



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:33 AM UTC

PDB ID : 4BST / pdb_00004bst
Title : Structure of the ectodomain of LGR5 in complex with R-spondin-1 (Fu1Fu2) in P6122 crystal form
Authors : Peng, W.C.; de Lau, W.; Forneris, F.; Granneman, J.C.M.; Huch, M.; Clevers, H.; Gros, P.
Deposited on : 2013-06-11
Resolution : 4.30 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

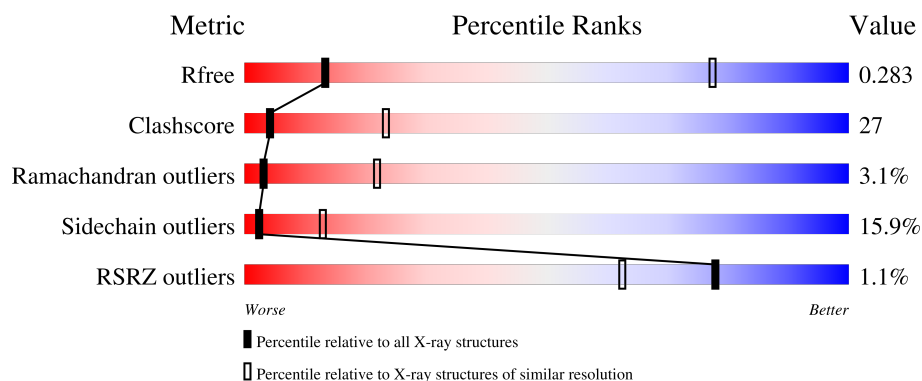
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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	539	2% 40% 32% 12% 15%
1	B	539	46% 31% 7% 15%
2	C	126	2% 30% 38% 12% 18%
2	D	126	2% 37% 32% 12% 17%
3	E	3	100%

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	A	1208	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8833 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 LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3585	2287	616	666	16			
1	B	458	Total	C	N	O	S	0	0	0
			3591	2290	617	667	17			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	HIS	-	expression tag	UNP O75473
A	9	HIS	-	expression tag	UNP O75473
A	10	HIS	-	expression tag	UNP O75473
A	11	HIS	-	expression tag	UNP O75473
A	12	HIS	-	expression tag	UNP O75473
A	13	HIS	-	expression tag	UNP O75473
A	14	GLU	-	expression tag	UNP O75473
A	15	ASN	-	expression tag	UNP O75473
A	16	LEU	-	expression tag	UNP O75473
A	17	TYR	-	expression tag	UNP O75473
A	18	PHE	-	expression tag	UNP O75473
A	19	GLN	-	expression tag	UNP O75473
A	20	GLY	-	expression tag	UNP O75473
A	21	SER	-	expression tag	UNP O75473
A	544	ALA	-	expression tag	UNP O75473
A	545	ALA	-	expression tag	UNP O75473
A	546	ALA	-	expression tag	UNP O75473
B	8	HIS	-	expression tag	UNP O75473
B	9	HIS	-	expression tag	UNP O75473
B	10	HIS	-	expression tag	UNP O75473
B	11	HIS	-	expression tag	UNP O75473
B	12	HIS	-	expression tag	UNP O75473
B	13	HIS	-	expression tag	UNP O75473
B	14	GLU	-	expression tag	UNP O75473

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	ASN	-	expression tag	UNP O75473
B	16	LEU	-	expression tag	UNP O75473
B	17	TYR	-	expression tag	UNP O75473
B	18	PHE	-	expression tag	UNP O75473
B	19	GLN	-	expression tag	UNP O75473
B	20	GLY	-	expression tag	UNP O75473
B	21	SER	-	expression tag	UNP O75473
B	544	ALA	-	expression tag	UNP O75473
B	545	ALA	-	expression tag	UNP O75473
B	546	ALA	-	expression tag	UNP O75473

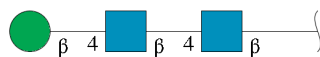
- Molecule 2 is a protein called R-SPONDIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	103	Total	C	N	O	S	0	0	0
			778	480	137	143	18			
2	D	104	Total	C	N	O	S	0	0	0
			784	483	138	145	18			

There are 20 discrepancies between the modelled and reference sequences:

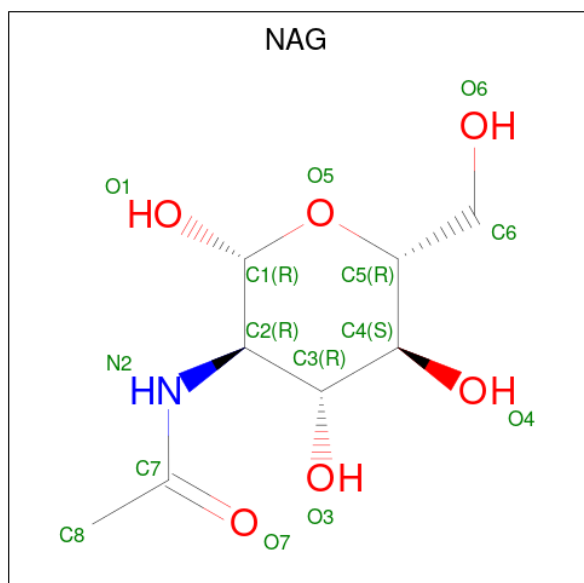
Chain	Residue	Modelled	Actual	Comment	Reference
C	29	GLY	-	expression tag	UNP Q2MKA7
C	30	SER	-	expression tag	UNP Q2MKA7
C	147	ALA	-	expression tag	UNP Q2MKA7
C	148	ALA	-	expression tag	UNP Q2MKA7
C	149	HIS	-	expression tag	UNP Q2MKA7
C	150	HIS	-	expression tag	UNP Q2MKA7
C	151	HIS	-	expression tag	UNP Q2MKA7
C	152	HIS	-	expression tag	UNP Q2MKA7
C	153	HIS	-	expression tag	UNP Q2MKA7
C	154	HIS	-	expression tag	UNP Q2MKA7
D	29	GLY	-	expression tag	UNP Q2MKA7
D	30	SER	-	expression tag	UNP Q2MKA7
D	147	ALA	-	expression tag	UNP Q2MKA7
D	148	ALA	-	expression tag	UNP Q2MKA7
D	149	HIS	-	expression tag	UNP Q2MKA7
D	150	HIS	-	expression tag	UNP Q2MKA7
D	151	HIS	-	expression tag	UNP Q2MKA7
D	152	HIS	-	expression tag	UNP Q2MKA7
D	153	HIS	-	expression tag	UNP Q2MKA7
D	154	HIS	-	expression tag	UNP Q2MKA7

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

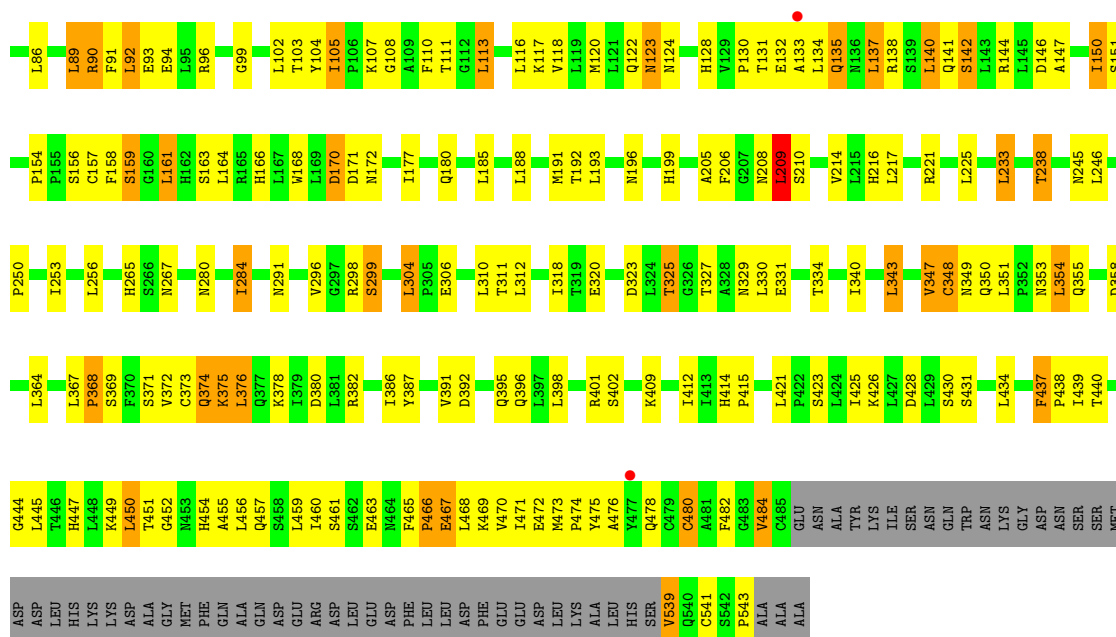


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

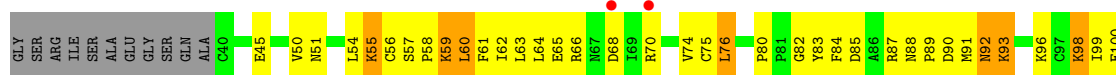
- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



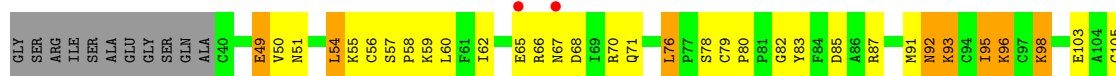
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		



• Molecule 2: R-SPONDIN-1



• Molecule 2: R-SPONDIN-1



• Molecule 3: beta-D-mannopyranose-(1-4)-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 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	131.10Å 131.10Å 531.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.17 – 4.30 48.17 – 4.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.17-4.30) 99.4 (48.17-4.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 4.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.243 , 0.268 0.250 , 0.283	Depositor DCC
R_{free} test set	991 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	180.2	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 192.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8833	wwPDB-VP
Average B, all atoms (Å ²)	213.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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, BMA

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	0.48	0/3665	1.04	13/4991 (0.3%)
1	B	0.45	0/3671	0.97	10/4999 (0.2%)
2	C	0.55	0/794	1.24	6/1066 (0.6%)
2	D	0.54	0/800	1.23	8/1074 (0.7%)
All	All	0.48	0/8930	1.05	37/12130 (0.3%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	129	CYS	CA-C-N	13.15	136.28	119.84
2	C	129	CYS	C-N-CA	13.15	136.28	119.84
1	A	439	ILE	N-CA-C	-11.67	102.62	113.71
2	D	129	CYS	CA-C-N	10.79	133.33	119.84
2	D	129	CYS	C-N-CA	10.79	133.33	119.84
1	A	84	ASN	CA-C-N	-10.69	109.94	120.52
1	A	84	ASN	C-N-CA	-10.69	109.94	120.52
1	B	70	TYR	CA-CB-CG	8.22	128.70	113.90
2	C	130	PRO	CA-C-N	8.09	136.26	121.70
2	C	130	PRO	C-N-CA	8.09	136.26	121.70
1	A	437	PHE	CA-C-N	-7.45	113.06	120.21
1	A	437	PHE	C-N-CA	-7.45	113.06	120.21
2	D	130	PRO	CA-C-N	7.29	134.82	121.70
2	D	130	PRO	C-N-CA	7.29	134.82	121.70
1	B	437	PHE	CA-C-N	7.17	127.09	120.21
1	B	437	PHE	C-N-CA	7.17	127.09	120.21
2	D	132	GLY	N-CA-C	-6.91	96.81	113.18
1	B	134	LEU	N-CA-C	6.59	121.21	112.25
2	C	82	GLY	N-CA-C	-6.32	106.71	114.92
1	A	66	VAL	CB-CA-C	6.26	121.56	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	79	CYS	CA-C-N	5.54	126.08	120.38
2	D	79	CYS	C-N-CA	5.54	126.08	120.38
1	A	151	SER	N-CA-C	-5.53	107.54	114.56
1	B	90	ARG	N-CA-C	5.46	122.44	110.80
2	D	117	GLY	N-CA-C	-5.43	108.23	115.40
1	A	421	LEU	CA-C-N	5.35	124.53	118.97
1	A	421	LEU	C-N-CA	5.35	124.53	118.97
1	B	105	ILE	CA-C-N	-5.31	115.11	120.21
1	B	105	ILE	C-N-CA	-5.31	115.11	120.21
1	A	83	PRO	N-CA-C	5.23	120.43	113.57
1	A	65	SER	N-CA-C	-5.23	102.11	109.96
1	A	66	VAL	N-CA-C	-5.11	98.72	109.34
1	B	450	LEU	N-CA-C	5.08	120.21	112.54
1	B	82	LEU	CA-C-N	-5.05	113.44	119.05
1	B	82	LEU	C-N-CA	-5.05	113.44	119.05
2	C	101	HIS	N-CA-C	5.03	118.68	112.24
1	A	362	ASN	N-CA-C	5.03	114.78	108.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3585	0	3593	212	0
1	B	3591	0	3597	163	0
2	C	778	0	744	55	0
2	D	784	0	749	62	0
3	E	39	0	34	5	0
4	A	42	0	39	1	0
4	B	14	0	13	0	0
All	All	8833	0	8769	479	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (479) 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:A:421:LEU:HG	1:A:424:LEU:HB2	1.34	1.05
1:B:104:TYR:OH	1:B:107:LYS:NZ	1.94	1.00
1:A:448:LEU:HD13	1:A:468:LEU:HD21	1.48	0.93
2:D:70:ARG:NH1	2:D:71:GLN:O	2.02	0.92
1:A:123:ASN:H	1:A:147:ALA:HB3	1.40	0.86
1:A:206:PHE:HB3	1:A:209:LEU:HD11	1.58	0.85
1:B:466:PRO:O	1:B:468:LEU:N	2.11	0.83
1:A:89:LEU:O	1:A:91:PHE:N	2.12	0.82
1:B:304:LEU:H	1:B:327:THR:HG22	1.45	0.82
1:A:208:ASN:O	1:A:210:SER:N	2.14	0.80
1:A:238:THR:HG22	1:A:261:GLU:HB3	1.61	0.80
1:A:310:LEU:HD11	1:A:312:LEU:HG	1.62	0.80
1:B:480:CYS:O	2:C:70:ARG:NH2	2.15	0.80
1:B:331:GLU:HA	1:B:354:LEU:HA	1.62	0.80
1:B:128:HIS:HA	1:B:150:ILE:HG12	1.64	0.79
2:D:139:THR:HG22	2:D:140:MET:H	1.48	0.79
2:C:50:VAL:HG23	2:C:51:ASN:HD22	1.47	0.78
1:A:402:SER:HB3	1:A:426:LYS:HB3	1.64	0.78
2:C:96:LYS:O	2:C:98:LYS:NZ	2.17	0.78
2:C:118:LEU:HD11	2:C:127:PRO:HG3	1.66	0.78
2:D:103:GLU:HG3	2:D:115:LYS:HG2	1.67	0.77
2:C:139:THR:OG1	2:C:140:MET:N	2.18	0.76
2:D:108:HIS:CG	2:D:109:ASN:H	2.03	0.76
1:A:453:ASN:HB3	1:A:456:LEU:HD23	1.67	0.75
2:D:119:TYR:CZ	2:D:142:CYS:HB2	2.21	0.75
1:A:345:GLN:CD	1:A:345:GLN:H	1.95	0.74
2:D:57:SER:HB3	2:D:60:LEU:HD13	1.69	0.74
2:C:130:PRO:HB3	2:C:131:GLU:HB2	1.70	0.74
1:B:206:PHE:HB3	1:B:209:LEU:HD11	1.70	0.73
2:C:108:HIS:O	2:C:110:PHE:N	2.21	0.73
1:A:434:LEU:HB2	1:A:456:LEU:HD21	1.69	0.72
1:A:100:ASN:O	1:A:124:ASN:ND2	2.21	0.72
1:A:442:LEU:HD11	1:A:445:LEU:HD22	1.70	0.72
1:B:170:ASP:N	1:B:170:ASP:OD1	2.23	0.72
1:A:475:TYR:HB2	1:A:477:TYR:HE1	1.55	0.72
1:A:190:ALA:HA	1:A:214:VAL:HG12	1.72	0.72
1:B:107:LYS:HE3	1:B:132:GLU:HB3	1.73	0.71
1:B:208:ASN:O	1:B:210:SER:N	2.24	0.71
1:B:82:LEU:HG	1:B:83:PRO:HD2	1.72	0.71
2:C:119:TYR:N	2:C:126:TYR:O	2.21	0.70
1:A:304:LEU:HD12	1:A:327:THR:HG21	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:CD1	1:A:113:LEU:HD11	2.22	0.69
1:A:450:LEU:HD13	1:A:474:PRO:HD3	1.74	0.69
1:A:481:ALA:HA	2:D:71:GLN:NE2	2.07	0.69
1:B:60:LEU:HG	1:B:82:LEU:HD13	1.75	0.69
1:B:154:PRO:HG2	1:B:157:CYS:HB3	1.74	0.69
1:B:476:ALA:HA	1:B:543:PRO:HB3	1.73	0.69
1:A:340:ILE:HG13	1:A:362:ASN:ND2	2.08	0.69
1:A:210:SER:HA	1:A:233:LEU:HA	1.74	0.69
2:C:60:LEU:HD23	2:C:75:CYS:HB3	1.74	0.69
1:A:82:LEU:N	1:A:82:LEU:HD12	2.08	0.68
1:B:284:ILE:HG12	1:B:306:GLU:OE2	1.92	0.68
1:B:454:HIS:O	1:B:457:GLN:NE2	2.26	0.68
2:D:70:ARG:HG3	2:D:70:ARG:HH11	1.59	0.68
1:A:154:PRO:HG2	1:A:157:CYS:HB3	1.75	0.68
1:B:122:GLN:O	1:B:124:ASN:ND2	2.26	0.67
2:D:119:TYR:HE1	2:D:141:GLU:HA	1.59	0.67
1:A:296:VAL:HG12	1:A:318:ILE:HG21	1.75	0.67
2:D:108:HIS:CD2	2:D:109:ASN:H	2.12	0.67
1:A:446:THR:HG23	1:A:447:HIS:ND1	2.10	0.67
2:C:63:LEU:HD22	2:C:76:LEU:HD11	1.76	0.67
2:D:108:HIS:CG	2:D:109:ASN:N	2.61	0.67
2:D:67:ASN:N	2:D:70:ARG:O	2.28	0.66
1:A:219:ASN:HD22	2:C:89:PRO:HD3	1.61	0.66
1:A:445:LEU:HD21	1:A:448:LEU:HD11	1.78	0.66
1:A:60:LEU:HD11	1:A:82:LEU:HD23	1.77	0.66
2:C:92:ASN:OD1	2:C:92:ASN:N	2.25	0.65
2:D:130:PRO:HA	2:D:131:GLU:HB2	1.76	0.65
1:B:444:GLY:HA2	1:B:467:GLU:CD	2.22	0.65
1:B:89:LEU:O	1:B:91:PHE:N	2.27	0.65
1:A:329:ASN:HA	1:A:353:ASN:HD21	1.62	0.65
1:B:70:TYR:HB2	1:B:94:GLU:HB3	1.78	0.64
1:B:374:GLN:O	1:B:375:LYS:HE2	1.97	0.64
1:A:40:CYS:HB3	1:A:48:LEU:HD11	1.79	0.64
1:A:96:ARG:HA	1:A:120:MET:HG2	1.80	0.64
1:A:84:ASN:N	1:A:84:ASN:OD1	2.31	0.63
1:A:353:ASN:HA	1:A:375:LYS:HD3	1.77	0.63
2:D:119:TYR:CE2	2:D:142:CYS:HB2	2.33	0.63
1:A:150:ILE:HG13	1:A:172:ASN:HB3	1.81	0.63
1:A:397:LEU:O	1:A:421:LEU:HD13	1.98	0.62
1:A:475:TYR:HB2	1:A:477:TYR:CE1	2.34	0.62
1:A:72:ASP:OD1	1:A:74:SER:OG	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:PRO:C	1:B:468:LEU:H	2.08	0.62
1:A:192:THR:OG1	2:C:106:PHE:HZ	1.82	0.62
2:C:55:LYS:HD2	2:C:56:CYS:H	1.65	0.62
1:B:378:LYS:HG3	1:B:402:SER:HB2	1.80	0.62
2:C:140:MET:O	2:C:140:MET:HG3	1.99	0.61
1:A:477:TYR:HD1	1:A:477:TYR:H	1.47	0.61
2:C:105:CYS:HB3	2:C:111:CYS:HA	1.83	0.61
1:A:170:ASP:OD1	1:A:170:ASP:N	2.31	0.61
1:B:484:VAL:HG11	1:B:541:CYS:HB3	1.83	0.61
2:C:105:CYS:HA	2:C:112:THR:H	1.65	0.61
1:B:158:PHE:HB3	1:B:161:LEU:HD11	1.82	0.60
1:A:388:GLU:N	1:A:388:GLU:OE1	2.34	0.60
1:A:465:PHE:HB3	1:A:468:LEU:HD12	1.83	0.60
1:B:265:HIS:O	1:B:267:ASN:ND2	2.35	0.60
1:B:460:ILE:HG12	1:B:478:GLN:HE21	1.66	0.60
2:C:62:ILE:HD11	2:C:93:LYS:HE3	1.84	0.60
1:B:135:GLN:N	1:B:135:GLN:CD	2.60	0.60
1:A:425:ILE:HD12	1:A:445:LEU:HA	1.83	0.60
1:B:380:ASP:OD2	1:B:382:ARG:NH1	2.35	0.60
2:C:50:VAL:HG23	2:C:51:ASN:ND2	2.15	0.60
1:B:144:ARG:HH22	2:D:106:PHE:HD1	1.49	0.60
1:A:105:ILE:HD13	1:A:130:PRO:HG3	1.83	0.59
1:B:311:THR:HA	1:B:334:THR:HG23	1.83	0.59
1:A:171:ASP:HA	1:A:195:LEU:HG	1.84	0.59
1:A:366:ASP:OD1	1:A:390:LYS:NZ	2.34	0.59
1:B:392:ASP:HA	1:B:395:GLN:HB2	1.84	0.59
1:A:231:ASP:OD1	1:A:231:ASP:N	2.34	0.59
1:B:351:LEU:HB3	1:B:354:LEU:CD2	2.33	0.59
1:A:261:GLU:HG3	1:A:285:THR:OG1	2.02	0.59
1:A:373:CYS:O	1:A:376:LEU:HD13	2.02	0.59
1:B:150:ILE:HG22	1:B:172:ASN:HB3	1.85	0.58
2:D:107:SER:OG	2:D:108:HIS:N	2.33	0.58
1:A:182:PHE:CZ	1:A:191:MET:HE1	2.39	0.58
1:B:107:LYS:HG3	1:B:132:GLU:HB3	1.85	0.58
2:C:61:PHE:CZ	2:C:85:ASP:HB3	2.38	0.58
2:D:98:LYS:HG3	2:D:108:HIS:CD2	2.38	0.58
1:B:329:ASN:OD1	1:B:353:ASN:ND2	2.37	0.58
1:A:74:SER:O	1:A:76:ASN:ND2	2.37	0.58
1:A:265:HIS:HA	1:A:291:ASN:HD21	1.69	0.57
1:A:484:VAL:HG21	1:A:541:CYS:HB3	1.86	0.57
1:B:81:LEU:HD12	1:B:82:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:LEU:HG	1:B:471:ILE:HD11	1.85	0.57
1:B:395:GLN:HG3	1:B:396:GLN:HG2	1.87	0.57
1:B:144:ARG:HD2	1:B:168:TRP:CG	2.40	0.57
1:A:192:THR:HA	1:A:216:HIS:HB2	1.86	0.57
1:A:458:SER:HB3	2:D:55:LYS:HE2	1.85	0.56
1:A:124:ASN:O	1:A:148:ASN:HA	2.04	0.56
1:A:66:VAL:HG22	1:A:67:PHE:H	1.70	0.56
1:A:302:GLN:HE22	1:A:323:ASP:HB3	1.69	0.56
2:C:45:GLU:N	2:C:45:GLU:OE1	2.38	0.56
1:A:225:LEU:HD21	1:A:250:PRO:HB3	1.87	0.56
1:A:387:TYR:C	1:A:410:ILE:HA	2.31	0.56
1:A:457:GLN:O	1:A:477:TYR:OH	2.17	0.56
1:B:70:TYR:CB	1:B:94:GLU:HB3	2.36	0.56
1:A:43:ASP:OD1	1:A:44:GLY:N	2.39	0.55
1:A:60:LEU:HD21	1:A:82:LEU:CD2	2.36	0.55
1:A:111:THR:C	1:A:113:LEU:H	2.14	0.55
1:B:457:GLN:HG3	1:B:475:TYR:HE2	1.71	0.55
1:A:144:ARG:HG2	1:A:168:TRP:CE3	2.41	0.55
1:A:131:THR:HA	1:A:154:PRO:HG3	1.89	0.55
1:B:164:LEU:HD23	1:B:185:LEU:HD21	1.88	0.55
1:A:113:LEU:HD12	1:A:116:LEU:HB2	1.88	0.55
1:A:110:PHE:O	1:A:113:LEU:HB2	2.07	0.55
1:A:198:ILE:HD13	1:A:222:ILE:HD11	1.89	0.55
1:A:77:ASN:HD22	4:A:1077:NAG:C7	2.19	0.55
1:A:433:LEU:N	1:A:453:ASN:OD1	2.38	0.55
1:A:420:THR:O	1:A:420:THR:OG1	2.13	0.55
1:B:107:LYS:CE	1:B:132:GLU:HB3	2.37	0.55
1:A:426:LYS:HG3	1:A:447:HIS:HB2	1.89	0.55
1:B:298:ARG:NE	1:B:320:GLU:OE1	2.33	0.54
2:C:100:GLU:OE1	2:C:100:GLU:N	2.40	0.54
1:B:445:LEU:O	1:B:467:GLU:HG2	2.07	0.54
1:A:147:ALA:HA	1:A:171:ASP:OD2	2.08	0.54
1:A:275:LYS:HE3	1:A:278:VAL:HB	1.89	0.54
1:A:52:CYS:HB3	1:A:55:LEU:HD21	1.89	0.54
1:A:480:CYS:SG	2:D:71:GLN:HB3	2.48	0.54
2:C:121:HIS:HB3	2:C:126:TYR:HE1	1.72	0.54
1:B:128:HIS:CA	1:B:150:ILE:HG12	2.35	0.54
1:B:349:ASN:OD1	1:B:350:GLN:N	2.40	0.54
1:B:355:GLN:O	1:B:376:LEU:HD12	2.07	0.54
2:C:121:HIS:CD2	2:C:122:LYS:HG2	2.42	0.54
1:A:392:ASP:HA	1:A:395:GLN:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:GLU:O	1:B:132:GLU:HG3	2.08	0.54
1:B:166:HIS:HE1	2:D:110:PHE:HE1	1.53	0.54
2:C:60:LEU:O	2:C:92:ASN:ND2	2.41	0.54
1:A:81:LEU:HA	1:A:82:LEU:CB	2.38	0.54
1:A:340:ILE:HG13	1:A:362:ASN:HD21	1.72	0.54
1:A:366:ASP:OD1	1:A:367:LEU:N	2.41	0.54
1:A:96:ARG:HB3	1:A:120:MET:HE2	1.89	0.53
1:A:415:PRO:HA	1:A:438:PRO:HB3	1.91	0.53
1:B:444:GLY:HA2	1:B:467:GLU:OE2	2.08	0.53
2:C:99:ILE:HD13	2:C:102:CYS:H	1.73	0.53
1:B:48:LEU:HG	1:B:68:THR:HA	1.89	0.53
1:B:144:ARG:HB3	1:B:168:TRP:CE3	2.43	0.53
1:B:177:ILE:HG21	1:B:205:ALA:HB1	1.90	0.53
1:B:69:SER:O	1:B:93:GLU:N	2.31	0.53
1:B:374:GLN:C	1:B:376:LEU:H	2.17	0.53
2:D:135:ALA:O	2:D:142:CYS:HA	2.09	0.53
1:A:362:ASN:O	1:A:384:ASN:HA	2.09	0.53
2:C:57:SER:OG	2:C:58:PRO:HD2	2.09	0.53
1:B:47:LEU:HB3	1:B:69:SER:HB3	1.90	0.53
1:B:52:CYS:HB2	1:B:73:LEU:HD23	1.91	0.53
1:A:389:ILE:HG13	1:A:389:ILE:O	2.10	0.52
1:A:425:ILE:HG13	1:A:446:THR:HG22	1.91	0.52
1:B:142:SER:HB2	1:B:166:HIS:HB2	1.90	0.52
1:B:348:CYS:HB2	1:B:372:VAL:HG23	1.91	0.52
2:D:108:HIS:C	2:D:110:PHE:H	2.18	0.52
2:D:51:ASN:HB2	2:D:54:LEU:HD11	1.91	0.52
1:B:147:ALA:HB2	2:D:87:ARG:CZ	2.40	0.52
1:A:392:ASP:HA	1:A:395:GLN:CG	2.40	0.52
1:B:43:ASP:OD1	1:B:44:GLY:N	2.42	0.52
1:B:351:LEU:HB3	1:B:354:LEU:HD21	1.90	0.52
2:C:108:HIS:C	2:C:110:PHE:H	2.18	0.52
2:D:93:LYS:NZ	2:D:95:ILE:HA	2.25	0.52
1:B:138:ARG:O	1:B:163:SER:OG	2.26	0.51
1:B:208:ASN:ND2	3:E:1:NAG:O7	2.42	0.51
1:A:354:LEU:HD21	1:A:356:VAL:O	2.10	0.51
2:C:84:PHE:HB2	2:C:106:PHE:O	2.11	0.51
1:A:332:SER:HA	1:A:356:VAL:HG22	1.92	0.51
2:C:63:LEU:HB3	2:C:74:VAL:HG13	1.91	0.51
2:D:95:ILE:HG13	2:D:95:ILE:O	2.11	0.51
1:A:99:GLY:HA2	1:A:123:ASN:HB3	1.92	0.51
1:B:250:PRO:HB2	1:B:253:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:GLU:HB3	1:B:82:LEU:HD11	1.91	0.51
1:B:144:ARG:HD2	1:B:168:TRP:CD2	2.46	0.51
1:A:69:SER:O	1:A:93:GLU:N	2.35	0.50
1:B:156:SER:O	1:B:159:SER:OG	2.27	0.50
1:B:188:LEU:HD21	1:B:191:MET:HB2	1.93	0.50
1:A:122:GLN:HB3	1:A:146:ASP:OD1	2.11	0.50
1:B:199:HIS:HA	1:B:221:ARG:O	2.10	0.50
2:C:59:LYS:HE2	2:C:87:ARG:NH1	2.27	0.50
1:A:138:ARG:HG3	1:A:139:SER:N	2.27	0.50
1:B:484:VAL:CG1	1:B:541:CYS:HB3	2.42	0.50
1:A:81:LEU:HA	1:A:82:LEU:HB3	1.93	0.50
1:A:459:LEU:HD11	2:D:54:LEU:HB3	1.94	0.50
1:B:450:LEU:N	1:B:472:GLU:OE1	2.45	0.50
1:A:144:ARG:HA	1:A:168:TRP:HB2	1.94	0.50
1:B:96:ARG:NE	1:B:120:MET:SD	2.85	0.50
1:B:168:TRP:CZ2	2:D:85:ASP:HB3	2.46	0.50
1:A:193:LEU:HB2	1:A:217:LEU:HD23	1.94	0.50
1:B:89:LEU:HD12	1:B:89:LEU:H	1.77	0.50
1:B:147:ALA:HA	1:B:171:ASP:HB3	1.94	0.50
1:B:267:ASN:HB2	1:B:291:ASN:ND2	2.27	0.50
1:B:431:SER:N	1:B:451:THR:O	2.41	0.50
2:C:56:CYS:SG	2:C:62:ILE:HG22	2.52	0.50
2:C:134:SER:OG	2:C:135:ALA:N	2.44	0.50
3:E:2:NAG:H62	3:E:3:BMA:H2	1.94	0.50
1:B:66:VAL:HG23	1:B:67:PHE:HD1	1.77	0.49
1:B:99:GLY:N	1:B:123:ASN:OD1	2.45	0.49
2:D:119:TYR:CZ	2:D:120:LEU:O	2.65	0.49
1:A:457:GLN:C	1:A:477:TYR:HH	2.15	0.49
1:B:343:LEU:HD13	1:B:364:LEU:HD21	1.94	0.49
1:A:178:PRO:HD2	1:A:182:PHE:CE1	2.47	0.49
1:A:304:LEU:HD12	1:A:327:THR:CG2	2.40	0.49
1:B:86:LEU:O	1:B:89:LEU:HD11	2.12	0.49
2:D:83:TYR:CD1	2:D:96:LYS:HA	2.47	0.49
1:A:319:THR:C	1:A:340:ILE:HG22	2.37	0.49
1:B:340:ILE:CD1	1:B:364:LEU:HG	2.43	0.49
2:C:118:LEU:HG	2:C:126:TYR:C	2.38	0.49
1:B:92:LEU:HD12	1:B:94:GLU:H	1.77	0.49
2:C:63:LEU:HD11	2:C:83:TYR:CE2	2.47	0.49
1:B:73:LEU:HB3	1:B:76:ASN:HD21	1.78	0.49
1:B:469:LYS:HG3	1:B:539:VAL:HA	1.94	0.49
1:B:460:ILE:HG12	1:B:478:GLN:NE2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:118:LEU:O	2:C:140:MET:HE1	2.12	0.49
1:A:214:VAL:HG23	1:A:238:THR:OG1	2.13	0.49
1:A:425:ILE:O	1:A:446:THR:HG22	2.13	0.49
1:B:132:GLU:HA	1:B:135:GLN:NE2	2.28	0.49
1:B:304:LEU:N	1:B:327:THR:HG22	2.22	0.49
1:B:374:GLN:O	1:B:376:LEU:N	2.46	0.49
1:B:459:LEU:HD12	2:C:54:LEU:HA	1.94	0.49
2:C:88:ASN:HB2	2:C:91:MET:O	2.13	0.49
1:A:208:ASN:OD1	1:A:208:ASN:N	2.46	0.48
1:A:343:LEU:HD13	1:A:364:LEU:HD21	1.95	0.48
1:B:180:GLN:H	1:B:180:GLN:CD	2.20	0.48
1:A:171:ASP:CA	1:A:195:LEU:HG	2.42	0.48
1:A:176:GLU:N	1:A:198:ILE:HG22	2.28	0.48
1:B:334:THR:HB	1:B:358:ASP:HB3	1.95	0.48
1:B:466:PRO:HG2	1:B:467:GLU:OE1	2.13	0.48
1:A:72:ASP:HB2	1:A:96:ARG:HD2	1.96	0.48
2:C:55:LYS:HD2	2:C:56:CYS:N	2.28	0.48
1:A:132:GLU:O	1:A:135:GLN:HB3	2.13	0.48
2:D:65:GLU:O	2:D:71:GLN:HA	2.13	0.48
1:A:93:GLU:HG3	1:A:117:LYS:HD3	1.96	0.48
1:B:445:LEU:HD12	1:B:468:LEU:HD13	1.95	0.48
2:C:103:GLU:OE1	2:C:115:LYS:NZ	2.47	0.48
1:A:65:SER:OG	1:A:66:VAL:O	2.24	0.48
1:A:147:ALA:N	1:A:171:ASP:OD1	2.40	0.48
1:A:158:PHE:CD2	1:A:185:LEU:HD11	2.49	0.48
1:A:239:LEU:HD22	1:A:241:LEU:HG	1.95	0.48
1:A:425:ILE:O	1:A:445:LEU:HD12	2.14	0.48
2:C:66:ARG:NH1	2:C:66:ARG:HB2	2.29	0.48
1:A:410:ILE:HD11	1:A:434:LEU:HD11	1.96	0.48
1:B:166:HIS:NE2	2:D:112:THR:OG1	2.46	0.48
2:D:50:VAL:O	2:D:70:ARG:NH2	2.47	0.48
2:D:119:TYR:CG	2:D:120:LEU:N	2.82	0.48
1:A:378:LYS:HD2	1:A:402:SER:OG	2.14	0.47
2:D:71:GLN:OE1	2:D:71:GLN:N	2.43	0.47
1:A:102:LEU:HD22	1:A:102:LEU:H	1.79	0.47
1:B:369:SER:C	1:B:371:SER:H	2.20	0.47
2:C:63:LEU:HD11	2:C:83:TYR:CZ	2.49	0.47
1:A:263:GLY:HA2	1:A:287:HIS:HB2	1.96	0.47
2:D:76:LEU:HD23	2:D:80:PRO:HD3	1.97	0.47
1:A:434:LEU:HB2	1:A:456:LEU:CD2	2.40	0.47
2:D:82:GLY:C	2:D:83:TYR:HD1	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:VAL:HG22	1:A:414:HIS:CG	2.49	0.47
1:B:66:VAL:HG23	1:B:67:PHE:CD1	2.50	0.47
2:D:119:TYR:CD1	2:D:120:LEU:N	2.83	0.47
1:A:131:THR:OG1	1:A:132:GLU:N	2.48	0.47
1:B:94:GLU:OE2	1:B:96:ARG:NH2	2.47	0.47
1:B:425:ILE:O	1:B:445:LEU:HB2	2.14	0.47
1:B:431:SER:HA	1:B:452:GLY:HA3	1.96	0.47
2:D:70:ARG:NH1	2:D:70:ARG:HG3	2.26	0.47
1:A:66:VAL:HG23	1:A:89:LEU:HA	1.97	0.47
1:A:236:LEU:HD23	1:A:256:LEU:HD13	1.96	0.47
1:A:310:LEU:HD12	1:A:311:THR:N	2.30	0.47
1:A:335:LEU:O	1:A:359:LEU:HA	2.15	0.47
1:A:365:GLU:N	1:A:365:GLU:OE1	2.47	0.47
1:A:49:ARG:HH22	1:A:72:ASP:HB2	1.80	0.47
1:B:428:ASP:CG	1:B:449:LYS:HB2	2.40	0.47
2:D:71:GLN:H	2:D:71:GLN:CD	2.22	0.46
1:A:60:LEU:HD11	1:A:82:LEU:CD2	2.43	0.46
1:B:473:MET:HG3	1:B:474:PRO:HD2	1.96	0.46
1:A:228:LYS:HZ3	1:A:254:ARG:HH21	1.62	0.46
1:A:265:HIS:HA	1:A:291:ASN:ND2	2.30	0.46
1:B:451:THR:N	1:B:472:GLU:OE1	2.43	0.46
2:D:76:LEU:HB3	2:D:78:SER:O	2.16	0.46
1:B:130:PRO:HB3	1:B:133:ALA:HB3	1.97	0.46
1:B:447:HIS:CE1	1:B:470:VAL:HB	2.51	0.46
2:C:80:PRO:O	2:C:83:TYR:HB2	2.16	0.46
1:A:83:PRO:HG2	1:A:84:ASN:OD1	2.16	0.46
1:B:108:GLY:HA2	1:B:111:THR:HG23	1.97	0.46
1:A:175:THR:C	1:A:198:ILE:HG22	2.41	0.46
1:A:425:ILE:HA	1:A:445:LEU:HB2	1.97	0.46
2:D:93:LYS:HZ2	2:D:95:ILE:HA	1.79	0.46
1:A:79:SER:HA	1:A:101:ALA:O	2.16	0.46
1:A:365:GLU:HG3	1:A:385:GLU:HB3	1.98	0.46
1:A:450:LEU:HD11	1:A:473:MET:SD	2.56	0.46
1:A:389:ILE:HD11	1:A:417:ALA:HB1	1.98	0.46
1:B:76:ASN:OD1	1:B:76:ASN:N	2.49	0.46
1:A:390:LYS:O	1:A:393:THR:HG22	2.16	0.46
1:B:53:SER:O	1:B:55:LEU:N	2.49	0.46
1:B:117:LYS:HE2	1:B:141:GLN:CD	2.41	0.46
1:B:463:GLU:C	1:B:465:PHE:H	2.24	0.46
1:A:42:PRO:HA	1:A:47:LEU:O	2.16	0.45
1:A:189:GLN:HA	1:A:212:LEU:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ILE:HD12	1:A:270:ARG:H	1.82	0.45
1:B:144:ARG:NH2	2:D:106:PHE:HD1	2.13	0.45
2:C:80:PRO:HD2	2:C:83:TYR:CD2	2.52	0.45
2:D:58:PRO:HB2	2:D:59:LYS:HG3	1.99	0.45
1:B:428:ASP:OD1	1:B:430:SER:N	2.40	0.45
1:A:389:ILE:HD11	1:A:417:ALA:CB	2.47	0.45
1:B:296:VAL:HB	1:B:318:ILE:HD11	1.98	0.45
1:A:113:LEU:HD13	1:A:113:LEU:HA	1.56	0.45
1:A:204:TYR:O	1:A:206:PHE:N	2.49	0.45
2:C:80:PRO:HD2	2:C:83:TYR:HD2	1.81	0.45
2:C:129:CYS:HA	2:C:130:PRO:HD2	1.60	0.45
1:A:463:GLU:O	1:A:464:ASN:ND2	2.50	0.45
1:B:135:GLN:HB3	1:B:159:SER:O	2.17	0.45
1:B:323:ASP:OD1	1:B:325:THR:OG1	2.34	0.45
1:A:60:LEU:HD21	1:A:82:LEU:HD23	1.99	0.45
1:A:61:PRO:HB2	1:A:64:LEU:CD2	2.47	0.45
1:A:348:CYS:HB2	1:A:372:VAL:HB	1.99	0.45
2:C:137:ASN:HD21	2:C:139:THR:HG22	1.82	0.45
3:E:1:NAG:H5	3:E:2:NAG:C7	2.47	0.45
1:A:65:SER:C	1:A:66:VAL:O	2.58	0.45
1:B:150:ILE:HD13	1:B:151:SER:N	2.32	0.45
2:D:129:CYS:HA	2:D:130:PRO:HD2	1.77	0.45
1:A:167:LEU:HD23	1:A:191:MET:HE3	1.98	0.45
1:A:177:ILE:HG21	1:A:205:ALA:HB1	1.98	0.45
1:A:477:TYR:CD1	1:A:477:TYR:N	2.85	0.45
1:B:437:PHE:CD1	1:B:438:PRO:O	2.70	0.45
2:C:59:LYS:HE2	2:C:87:ARG:HH11	1.82	0.45
1:A:345:GLN:H	1:A:345:GLN:NE2	2.15	0.44
1:B:140:LEU:HD12	1:B:164:LEU:HD13	1.98	0.44
2:C:130:PRO:CB	2:C:131:GLU:HB2	2.42	0.44
2:D:134:SER:OG	2:D:135:ALA:N	2.49	0.44
3:E:2:NAG:H62	3:E:3:BMA:C2	2.47	0.44
1:B:135:GLN:C	1:B:137:LEU:H	2.25	0.44
2:D:56:CYS:SG	2:D:62:ILE:HG12	2.57	0.44
1:A:469:LYS:HZ2	1:A:539:VAL:N	2.16	0.44
1:B:353:ASN:N	1:B:375:LYS:HE3	2.33	0.44
2:C:115:LYS:HD3	2:C:116:GLU:H	1.82	0.44
1:A:50:VAL:HB	1:A:71:LEU:HD13	1.99	0.44
1:A:60:LEU:H	1:A:60:LEU:HG	1.39	0.44
1:A:182:PHE:HE2	1:A:191:MET:SD	2.41	0.44
1:B:70:TYR:HA	1:B:92:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:HIS:CE1	2:D:110:PHE:HE1	2.34	0.44
1:B:461:SER:C	1:B:482:PHE:HE1	2.26	0.44
2:D:119:TYR:HE1	2:D:141:GLU:CA	2.27	0.44
1:B:374:GLN:C	1:B:376:LEU:N	2.76	0.44
1:A:87:PRO:HB2	1:A:112:GLY:HA3	2.00	0.44
2:D:50:VAL:HG23	2:D:51:ASN:CG	2.43	0.44
1:A:310:LEU:CD1	1:A:312:LEU:HG	2.41	0.44
1:B:66:VAL:O	1:B:67:PHE:HB2	2.18	0.44
1:B:471:ILE:O	1:B:541:CYS:HA	2.18	0.44
1:A:222:ILE:HG12	1:A:244:ASN:OD1	2.18	0.43
1:B:367:LEU:HA	1:B:368:PRO:HD3	1.83	0.43
1:A:233:LEU:HD13	1:A:236:LEU:HB2	2.00	0.43
1:A:542:SER:HA	1:A:543:PRO:HD2	1.87	0.43
1:B:398:LEU:O	1:B:423:SER:OG	2.19	0.43
2:C:59:LYS:HE3	2:C:59:LYS:HA	1.99	0.43
2:D:57:SER:OG	2:D:58:PRO:HD2	2.18	0.43
2:D:119:TYR:OH	2:D:142:CYS:HB2	2.17	0.43
1:A:49:ARG:HH11	1:A:70:TYR:C	2.26	0.43
1:A:100:ASN:H	1:A:124:ASN:HD21	1.66	0.43
1:A:385:GLU:HG2	1:A:409:LYS:HD2	2.00	0.43
1:A:425:ILE:HG13	1:A:446:THR:CG2	2.48	0.43
1:B:466:PRO:C	1:B:468:LEU:N	2.74	0.43
1:A:176:GLU:HG2	1:A:200:HIS:CE1	2.54	0.43
1:B:299:SER:O	1:B:299:SER:OG	2.35	0.43
1:A:476:ALA:HA	1:A:543:PRO:HB3	2.00	0.43
1:B:107:LYS:HE3	1:B:132:GLU:CB	2.45	0.43
1:B:135:GLN:C	1:B:137:LEU:N	2.72	0.43
1:A:82:LEU:HD11	1:A:85:PRO:HA	2.00	0.43
1:A:90:ARG:HG3	1:A:91:PHE:CE2	2.54	0.43
2:D:49:GLU:OE1	2:D:49:GLU:N	2.52	0.43
1:A:352:PRO:O	1:A:354:LEU:N	2.52	0.43
1:A:471:ILE:O	1:A:541:CYS:HA	2.19	0.43
1:B:137:LEU:H	1:B:137:LEU:HD12	1.84	0.43
2:C:130:PRO:HA	2:C:131:GLU:CG	2.48	0.43
1:A:457:GLN:HG2	1:A:475:TYR:HE2	1.83	0.42
1:B:59:GLU:HA	1:B:78:ILE:HD12	2.01	0.42
1:B:130:PRO:CB	1:B:133:ALA:HB3	2.49	0.42
1:A:138:ARG:HG3	1:A:139:SER:OG	2.18	0.42
1:B:156:SER:C	1:B:159:SER:HG	2.25	0.42
1:B:233:LEU:HD13	1:B:233:LEU:H	1.84	0.42
1:A:178:PRO:O	1:A:182:PHE:HD1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASN:O	1:A:267:ASN:HA	2.20	0.42
1:A:468:LEU:HD23	1:A:468:LEU:HA	1.76	0.42
2:D:92:ASN:OD1	2:D:92:ASN:N	2.51	0.42
2:D:121:HIS:N	2:D:124:ARG:O	2.50	0.42
1:A:66:VAL:O	1:A:67:PHE:HD1	2.03	0.42
1:A:319:THR:HG23	1:A:320:GLU:CD	2.45	0.42
1:A:362:ASN:CG	1:A:363:LEU:H	2.26	0.42
1:B:48:LEU:HD23	1:B:67:PHE:HB2	2.01	0.42
1:B:193:LEU:HB2	1:B:217:LEU:HD23	2.02	0.42
2:D:51:ASN:HB2	2:D:54:LEU:CD1	2.49	0.42
1:B:138:ARG:HH12	1:B:163:SER:HB3	1.84	0.42
1:A:170:ASP:O	1:A:172:ASN:ND2	2.53	0.42
1:A:426:LYS:HD2	1:A:447:HIS:CD2	2.55	0.42
1:A:387:TYR:CD1	1:A:388:GLU:HB3	2.55	0.42
1:A:376:LEU:HD23	1:A:379:ILE:HD11	2.02	0.41
1:A:447:HIS:C	1:A:448:LEU:HD12	2.44	0.41
1:B:415:PRO:HA	1:B:438:PRO:HB3	2.01	0.41
1:B:480:CYS:C	1:B:482:PHE:N	2.79	0.41
2:C:118:LEU:HA	2:C:118:LEU:HD12	1.76	0.41
2:C:129:CYS:O	2:C:130:PRO:O	2.38	0.41
1:A:146:ASP:O	1:A:148:ASN:ND2	2.53	0.41
1:A:238:THR:CG2	1:A:261:GLU:HB3	2.41	0.41
1:B:150:ILE:HG22	1:B:172:ASN:CB	2.48	0.41
1:A:111:THR:C	1:A:113:LEU:N	2.78	0.41
1:A:155:PRO:HA	1:A:181:ALA:HB2	2.02	0.41
1:A:434:LEU:O	1:A:455:ALA:HB3	2.20	0.41
1:A:453:ASN:CB	1:A:456:LEU:HD23	2.46	0.41
1:B:123:ASN:H	1:B:147:ALA:HB3	1.85	0.41
1:B:214:VAL:HA	1:B:238:THR:HG22	2.01	0.41
1:A:82:LEU:HD11	1:A:85:PRO:CA	2.50	0.41
1:A:128:HIS:N	1:A:150:ILE:HG22	2.36	0.41
1:B:107:LYS:HE3	1:B:132:GLU:N	2.35	0.41
2:C:110:PHE:CD2	2:C:123:GLY:HA3	2.55	0.41
1:A:98:ALA:HB2	1:A:122:GLN:HG3	2.03	0.41
1:B:110:PHE:HA	1:B:113:LEU:HD22	2.02	0.41
2:D:108:HIS:C	2:D:110:PHE:N	2.78	0.41
1:A:228:LYS:NZ	1:A:254:ARG:HH21	2.18	0.41
1:A:480:CYS:SG	2:D:66:ARG:HD2	2.61	0.41
1:B:434:LEU:O	1:B:455:ALA:HB3	2.21	0.41
2:D:129:CYS:O	2:D:130:PRO:O	2.38	0.41
1:A:99:GLY:CA	1:A:123:ASN:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ASN:HA	1:B:147:ALA:O	2.21	0.41
1:B:146:ASP:HB3	1:B:168:TRP:HB3	2.03	0.41
1:B:192:THR:HA	1:B:216:HIS:HB2	2.03	0.41
1:B:340:ILE:HD12	1:B:340:ILE:O	2.20	0.41
1:B:387:TYR:HA	1:B:409:LYS:O	2.20	0.41
1:B:414:HIS:CG	1:B:415:PRO:HD2	2.56	0.41
2:D:82:GLY:HA2	2:D:103:GLU:O	2.21	0.41
2:D:140:MET:HE2	2:D:140:MET:HB3	1.93	0.41
1:A:66:VAL:CG2	1:A:89:LEU:HA	2.51	0.41
1:A:75:MET:SD	1:A:99:GLY:HA3	2.61	0.41
1:A:311:THR:HA	1:A:334:THR:HG23	2.03	0.41
1:A:368:PRO:HD2	1:A:370:PHE:HE1	1.85	0.41
1:B:172:ASN:O	1:B:196:ASN:HA	2.21	0.41
1:B:310:LEU:HD12	1:B:310:LEU:HA	1.85	0.41
1:B:426:LYS:CB	1:B:447:HIS:HB2	2.51	0.41
1:B:468:LEU:HG	1:B:471:ILE:CD1	2.51	0.41
1:A:176:GLU:CA	1:A:198:ILE:HG22	2.51	0.40
1:A:477:TYR:CE2	2:D:91:MET:HE1	2.57	0.40
1:A:200:HIS:HA	1:A:224:SER:O	2.21	0.40
1:A:295:PHE:HB2	1:A:317:GLN:HB2	2.03	0.40
1:A:369:SER:C	1:A:371:SER:H	2.29	0.40
3:E:1:NAG:H61	3:E:2:NAG:H82	2.04	0.40
1:A:120:MET:HA	1:A:144:ARG:HB2	2.03	0.40
1:A:302:GLN:OE1	1:A:325:THR:N	2.55	0.40
1:A:62:SER:OG	1:A:63:ASN:N	2.53	0.40
1:A:381:LEU:O	1:A:384:ASN:ND2	2.52	0.40
1:B:367:LEU:HD11	1:B:386:ILE:HD13	2.03	0.40
1:B:391:VAL:HG13	1:B:392:ASP:N	2.37	0.40

There are no symmetry-related clashes.

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	453/539 (84%)	388 (86%)	57 (13%)	8 (2%)	6	33
1	B	454/539 (84%)	378 (83%)	63 (14%)	13 (3%)	3	23
2	C	101/126 (80%)	82 (81%)	14 (14%)	5 (5%)	1	16
2	D	102/126 (81%)	82 (80%)	12 (12%)	8 (8%)	1	10
All	All	1110/1330 (84%)	930 (84%)	146 (13%)	34 (3%)	3	22

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	A	90	ARG
1	A	209	LEU
1	A	353	ASN
1	B	66	VAL
1	B	90	ARG
1	B	123	ASN
1	B	209	LEU
1	B	467	GLU
2	C	109	ASN
2	C	129	CYS
2	C	130	PRO
2	C	131	GLU
2	C	133	SER
2	D	129	CYS
2	D	130	PRO
2	D	133	SER
2	D	142	CYS
1	B	43	ASP
1	B	53	SER
1	B	54	ASP
2	D	109	ASN
1	B	466	PRO
2	D	131	GLU
1	A	82	LEU
1	B	64	LEU
2	D	137	ASN
1	A	66	VAL
1	B	374	GLN
2	D	135	ALA
1	A	87	PRO
1	A	368	PRO
1	B	347	VAL

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Mol	Chain	Res	Type
1	B	368	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	414/484 (86%)	339 (82%)	75 (18%)	2	10
1	B	415/484 (86%)	361 (87%)	54 (13%)	4	17
2	C	89/105 (85%)	71 (80%)	18 (20%)	1	8
2	D	90/105 (86%)	77 (86%)	13 (14%)	3	15
All	All	1008/1178 (86%)	848 (84%)	160 (16%)	2	13

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	CYS
1	A	36	THR
1	A	47	LEU
1	A	55	LEU
1	A	60	LEU
1	A	64	LEU
1	A	66	VAL
1	A	74	SER
1	A	76	ASN
1	A	81	LEU
1	A	82	LEU
1	A	84	ASN
1	A	89	LEU
1	A	90	ARG
1	A	92	LEU
1	A	93	GLU
1	A	102	LEU
1	A	103	THR
1	A	113	LEU
1	A	116	LEU

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Mol	Chain	Res	Type
1	A	118	VAL
1	A	121	LEU
1	A	135	GLN
1	A	150	ILE
1	A	153	VAL
1	A	159	SER
1	A	170	ASP
1	A	174	LEU
1	A	175	THR
1	A	195	LEU
1	A	198	ILE
1	A	208	ASN
1	A	209	LEU
1	A	214	VAL
1	A	225	LEU
1	A	228	LYS
1	A	231	ASP
1	A	233	LEU
1	A	238	THR
1	A	302	GLN
1	A	304	LEU
1	A	310	LEU
1	A	312	LEU
1	A	318	ILE
1	A	325	THR
1	A	327	THR
1	A	336	THR
1	A	340	ILE
1	A	343	LEU
1	A	347	VAL
1	A	348	CYS
1	A	356	VAL
1	A	373	CYS
1	A	378	LYS
1	A	381	LEU
1	A	388	GLU
1	A	389	ILE
1	A	391	VAL
1	A	402	SER
1	A	410	ILE
1	A	420	THR
1	A	421	LEU

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Mol	Chain	Res	Type
1	A	424	LEU
1	A	425	ILE
1	A	433	LEU
1	A	440	THR
1	A	445	LEU
1	A	450	LEU
1	A	456	LEU
1	A	458	SER
1	A	459	LEU
1	A	460	ILE
1	A	462	SER
1	A	477	TYR
1	A	478	GLN
1	B	40	CYS
1	B	60	LEU
1	B	64	LEU
1	B	65	SER
1	B	70	TYR
1	B	77	ASN
1	B	82	LEU
1	B	89	LEU
1	B	92	LEU
1	B	102	LEU
1	B	103	THR
1	B	105	ILE
1	B	113	LEU
1	B	116	LEU
1	B	118	VAL
1	B	131	THR
1	B	135	GLN
1	B	137	LEU
1	B	140	LEU
1	B	142	SER
1	B	150	ILE
1	B	159	SER
1	B	161	LEU
1	B	170	ASP
1	B	209	LEU
1	B	225	LEU
1	B	233	LEU
1	B	238	THR
1	B	245	ASN

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Mol	Chain	Res	Type
1	B	246	LEU
1	B	256	LEU
1	B	280	ASN
1	B	284	ILE
1	B	299	SER
1	B	304	LEU
1	B	312	LEU
1	B	325	THR
1	B	330	LEU
1	B	343	LEU
1	B	347	VAL
1	B	348	CYS
1	B	354	LEU
1	B	373	CYS
1	B	375	LYS
1	B	376	LEU
1	B	401	ARG
1	B	412	ILE
1	B	421	LEU
1	B	439	ILE
1	B	440	THR
1	B	456	LEU
1	B	480	CYS
1	B	484	VAL
1	B	539	VAL
2	C	55	LYS
2	C	59	LYS
2	C	60	LEU
2	C	64	LEU
2	C	65	GLU
2	C	68	ASP
2	C	76	LEU
2	C	90	ASP
2	C	92	ASN
2	C	93	LYS
2	C	98	LYS
2	C	102	CYS
2	C	105	CYS
2	C	108	HIS
2	C	109	ASN
2	C	112	THR
2	C	115	LYS

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Mol	Chain	Res	Type
2	C	139	THR
2	D	49	GLU
2	D	54	LEU
2	D	68	ASP
2	D	76	LEU
2	D	92	ASN
2	D	93	LYS
2	D	95	ILE
2	D	96	LYS
2	D	98	LYS
2	D	105	CYS
2	D	107	SER
2	D	112	THR
2	D	120	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	HIS
1	A	265	HIS
1	A	294	GLN
1	A	345	GLN
1	A	355	GLN
1	A	443	HIS
1	A	464	ASN
1	B	37	HIS
1	B	124	ASN
1	B	135	GLN
1	B	136	ASN
1	B	219	ASN
1	B	268	ASN
1	B	313	ASN
1	B	377	GLN
2	C	51	ASN
2	C	71	GLN
2	D	88	ASN

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 ⓘ

3 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$
3	NAG	E	1	3,1	14,14,15	0.92	1 (7%)	17,19,21	1.72	3 (17%)
3	NAG	E	2	3	14,14,15	1.82	1 (7%)	17,19,21	1.08	1 (5%)
3	BMA	E	3	3	11,11,12	1.39	3 (27%)	15,15,17	2.26	4 (26%)

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	E	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	O5-C1	-6.64	1.32	1.43
3	E	3	BMA	O5-C5	2.73	1.48	1.43
3	E	1	NAG	C1-C2	2.62	1.55	1.52
3	E	3	BMA	C1-C2	2.35	1.57	1.52
3	E	3	BMA	O5-C1	2.04	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	BMA	C1-O5-C5	7.00	121.57	112.19
3	E	1	NAG	C2-N2-C7	4.10	128.40	122.90
3	E	1	NAG	O4-C4-C3	3.62	118.92	110.38
3	E	3	BMA	C1-C2-C3	2.86	113.80	109.64
3	E	1	NAG	C1-C2-N2	2.60	114.53	110.43
3	E	2	NAG	C3-C4-C5	2.59	114.94	110.23
3	E	3	BMA	O2-C2-C3	-2.48	105.02	110.15
3	E	3	BMA	O5-C1-C2	2.45	116.63	110.79

There are no chirality outliers.

All (4) torsion outliers are listed below:

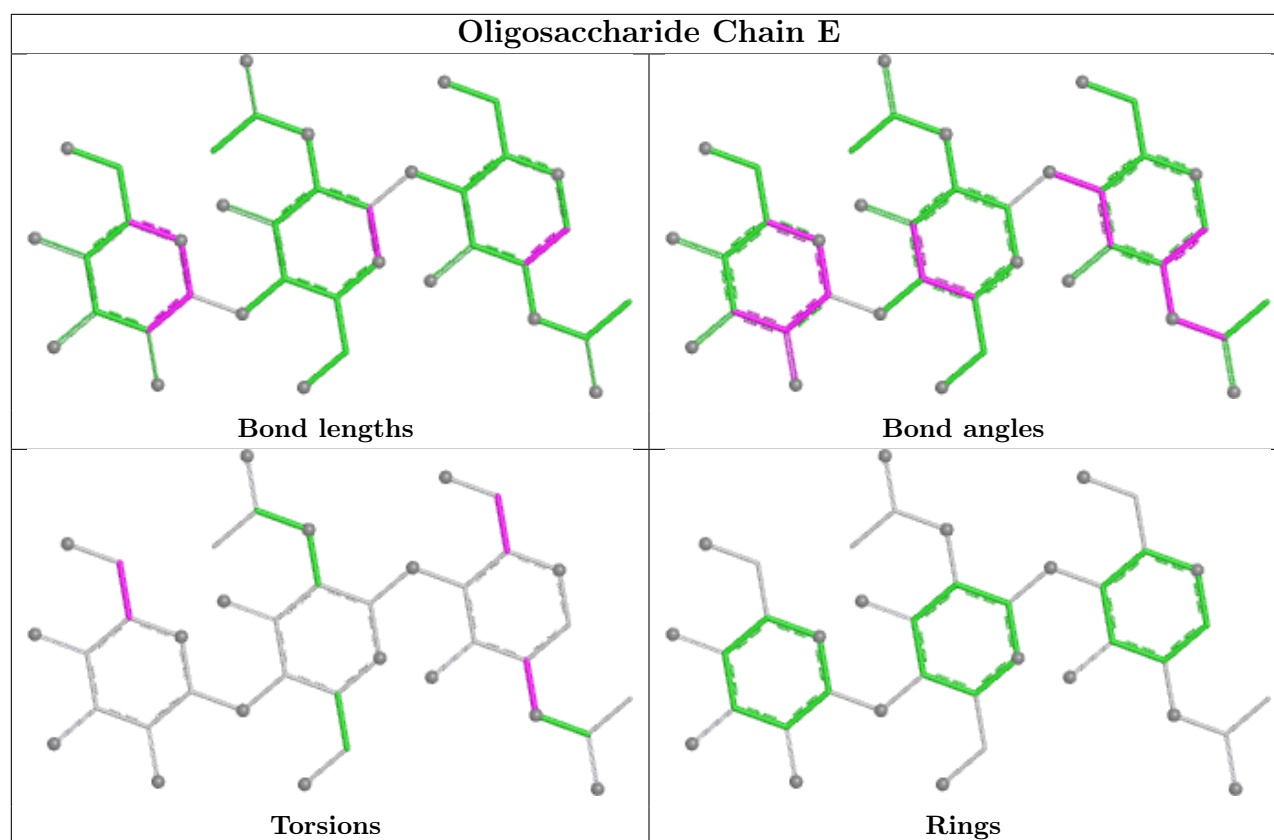
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C1-C2-N2-C7
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	3	BMA	2	0
3	E	1	NAG	3	0
3	E	2	NAG	4	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	1077	1	14,14,15	0.69	1 (7%)	17,19,21	0.64	0
4	NAG	A	1208	1	14,14,15	0.55	0	17,19,21	0.54	0
4	NAG	A	1077	1	14,14,15	0.47	0	17,19,21	0.49	0
4	NAG	A	1063	1	14,14,15	0.21	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1077	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1208	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	A	1077	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1063	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1077	NAG	C1-C2	2.26	1.55	1.52

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1208	NAG	C1

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1208	NAG	O5-C5-C6-O6
4	B	1077	NAG	O5-C5-C6-O6
4	B	1077	NAG	C4-C5-C6-O6
4	A	1208	NAG	C4-C5-C6-O6
4	A	1208	NAG	C3-C2-N2-C7
4	A	1063	NAG	C1-C2-N2-C7
4	A	1208	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1077	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	457/539 (84%)	-0.27	6 (1%) 75 59	131, 205, 257, 372	0
1	B	458/539 (84%)	-0.33	2 (0%) 88 77	135, 205, 259, 373	0
2	C	103/126 (81%)	-0.23	2 (1%) 66 51	165, 243, 334, 392	0
2	D	104/126 (82%)	-0.26	2 (1%) 66 51	176, 245, 333, 390	0
All	All	1122/1330 (84%)	-0.29	12 (1%) 78 62	131, 210, 288, 392	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	477	TYR	3.3
1	A	81	LEU	3.0
1	A	205	ALA	2.8
2	D	65	GLU	2.8
1	A	82	LEU	2.8
2	C	70	ARG	2.5
1	A	202	PRO	2.5
1	A	389	ILE	2.4
1	A	103	THR	2.4
1	B	133	ALA	2.2
2	C	68	ASP	2.1
2	D	67	ASN	2.0

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

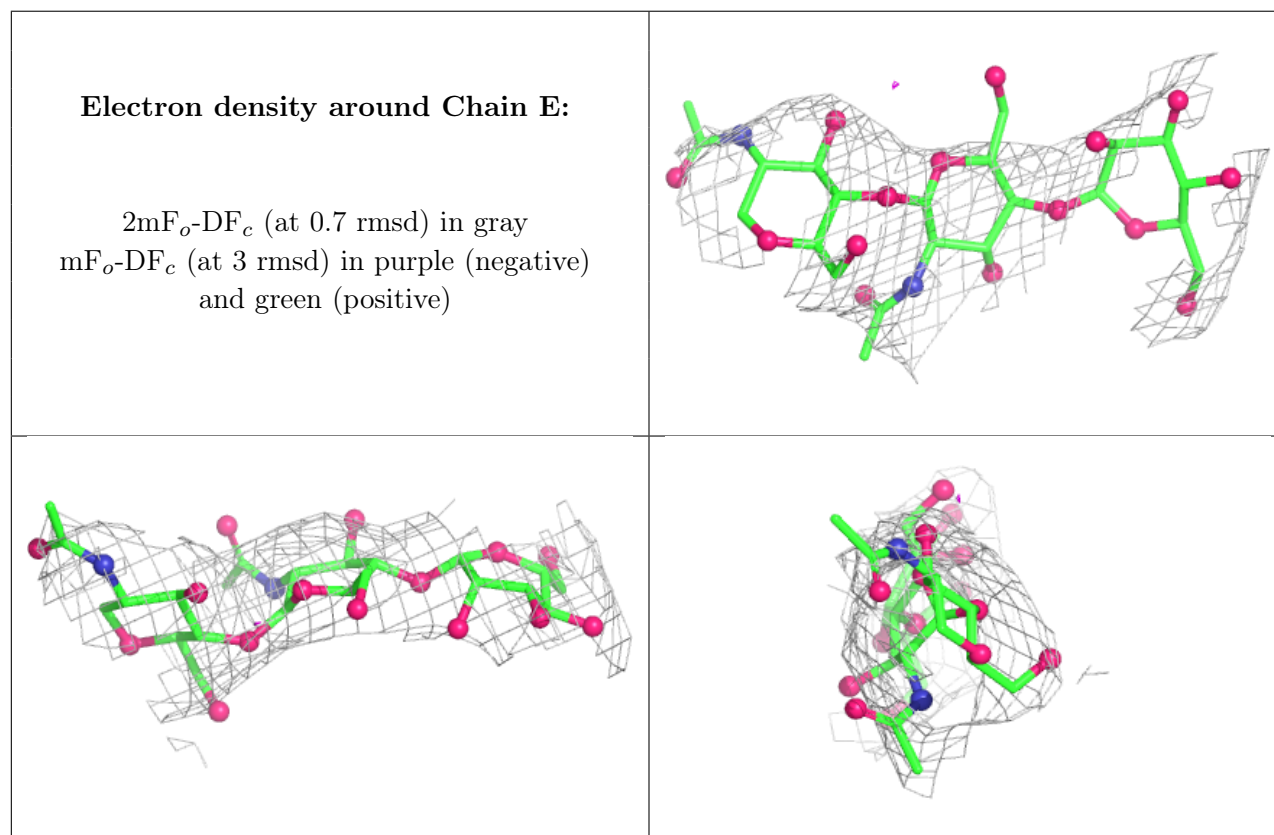
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
3	NAG	E	2	14/15	0.29	0.08	179,259,273,274	0
3	BMA	E	3	11/12	0.55	0.09	206,247,350,359	0
3	NAG	E	1	14/15	0.84	0.06	120,232,277,284	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
4	NAG	A	1063	14/15	0.40	0.06	182,291,310,317	0
4	NAG	A	1208	14/15	0.53	0.07	227,283,330,353	0
4	NAG	A	1077	14/15	0.55	0.08	199,261,288,316	0
4	NAG	B	1077	14/15	0.58	0.10	216,285,322,322	0

6.5 Other polymers [i](#)

There are no such residues in this entry.