	4.3
3	D	10	VAL	4.3
2	C	184	SER	4.3
1	A	532	TYR	4.2
1	A	531	GLU	4.2
1	A	551	SER	4.2
3	D	127	GLN	4.2
1	A	255	ASP	4.2
2	C	143	GLY	4.2
2	C	177	SER	4.2
3	D	190	GLU	4.1
2	C	196	GLN	4.1
2	C	129	ALA	4.1
1	B	522	CYS	4.1
1	B	253	ASN	4.1
2	H	138	GLY	4.1
3	D	164	GLU	4.1
2	C	176	SER	4.1

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Mol	Chain	Res	Type	RSRZ
3	D	165	SER	4.1
3	D	123	PRO	4.1
3	L	123	PRO	4.0
2	H	123	PRO	4.0
2	C	174	LEU	4.0
2	H	134	SER	4.0
3	L	162	SER	4.0
2	C	145	LEU	3.9
1	A	259	SER	3.9
3	D	196	ALA	3.9
3	L	155	ASN	3.9
1	A	527	GLY	3.9
3	D	174	SER	3.9
1	A	552	VAL	3.8
2	C	198	TYR	3.8
1	B	260	MET	3.8
3	D	121	PHE	3.8
2	C	203	ASN	3.8
3	D	179	SER	3.8
3	D	197	CYS	3.8
3	D	153	VAL	3.7
2	C	199	ILE	3.7
3	D	146	GLU	3.7
3	L	185	SER	3.7
3	D	177	SER	3.7
2	C	213	LYS	3.7
2	C	187	THR	3.7
2	C	167	VAL	3.7
3	D	183	THR	3.7
2	H	135	THR	3.6
1	B	296	HIS	3.6
3	L	66	GLY	3.6
3	D	113	VAL	3.6
2	H	174	LEU	3.6
1	B	255	ASP	3.6
3	D	172	LYS	3.6
3	D	178	LEU	3.6
3	D	114	ALA	3.5
2	C	132	SER	3.5
2	C	200	CYS	3.5
2	C	124	SER	3.5
3	D	128	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
3	D	142	PHE	3.5
1	B	550	GLY	3.5
2	C	157	SER	3.5
2	C	214	LYS	3.4
2	C	170	PHE	3.4
3	D	212	PHE	3.4
2	C	161	GLY	3.4
1	B	563	VAL	3.4
3	D	133	ALA	3.4
1	A	528	LEU	3.4
1	A	561	GLN	3.4
1	B	259	SER	3.3
2	C	136	SER	3.3
1	B	560	ASP	3.3
1	A	251	THR	3.3
3	L	183	THR	3.3
3	D	194	VAL	3.3
3	D	117	SER	3.3
3	D	170	ASP	3.3
1	B	1	THR	3.3
3	D	184	LEU	3.3
2	C	156	VAL	3.3
2	C	158	TRP	3.3
2	H	151	PRO	3.2
1	A	296	HIS	3.2
2	C	175	GLN	3.2
1	B	251	THR	3.2
3	D	208	VAL	3.2
1	A	101	LEU	3.2
1	A	313	SER	3.2
1	A	257	PHE	3.2
1	B	315	PRO	3.2
1	B	302	ALA	3.2
1	B	555	PHE	3.2
1	B	553	THR	3.2
1	B	554	CYS	3.1
1	B	295	LEU	3.1
3	D	167	THR	3.1
3	D	191	LYS	3.1
2	C	181	SER	3.1
3	D	182	LEU	3.1
3	L	197	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	164	THR	3.1
3	D	211	SER	3.1
2	C	123	PRO	3.1
3	D	131	GLY	3.0
2	C	195	THR	3.0
3	D	175	THR	3.0
2	C	191	SER	3.0
2	H	129	ALA	3.0
1	B	254	THR	3.0
3	D	18	ILE	3.0
1	A	539	LEU	2.9
2	C	182	LEU	2.9
1	A	541	CYS	2.9
2	C	193	LEU	2.9
3	D	143	TYR	2.9
3	D	209	THR	2.9
1	B	261	PRO	2.9
1	B	312	CYS	2.9
2	C	146	VAL	2.9
2	H	137	GLY	2.9
1	A	260	MET	2.9
2	H	178	GLY	2.9
3	D	65	SER	2.8
2	C	189	PRO	2.8
1	B	559	ALA	2.8
1	A	524	VAL	2.8
3	D	192	HIS	2.8
2	H	88	SER	2.8
1	B	525	LEU	2.8
1	A	546	GLN	2.8
3	L	82	ALA	2.8
1	B	258	GLU	2.8
3	D	166	VAL	2.7
1	A	315	PRO	2.7
2	H	182	LEU	2.7
2	C	134	SER	2.7
3	D	134	SER	2.7
1	A	305	GLY	2.7
2	C	201	ASN	2.7
2	C	172	ALA	2.7
3	D	22	CYS	2.7
3	L	134	SER	2.7

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Mol	Chain	Res	Type	RSRZ
3	D	67	SER	2.7
3	L	186	LYS	2.7
2	C	148	ASP	2.7
2	C	188	VAL	2.7
3	L	157	LEU	2.7
3	D	70	GLY	2.7
3	L	52	ASP	2.7
2	C	144	CYS	2.6
2	C	162	ALA	2.6
1	A	261	PRO	2.6
1	B	547	PRO	2.6
1	B	305	GLY	2.6
1	A	316	CYS	2.6
1	A	562	CYS	2.6
3	L	184	LEU	2.6
2	H	136	SER	2.6
1	A	542	HIS	2.6
2	C	147	LYS	2.6
2	C	117	SER	2.6
1	B	257	PHE	2.6
1	B	161	LEU	2.6
2	C	216	GLU	2.6
2	H	209	THR	2.6
3	L	181	THR	2.6
1	A	557	PRO	2.6
1	B	561	GLN	2.5
3	L	160	GLY	2.5
1	A	258	GLU	2.5
2	C	120	THR	2.5
1	B	546	GLN	2.5
3	L	194	VAL	2.5
2	H	89	ASP	2.5
2	H	179	LEU	2.5
1	B	313	SER	2.5
2	H	140	ALA	2.5
3	D	82	ALA	2.5
2	H	194	GLY	2.5
3	D	78	SER	2.5
2	H	197	THR	2.5
2	C	209	THR	2.5
1	A	157	LEU	2.5
3	L	14	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	320	CYS	2.4
3	D	150	GLN	2.4
1	B	562	CYS	2.4
2	C	121	LYS	2.4
1	B	157	LEU	2.4
3	D	176	TYR	2.4
2	H	150	PHE	2.4
2	C	1	GLU	2.4
1	B	545	CYS	2.4
2	C	155	THR	2.4
1	A	312	CYS	2.4
3	D	210	LYS	2.4
2	H	142	LEU	2.4
3	L	128	LEU	2.4
1	A	548	GLN	2.3
1	A	534	ASN	2.3
3	D	154	ASP	2.3
3	L	191	LYS	2.3
1	B	364	ALA	2.3
2	H	160	SER	2.3
3	D	9	SER	2.3
3	L	143	TYR	2.3
1	A	549	ASN	2.3
1	B	262	ASN	2.3
3	L	182	LEU	2.3
3	D	203	GLY	2.3
1	A	555	PHE	2.3
1	A	529	PRO	2.2
3	L	206	SER	2.2
3	D	186	LYS	2.2
3	D	81	GLN	2.2
3	D	125	ASP	2.2
1	B	494	ALA	2.2
1	B	556	GLY	2.2
3	L	207	PRO	2.2
2	C	131	SER	2.2
1	B	68	GLN	2.2
1	B	528	LEU	2.2
3	D	111	GLY	2.2
2	H	149	TYR	2.2
1	A	558	GLU	2.2
2	C	159	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	545	CYS	2.2
1	B	541	CYS	2.2
2	H	139	THR	2.2
2	C	116	SER	2.2
1	A	297	ASN	2.2
1	B	529	PRO	2.2
1	A	320	CYS	2.2
1	A	560	ASP	2.2
3	D	68	LYS	2.1
1	B	158	ALA	2.1
2	H	141	ALA	2.1
2	H	122	GLY	2.1
3	D	66	GLY	2.1
3	L	176	TYR	2.1
2	C	210	LYS	2.1
3	L	150	GLN	2.1
1	B	239	SER	2.1
3	L	67	SER	2.1
2	H	173	VAL	2.1
1	A	367	THR	2.1
1	B	367	THR	2.1
2	C	149	TYR	2.1
3	L	81	GLN	2.1
1	A	386	GLY	2.1
2	C	151	PRO	2.1
3	D	84	ASP	2.1
2	C	118	ALA	2.1
2	H	217	PRO	2.1
3	L	199	VAL	2.0
2	H	207	SER	2.0
3	D	213	ASN	2.0
3	D	206	SER	2.0
2	H	172	ALA	2.0
1	A	526	GLN	2.0
2	C	62	GLN	2.0
2	H	128	LEU	2.0

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

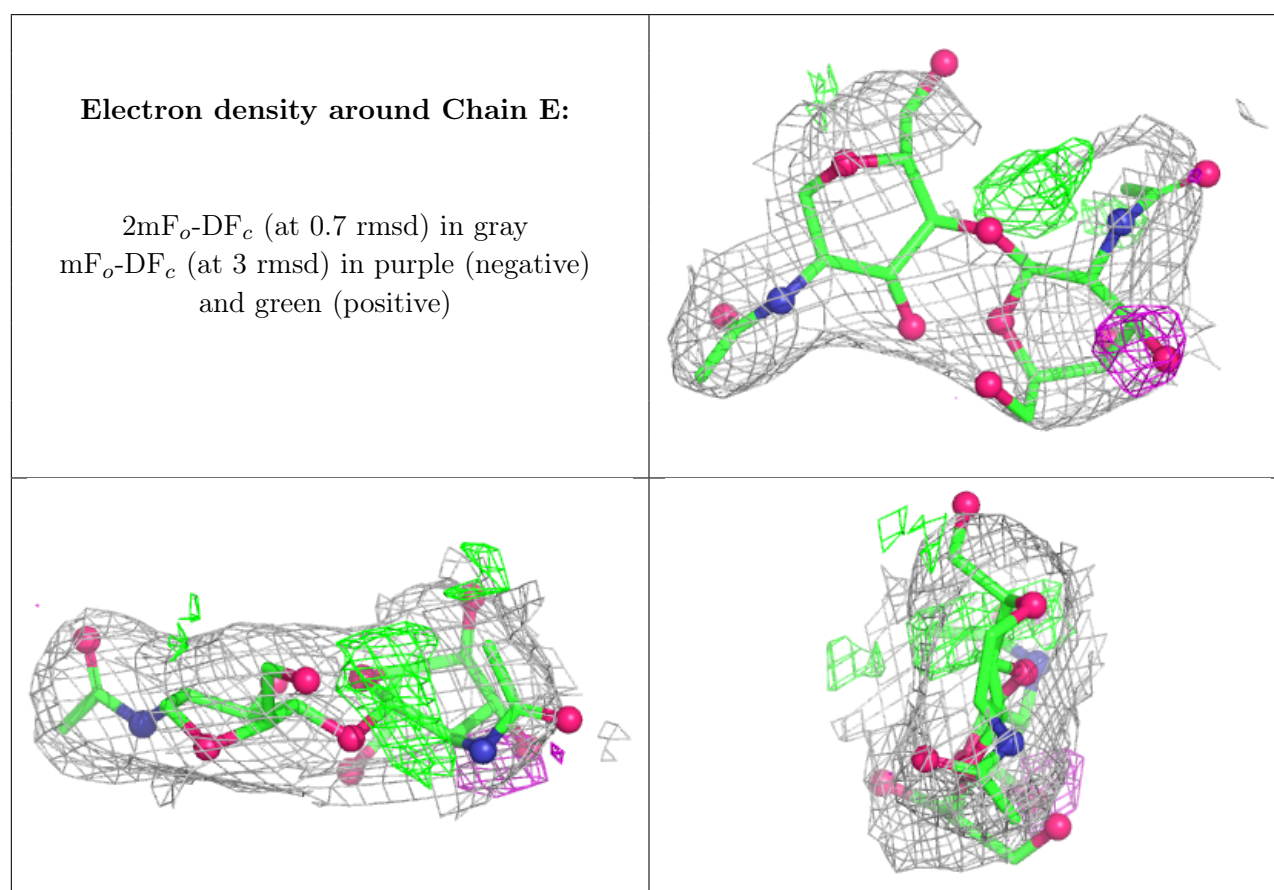
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	E	1	14/15	-	-	47,59,69,73	0
4	NAG	E	2	14/15	-	-	80,88,108,108	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	B	1001	14/15	0.52	0.26	57,60,76,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.