



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:12 PM GMT

PDB ID : 4BST
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

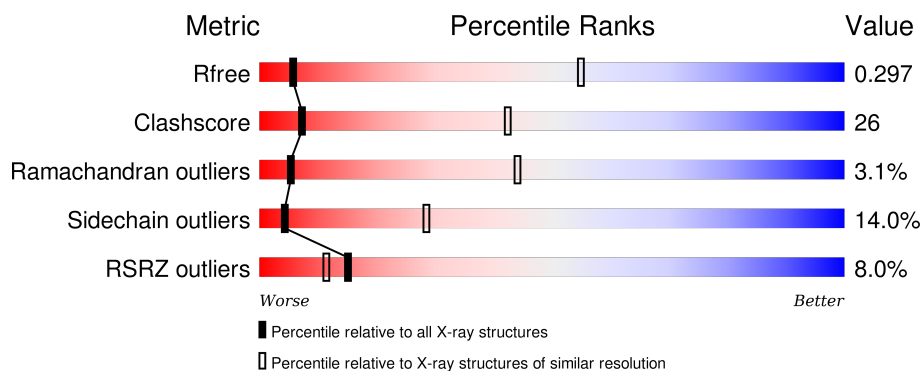
1 Overall quality at a glance ⓘ

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}	91344	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>4%</div> <div>42%</div> <div>33%</div> <div>8%</div> <div>15%</div> </div>
1	B	539	<div> <div>9%</div> <div>47%</div> <div>31%</div> <div>6%</div> <div>15%</div> </div>
2	C	126	<div> <div>7%</div> <div>33%</div> <div>36%</div> <div>13%</div> <div>18%</div> </div>
2	D	126	<div> <div>11%</div> <div>40%</div> <div>30%</div> <div>10%</div> <div>17%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	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

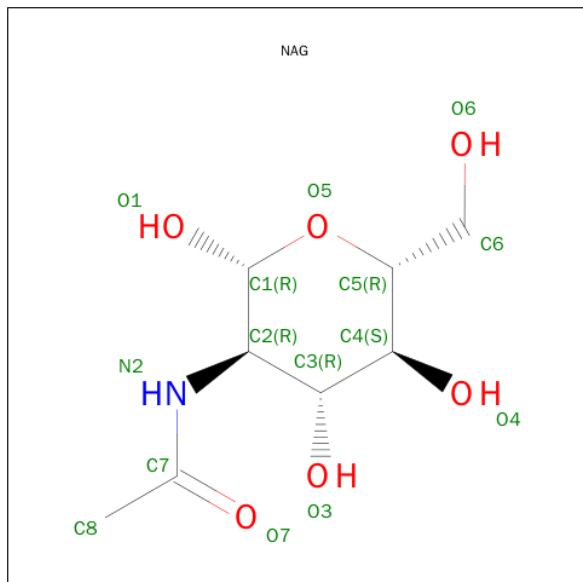
- Molecule 2 is a protein called R-SPONDIN-1.

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

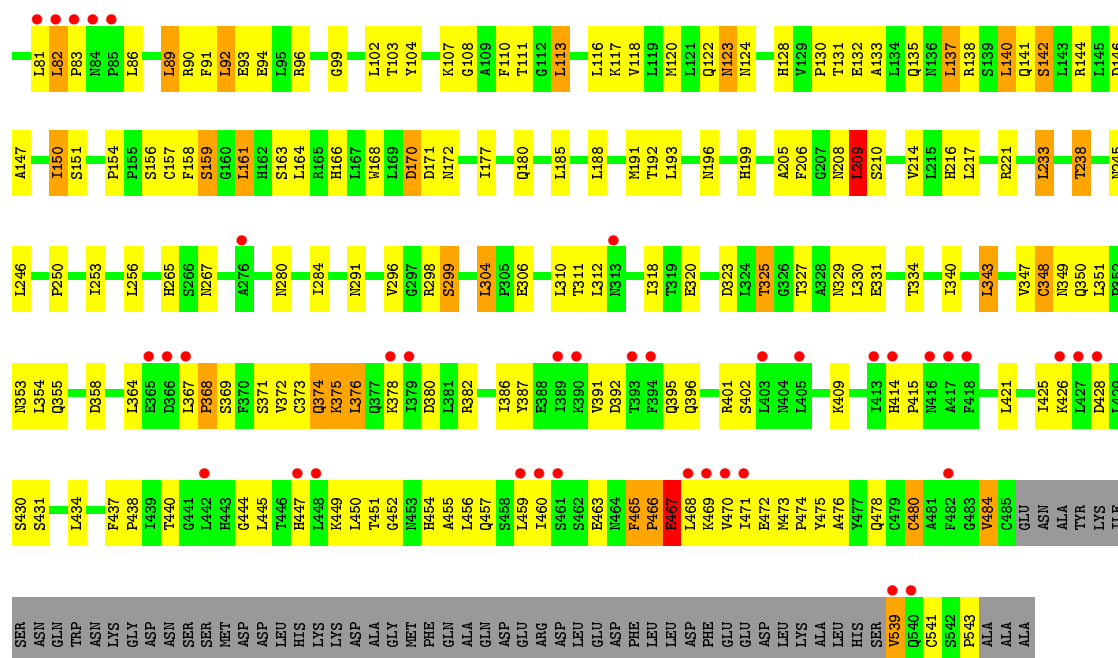
- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



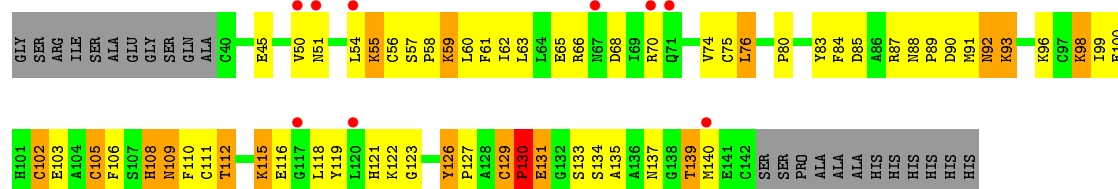
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

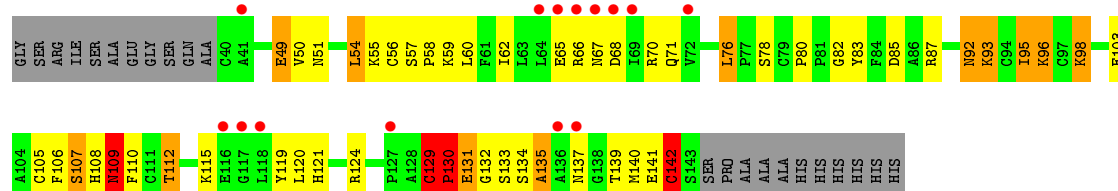
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	3	Total	C	N	O	0	0
			39	22	2	15		



• Molecule 2: R-SPONDIN-1



• Molecule 2: R-SPONDIN-1



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) 99.6 (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 0.264 , 0.297	Depositor DCC
R_{free} test set	991 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	180.2	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 203.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 19366 reflections	Xtriage
F_o, F_c correlation	0.88	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.37	0/3665	0.74	9/4991 (0.2%)
1	B	0.35	0/3671	0.65	3/4999 (0.1%)
2	C	0.45	0/794	0.83	1/1066 (0.1%)
2	D	0.50	0/800	0.82	4/1074 (0.4%)
All	All	0.38	0/8930	0.72	17/12130 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	TYR	CA-CB-CG	8.05	128.70	113.40
1	A	195	LEU	CA-CB-CG	7.31	132.12	115.30
1	A	198	ILE	CG1-CB-CG2	-6.96	96.08	111.40
1	A	81	LEU	CA-CB-CG	6.61	130.50	115.30
2	D	132	GLY	N-CA-C	-6.52	96.81	113.10
1	A	310	LEU	CA-CB-CG	6.31	129.81	115.30
1	A	92	LEU	CA-CB-CG	6.28	129.74	115.30
2	D	142	CYS	CA-CB-SG	6.01	124.82	114.00
2	C	130	PRO	C-N-CA	5.83	136.26	121.70
2	D	129	CYS	CA-CB-SG	5.49	123.89	114.00
1	A	102	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	60	LEU	CA-CB-CG	5.41	127.73	115.30
1	A	312	LEU	CA-CB-CG	5.38	127.67	115.30
1	A	66	VAL	CB-CA-C	5.35	121.56	111.40
1	B	140	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	113	LEU	CB-CG-CD1	-5.26	102.05	111.00
2	D	130	PRO	C-N-CA	5.25	134.82	121.70

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	202	0
1	B	3591	0	3597	156	0
2	C	778	0	744	55	0
2	D	784	0	749	57	0
3	A	42	0	39	1	0
3	B	14	0	13	0	0
4	B	39	0	34	5	0
All	All	8833	0	8769	457	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 26.

All (457) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:108:HIS:CG	2:D:109:ASN:H	2.03	0.76
2:C:139:THR:OG1	2:C:140:MET:N	2.18	0.76
2:D:119:TYR:CZ	2:D:142:CYS:HB2	2.21	0.75
1:A:453:ASN:HB3	1:A:456:LEU:HD23	1.67	0.75
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:OD1	1:B:170:ASP:N	2.23	0.72
1:A:475:TYR:HB2	1:A:477:TYR:HE1	1.55	0.72
2:C:96:LYS:O	2:C:98:LYS:NZ	2.17	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
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:345:GLN:CD	1:A:345:GLN:H	1.95	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:454:HIS:O	1:B:457:GLN:NE2	2.26	0.68
1:B:284:ILE:HG12	1:B:306:GLU:OE2	1.92	0.68
2:D:70:ARG:HH11	2:D:70:ARG:HG3	1.59	0.68
1:A:154:PRO:HG2	1:A:157:CYS:HB3	1.75	0.68
2:D:119:TYR:HE1	2:D:141:GLU:HA	1.59	0.67
1:B:122:GLN:O	1:B:124:ASN:ND2	2.26	0.67
2:D:108:HIS:CD2	2:D:109:ASN:H	2.12	0.67
1:A:296:VAL:HG12	1:A:318:ILE:HG21	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:445:LEU:HD21	1:A:448:LEU:HD11	1.78	0.66
1:A:219:ASN:HD22	2:C:89:PRO:HD3	1.61	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: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:374:GLN:O	1:B:375:LYS:HE2	1.97	0.64
1:B:70:TYR:HB2	1:B:94:GLU:HB3	1.78	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:353:ASN:HA	1:A:375:LYS:HD3	1.77	0.63
1:A:84:ASN:N	1:A:84:ASN:OD1	2.31	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
2:C:140:MET:O	2:C:140:MET:HG3	1.99	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
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
1:A:477:TYR:H	1:A:477:TYR:HD1	1.47	0.61
2:C:105:CYS:HB3	2:C:111:CYS:HA	1.83	0.61
1:A:170:ASP:N	1:A:170:ASP:OD1	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:465:PHE:HB3	1:A:468:LEU:HD12	1.83	0.60
1:B:444:GLY:HA2	1:B:467:GLU:CD	2.22	0.60
1:A:388:GLU:N	1:A:388:GLU:OE1	2.34	0.60
1:B:265:HIS:O	1:B:267:ASN:ND2	2.35	0.60
2:C:62:ILE:HD11	2:C:93:LYS:HE3	1.84	0.60
1:B:460:ILE:HG12	1:B:478:GLN:HE21	1.66	0.60
1:A:425:ILE:HD12	1:A:445:LEU:HA	1.83	0.60
2:C:50:VAL:HG23	2:C:51:ASN:ND2	2.15	0.60
1:B:380:ASP:OD2	1:B:382:ARG:NH1	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:107:SER:OG	2:D:108:HIS:N	2.33	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:N	1:A:231:ASP:OD1	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
1:B:107:LYS:HG3	1:B:132:GLU:HB3	1.85	0.58
2:D:98:LYS:HG3	2:D:108:HIS:CD2	2.38	0.58
2:C:61:PHE:CZ	2:C:85:ASP:HB3	2.38	0.58
1:B:329:ASN:OD1	1:B:353:ASN:ND2	2.37	0.58
1:A:457:GLN:O	1:A:477:TYR:OH	2.17	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:B:466:PRO:C	1:B:468:LEU:H	2.08	0.57
1:B:81:LEU:HD12	1:B:82:LEU:HB2	1.86	0.57
1:A:484:VAL:HG21	1:A:541:CYS:HB3	1.86	0.57
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
2:C:45:GLU:N	2:C:45:GLU:OE1	2.38	0.56
1:A:302:GLN:HE22	1:A:323:ASP:HB3	1.69	0.56
1:B:70:TYR:CB	1:B:94:GLU:HB3	2.36	0.56
1:A:225:LEU:HD21	1:A:250:PRO:HB3	1.87	0.56
1:A:60:LEU:HD21	1:A:82:LEU:CD2	2.36	0.55
1:B:457:GLN:HG3	1:B:475:TYR:HE2	1.71	0.55
1:A:43:ASP:OD1	1:A:44:GLY:N	2.39	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:B:135:GLN:N	1:B:135:GLN:CD	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASN:HD22	3:A:1077:NAG:C7	2.19	0.55
1:A:433:LEU:N	1:A:453:ASN:OD1	2.38	0.55
1:B:107:LYS:CE	1:B:132:GLU:HB3	2.37	0.55
1:A:420:THR:O	1:A:420:THR:OG1	2.13	0.55
1:A:426:LYS:HG3	1:A:447:HIS:HB2	1.89	0.55
2:C:100:GLU:N	2:C:100:GLU:OE1	2.40	0.54
1:B:298:ARG:NE	1:B:320:GLU:OE1	2.33	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: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:A:52:CYS:HB3	1:A:55:LEU:HD21	1.89	0.54
1:B:128:HIS:CA	1:B:150:ILE:HG12	2.35	0.54
1:B:355:GLN:O	1:B:376:LEU:HD12	2.07	0.54
1:B:349:ASN:OD1	1:B:350:GLN:N	2.40	0.54
2:C:121:HIS:CD2	2:C:122:LYS:HG2	2.42	0.54
1:B:132:GLU:O	1:B:132:GLU:HG3	2.08	0.54
1:A:392:ASP:HA	1:A:395:GLN:HG2	1.89	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:340:ILE:HG13	1:A:362:ASN:HD21	1.72	0.54
1:A:81:LEU:HA	1:A:82:LEU:CB	2.38	0.54
1:A:366:ASP:OD1	1:A:367:LEU:N	2.41	0.54
1:B:444:GLY:HA2	1:B:467:GLU:OE2	2.08	0.53
1:A:415:PRO:HA	1:A:438:PRO:HB3	1.91	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
2:D:135:ALA:O	2:D:142:CYS:HA	2.09	0.53
1:B:69:SER:O	1:B:93:GLU:N	2.31	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: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:A:389:ILE:HG13	1:A:389:ILE:O	2.10	0.52
1:B:348:CYS:HB2	1:B:372:VAL:HG23	1.91	0.52
2:D:51:ASN:HB2	2:D:54:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ALA:HB2	2:D:87:ARG:CZ	2.40	0.52
1:B:351:LEU:HB3	1:B:354:LEU:HD21	1.90	0.52
1:A:392:ASP:HA	1:A:395:GLN:CG	2.40	0.52
2:D:93:LYS:NZ	2:D:95:ILE:HA	2.25	0.52
1:B:43:ASP:OD1	1:B:44:GLY:N	2.42	0.52
1:B:208:ASN:ND2	4:B:1208:NAG:O7	2.42	0.51
1:A:354:LEU:HD21	1:A:356:VAL:O	2.10	0.51
1:A:387:TYR:C	1:A:410:ILE:HA	2.31	0.51
2:C:84:PHE:HB2	2:C:106:PHE:O	2.11	0.51
2:C:63:LEU:HB3	2:C:74:VAL:HG13	1.91	0.51
2:D:95:ILE:O	2:D:95:ILE:HG13	2.11	0.51
1:A:332:SER:HA	1:A:356:VAL:HG22	1.92	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
1:B:59:GLU:HB3	1:B:82:LEU:HD11	1.91	0.51
1:A:111:THR:C	1:A:113:LEU:H	2.14	0.51
1:B:144:ARG:HD2	1:B:168:TRP:CD2	2.46	0.51
1:B:156:SER:O	1:B:159:SER:OG	2.27	0.50
1:A:69:SER:O	1:A:93:GLU:N	2.35	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:B:484:VAL:CG1	1:B:541:CYS:HB3	2.42	0.50
1:A:138:ARG:HG3	1:A:139:SER:N	2.27	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:B:96:ARG:NE	1:B:120:MET:SD	2.85	0.50
1:A:144:ARG:HA	1:A:168:TRP:HB2	1.94	0.50
1:B:168:TRP:CZ2	2:D:85:ASP:HB3	2.46	0.50
4:B:1209:NAG:H62	4:B:1210:BMA:H2	1.94	0.50
1:B:89:LEU:H	1:B:89:LEU:HD12	1.77	0.50
2:C:56:CYS:SG	2:C:62:ILE:HG22	2.52	0.50
1:B:267:ASN:HB2	1:B:291:ASN:ND2	2.27	0.50
1:B:147:ALA:HA	1:B:171:ASP:HB3	1.94	0.50
1:B:431:SER:N	1:B:451:THR:O	2.41	0.50
1:A:193:LEU:HB2	1:A:217:LEU:HD23	1.94	0.50
2:C:134:SER:OG	2:C:135:ALA:N	2.44	0.50
2:D:119:TYR:CZ	2:D:120:LEU:O	2.65	0.49
1:B:66:VAL:HG23	1:B:67:PHE:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:GLY:N	1:B:123:ASN:OD1	2.45	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
2:D:83:TYR:CD1	2:D:96:LYS:HA	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
1:B:340:ILE:CD1	1:B:364:LEU:HG	2.43	0.49
2:C:63:LEU:HD11	2:C:83:TYR:CE2	2.47	0.49
1:B:92:LEU:HD12	1:B:94:GLU:H	1.77	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
1:B:132:GLU:HA	1:B:135:GLN:NE2	2.28	0.49
1:A:425:ILE:O	1:A:446:THR:HG22	2.13	0.49
1:B:304:LEU:N	1:B:327:THR:HG22	2.22	0.49
1:A:214:VAL:HG23	1:A:238:THR:OG1	2.13	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:N	1:A:208:ASN:OD1	2.46	0.48
1:A:343:LEU:HD13	1:A:364:LEU:HD21	1.95	0.48
1:A:171:ASP:CA	1:A:195:LEU:HG	2.42	0.48
1:B:466:PRO:HG2	1:B:467:GLU:OE1	2.13	0.48
1:B:334:THR:HB	1:B:358:ASP:HB3	1.95	0.48
1:A:176:GLU:N	1:A:198:ILE:HG22	2.28	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
2:D:65:GLU:O	2:D:71:GLN:HA	2.13	0.48
1:A:132:GLU:O	1:A:135:GLN:HB3	2.13	0.48
1:B:445:LEU:HD12	1:B:468:LEU:HD13	1.95	0.48
1:A:93:GLU:HG3	1:A:117:LYS:HD3	1.96	0.48
2:C:103:GLU:OE1	2:C:115:LYS:NZ	2.47	0.48
1:A:425:ILE:O	1:A:445:LEU:HD12	2.14	0.48
1:A:147:ALA:N	1:A:171:ASP:OD1	2.40	0.48
1:A:65:SER:OG	1:A:66:VAL:O	2.24	0.48
2:C:66:ARG:NH1	2:C:66:ARG:HB2	2.29	0.48
1:A:239:LEU:HD22	1:A:241:LEU:HG	1.95	0.48
1:A:158:PHE:CD2	1:A:185:LEU:HD11	2.49	0.48
2:D:50:VAL:O	2:D:70:ARG:NH2	2.47	0.48
1:B:166:HIS:NE2	2:D:112:THR:OG1	2.46	0.48
2:D:108:HIS:C	2:D:110:PHE:H	2.18	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ILE:HD11	1:A:434:LEU:HD11	1.96	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
2:C:63:LEU:HD11	2:C:83:TYR:CZ	2.49	0.47
1:B:374:GLN:C	1:B:376:LEU:H	2.17	0.47
1:A:102:LEU:H	1:A:102:LEU:HD22	1.79	0.47
2:C:108:HIS:C	2:C:110:PHE:H	2.18	0.47
1:A:192:THR:HG1	2:C:106:PHE:HZ	1.60	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:119:TYR:CD1	2:D:120:LEU:N	2.83	0.47
1:B:66:VAL:HG23	1:B:67:PHE:CD1	2.50	0.47
1:A:391:VAL:HG22	1:A:414:HIS:CG	2.49	0.47
2:D:70:ARG:HG3	2:D:70:ARG:NH1	2.26	0.47
1:B:425:ILE:O	1:B:445:LEU:HB2	2.14	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:431:SER:HA	1:B:452:GLY:HA3	1.96	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:365:GLU:N	1:A:365:GLU:OE1	2.47	0.47
1:A:469:LYS:HZ2	1:A:539:VAL:N	2.13	0.47
1:A:335:LEU:O	1:A:359:LEU:HA	2.15	0.47
1:A:49:ARG:HH22	1:A:72:ASP:HB2	1.80	0.47
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: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
2:C:80:PRO:O	2:C:83:TYR:HB2	2.16	0.46
1:B:447:HIS:CE1	1:B:470:VAL:HB	2.51	0.46
1:B:130:PRO:HB3	1:B:133:ALA:HB3	1.97	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:B:138:ARG:O	1:B:163:SER:OG	2.26	0.46
1:A:425:ILE:HA	1:A:445:LEU:HB2	1.97	0.46
1:A:450:LEU:HD11	1:A:473:MET:SD	2.56	0.46
1:A:365:GLU:HG3	1:A:385:GLU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:SER:HA	1:A:101:ALA:O	2.16	0.46
1:B:76:ASN:OD1	1:B:76:ASN:N	2.49	0.46
1:A:389:ILE:HD11	1:A:417:ALA:HB1	1.98	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:A:42:PRO:HA	1:A:47:LEU:O	2.16	0.45
2:D:58:PRO:HB2	2:D:59:LYS:HG3	1.99	0.45
2:C:80:PRO:HD2	2:C:83:TYR:CD2	2.52	0.45
1:B:144:ARG:NH2	2:D:106:PHE:HD1	2.13	0.45
1:A:189:GLN:HA	1:A:212:LEU:HA	1.98	0.45
1:A:269:ILE:HD12	1:A:270:ARG:H	1.82	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:204:TYR:O	1:A:206:PHE:N	2.49	0.45
2:C:129:CYS:HA	2:C:130:PRO:HD2	1.60	0.45
1:A:113:LEU:HA	1:A:113:LEU:HD13	1.56	0.45
2:C:80:PRO:HD2	2:C:83:TYR:HD2	1.81	0.45
1:B:135:GLN:HB3	1:B:159:SER:O	2.17	0.45
1:A:463:GLU:O	1:A:464:ASN:ND2	2.50	0.45
1:B:323:ASP:OD1	1:B:325:THR:OG1	2.34	0.45
2:C:137:ASN:HD21	2:C:139:THR:HG22	1.82	0.45
4:B:1208:NAG:H5	4:B:1209:NAG:C7	2.47	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
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:477:TYR:N	1:A:477:TYR:CD1	2.85	0.45
2:C:59:LYS:HE2	2:C:87:ARG:HH11	1.82	0.45
1:A:177:ILE:HG21	1:A:205:ALA:HB1	1.98	0.45
1:B:437:PHE:CD1	1:B:438:PRO:O	2.70	0.45
2:D:134:SER:OG	2:D:135:ALA:N	2.49	0.44
2:C:130:PRO:CB	2:C:131:GLU:HB2	2.42	0.44
4:B:1209:NAG:H62	4:B:1210:BMA:C2	2.47	0.44
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:D:56:CYS:SG	2:D:62:ILE:HG12	2.57	0.44
1:A:319:THR:C	1:A:340:ILE:HG22	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:HG	1:A:60:LEU:H	1.39	0.44
1:A:182:PHE:HE2	1:A:191:MET:SD	2.41	0.44
1:A:50:VAL:HB	1:A:71:LEU:HD13	1.99	0.44
1:B:166:HIS:CE1	2:D:110:PHE:HE1	2.34	0.44
2:D:119:TYR:HE1	2:D:141:GLU:CA	2.27	0.44
1:B:70:TYR:HA	1:B:92:LEU:CD1	2.47	0.44
2:C:118:LEU:HG	2:C:126:TYR:C	2.38	0.44
1:A:87:PRO:HB2	1:A:112:GLY:HA3	2.00	0.44
1:B:471:ILE:O	1:B:541:CYS:HA	2.18	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:180:GLN:CD	1:B:180:GLN:H	2.20	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
2:D:119:TYR:OH	2:D:142:CYS:HB2	2.17	0.43
2:D:57:SER:OG	2:D:58:PRO:HD2	2.18	0.43
2:C:59:LYS:HA	2:C:59:LYS:HE3	1.99	0.43
1:A:542:SER:HA	1:A:543:PRO:HD2	1.87	0.43
1:A:425:ILE:HG13	1:A:446:THR:CG2	2.48	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:176:GLU:HG2	1:A:200:HIS:CE1	2.54	0.43
1:B:299:SER:OG	1:B:299:SER:O	2.35	0.43
1:B:107:LYS:HE3	1:B:132:GLU:CB	2.45	0.43
1:A:476:ALA:HA	1:A:543:PRO:HB3	2.00	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
1:B:369:SER:C	1:B:371:SER:H	2.20	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:B:137:LEU:HD12	1:B:137:LEU:H	1.84	0.43
2:C:130:PRO:HA	2:C:131:GLU:CG	2.48	0.43
1:A:471:ILE:O	1:A:541:CYS:HA	2.19	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
2:D:82:GLY:C	2:D:83:TYR:HD1	2.23	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:233:LEU:HD13	1:B:233:LEU:H	1.84	0.42
1:A:468:LEU:HA	1:A:468:LEU:HD23	1.76	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:178:PRO:O	1:A:182:PHE:HD1	2.02	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:B:48:LEU:HD23	1:B:67:PHE:HB2	2.01	0.42
2:D:51:ASN:HB2	2:D:54:LEU:CD1	2.49	0.42
1:B:193:LEU:HB2	1:B:217:LEU:HD23	2.02	0.42
1:B:138:ARG:HH12	1:B:163:SER:HB3	1.84	0.42
1:B:428:ASP:CG	1:B:449:LYS:HB2	2.40	0.42
1:B:135:GLN:C	1:B:137:LEU:N	2.72	0.42
1:A:426:LYS:HD2	1:A:447:HIS:CD2	2.55	0.42
1:A:170:ASP:O	1:A:172:ASN:ND2	2.53	0.42
2:D:71:GLN:CD	2:D:71:GLN:H	2.22	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:B:415:PRO:HA	1:B:438:PRO:HB3	2.01	0.41
2:C:118:LEU:HD12	2:C:118:LEU:HA	1.76	0.41
2:C:129:CYS:O	2:C:130:PRO:O	2.38	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:146:ASP:O	1:A:148:ASN:ND2	2.53	0.41
1:A:228:LYS:NZ	1:A:254:ARG:HH21	2.18	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:155:PRO:HA	1:A:181:ALA:HB2	2.02	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: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:A:175:THR:C	1:A:198:ILE:HG22	2.41	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
1:A:228:LYS:HZ1	1:A:254:ARG:HE	1.69	0.41
1:A:62:SER:OG	1:A:63:ASN:N	2.53	0.41
1:A:480:CYS:SG	2:D:66:ARG:HD2	2.61	0.41
2:D:129:CYS:O	2:D:130:PRO:O	2.38	0.41
1:B:434:LEU:O	1:B:455:ALA:HB3	2.21	0.41
1:B:463:GLU:C	1:B:465:PHE:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLY:CA	1:A:123:ASN:HB3	2.50	0.41
2:D:82:GLY:HA2	2:D:103:GLU:O	2.21	0.41
1:B:146:ASP:HB3	1:B:168:TRP:HB3	2.03	0.41
1:B:123:ASN:HA	1:B:147:ALA:O	2.21	0.41
1:B:340:ILE:O	1:B:340:ILE:HD12	2.20	0.41
1:B:414:HIS:CG	1:B:415:PRO:HD2	2.56	0.41
1:B:387:TYR:HA	1:B:409:LYS:O	2.20	0.41
1:B:117:LYS:HE2	1:B:141:GLN:CD	2.41	0.41
1:B:192:THR:HA	1:B:216:HIS:HB2	2.03	0.41
1:A:75:MET:SD	1:A:99:GLY:HA3	2.61	0.41
1:B:468:LEU:HG	1:B:471:ILE:CD1	2.51	0.41
1:A:66:VAL:CG2	1:A:89:LEU:HA	2.51	0.41
1:A:311:THR:HA	1:A:334:THR:HG23	2.03	0.41
1:B:172:ASN:O	1:B:196:ASN:HA	2.21	0.41
1:B:426:LYS:CB	1:B:447:HIS:HB2	2.51	0.41
1:A:368:PRO:HD2	1:A:370:PHE:HE1	1.85	0.41
1:B:310:LEU:HD12	1:B:310:LEU:HA	1.85	0.41
1:A:176:GLU:CA	1:A:198:ILE:HG22	2.51	0.40
4:B:1208:NAG:H61	4:B:1209:NAG:H82	2.04	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: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: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:A:65:SER:C	1:A:66:VAL:O	2.58	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	453/539 (84%)	388 (86%)	57 (13%)	8 (2%)	11	55
1	B	454/539 (84%)	378 (83%)	63 (14%)	13 (3%)	6	45
2	C	101/126 (80%)	82 (81%)	14 (14%)	5 (5%)	3	31
2	D	102/126 (81%)	82 (80%)	12 (12%)	8 (8%)	1	20
All	All	1110/1330 (84%)	930 (84%)	146 (13%)	34 (3%)	5	44

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%)	350 (84%)	64 (16%)	3	24
1	B	415/484 (86%)	368 (89%)	47 (11%)	7	36
2	C	89/105 (85%)	72 (81%)	17 (19%)	2	14
2	D	90/105 (86%)	77 (86%)	13 (14%)	4	27
All	All	1008/1178 (86%)	867 (86%)	141 (14%)	4	28

All (141) 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	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
1	A	118	VAL

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Mol	Chain	Res	Type
1	A	121	LEU
1	A	135	GLN
1	A	152	TYR
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	214	VAL
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	343	LEU
1	A	348	CYS
1	A	356	VAL
1	A	373	CYS
1	A	381	LEU
1	A	389	ILE
1	A	402	SER
1	A	420	THR
1	A	421	LEU
1	A	424	LEU
1	A	433	LEU
1	A	440	THR
1	A	445	LEU
1	A	447	HIS
1	A	450	LEU
1	A	458	SER
1	A	459	LEU
1	A	460	ILE

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Mol	Chain	Res	Type
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	113	LEU
1	B	116	LEU
1	B	118	VAL
1	B	131	THR
1	B	137	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	233	LEU
1	B	238	THR
1	B	245	ASN
1	B	246	LEU
1	B	256	LEU
1	B	280	ASN
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	348	CYS
1	B	373	CYS
1	B	375	LYS
1	B	376	LEU
1	B	401	ARG
1	B	421	LEU

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Mol	Chain	Res	Type
1	B	440	THR
1	B	456	LEU
1	B	465	PHE
1	B	467	GLU
1	B	480	CYS
1	B	484	VAL
1	B	539	VAL
2	C	55	LYS
2	C	59	LYS
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
2	C	126	TYR
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	109	ASN
2	D	112	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN

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Mol	Chain	Res	Type
1	A	162	HIS
1	A	265	HIS
1	A	464	ASN
1	B	135	GLN
1	B	313	ASN
1	B	478	GLN
2	C	51	ASN
2	C	71	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

3 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	1208	1,4	14,14,15	0.89	1 (7%)	15,19,21	1.68	3 (20%)
4	NAG	B	1209	4	14,14,15	1.83	1 (7%)	15,19,21	1.07	2 (13%)
4	BMA	B	1210	4	11,11,12	1.36	3 (27%)	14,15,17	2.59	4 (28%)

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	1208	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1209	4	-	0/6/23/26	0/1/1/1
4	BMA	B	1210	4	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1209	NAG	O5-C1	-6.68	1.32	1.43
4	B	1210	BMA	O5-C1	2.03	1.47	1.43
4	B	1210	BMA	C1-C2	2.36	1.57	1.52
4	B	1210	BMA	O5-C5	2.41	1.48	1.43
4	B	1208	NAG	C1-C2	2.49	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1210	BMA	O2-C2-C3	-2.54	105.02	110.12
4	B	1209	NAG	C1-O5-C5	-2.02	109.68	112.25
4	B	1208	NAG	C1-O5-C5	2.03	114.83	112.25
4	B	1209	NAG	C3-C4-C5	2.72	114.94	110.20
4	B	1210	BMA	O5-C1-C2	3.56	116.63	110.86
4	B	1210	BMA	C1-C2-C3	3.60	113.80	109.54
4	B	1208	NAG	O4-C4-C3	3.81	118.92	110.34
4	B	1208	NAG	C2-N2-C7	4.17	128.40	123.04
4	B	1210	BMA	C1-O5-C5	7.35	121.57	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1208	NAG	3	0
4	B	1209	NAG	4	0
4	B	1210	BMA	2	0

5.6 Ligand geometry

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	$\# Z > 2$
3	NAG	A	1063	1	14,14,15	0.20	0	15,19,21	0.28	0
3	NAG	A	1077	1	14,14,15	0.45	0	15,19,21	0.35	0
3	NAG	A	1208	1	14,14,15	0.53	0	15,19,21	0.35	0
3	NAG	B	1077	1	14,14,15	0.65	1 (7%)	15,19,21	0.47	0

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1077	NAG	C1-C2	2.14	1.55	1.52

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1208	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	457/539 (84%)	0.15	20 (4%) 38 29	131, 205, 257, 372	0
1	B	458/539 (84%)	0.43	47 (10%) 9 7	135, 205, 259, 373	0
2	C	103/126 (81%)	0.45	9 (8%) 13 10	165, 243, 334, 392	0
2	D	104/126 (82%)	0.75	14 (13%) 4 5	176, 245, 333, 390	0
All	All	1122/1330 (84%)	0.35	90 (8%) 15 11	131, 210, 288, 392	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	539	VAL	6.0
1	A	83	PRO	5.6
1	B	82	LEU	5.2
2	D	67	ASN	5.0
1	B	60	LEU	4.9
1	B	59	GLU	4.9
1	A	61	PRO	4.7
1	B	61	PRO	4.6
1	B	83	PRO	4.6
2	D	68	ASP	4.5
2	D	65	GLU	4.5
1	B	84	ASN	4.4
1	A	228	LYS	4.2
1	B	460	ILE	4.2
1	A	227	LYS	4.1
1	A	60	LEU	3.9
1	B	540	GLN	3.9
1	B	427	LEU	3.9
1	B	64	LEU	3.7
1	A	81	LEU	3.7
1	A	82	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	C	70	ARG	3.5
2	C	51	ASN	3.4
1	B	403	LEU	3.4
1	A	54	ASP	3.4
2	D	117	GLY	3.3
1	B	448	LEU	3.3
1	B	81	LEU	3.3
2	D	116	GLU	3.1
1	A	59	GLU	3.1
1	B	33	GLY	3.0
1	B	469	LYS	2.9
1	B	471	ILE	2.9
1	B	417	ALA	2.9
1	A	57	LEU	2.9
2	D	69	ILE	2.8
1	B	365	GLU	2.8
2	D	66	ARG	2.8
1	A	226	GLY	2.8
1	B	413	ILE	2.7
1	B	470	VAL	2.7
2	D	41	ALA	2.7
2	C	140	MET	2.7
2	C	71	GLN	2.7
2	D	127	PRO	2.7
2	C	50	VAL	2.6
1	B	390	LYS	2.6
1	B	85	PRO	2.6
1	B	389	ILE	2.6
1	B	482	PHE	2.6
1	A	80	GLN	2.5
1	B	468	LEU	2.5
2	D	118	LEU	2.5
1	B	73	LEU	2.4
1	B	447	HIS	2.4
1	A	204	TYR	2.4
2	D	136	ALA	2.4
1	B	418	PHE	2.4
2	C	117	GLY	2.3
1	A	249	PHE	2.3
1	B	276	ALA	2.3
1	B	313	ASN	2.3
1	B	62	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	72	VAL	2.3
2	C	120	LEU	2.3
1	B	379	ILE	2.3
2	C	67	ASN	2.3
1	B	394	PHE	2.3
1	A	62	SER	2.2
1	B	428	ASP	2.2
1	B	50	VAL	2.2
2	C	54	LEU	2.2
1	A	64	LEU	2.2
1	B	414	HIS	2.2
1	B	459	LEU	2.2
1	B	461	SER	2.2
2	D	64	LEU	2.2
1	B	378	LYS	2.1
1	A	205	ALA	2.1
1	B	416	ASN	2.1
2	D	137	ASN	2.1
1	B	405	LEU	2.1
1	A	230	PHE	2.1
1	B	366	ASP	2.1
1	B	393	THR	2.1
1	B	426	LYS	2.1
1	A	50	VAL	2.0
1	B	442	LEU	2.0
1	A	482	PHE	2.0
1	B	367	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	BMA	B	1210	11/12	0.51	0.93	-	206,247,350,359	0
4	NAG	B	1208	14/15	0.91	0.34	-	120,232,277,284	0
4	NAG	B	1209	14/15	0.82	0.32	-	179,259,273,274	0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	1077	14/15	0.73	0.70	-	199,261,288,316	0
3	NAG	B	1077	14/15	0.71	0.25	-	216,285,322,322	0
3	NAG	A	1063	14/15	0.67	0.24	-	182,291,310,317	0
3	NAG	A	1208	14/15	0.88	0.27	-	227,283,330,353	0

6.5 Other polymers [i](#)

There are no such residues in this entry.