



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:08 PM GMT

PDB ID : 4KNG  
Title : Crystal structure of human LGR5-RSPO1-RNF43  
Authors : Chen, P.H.; He, X.  
Deposited on : 2013-05-09  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

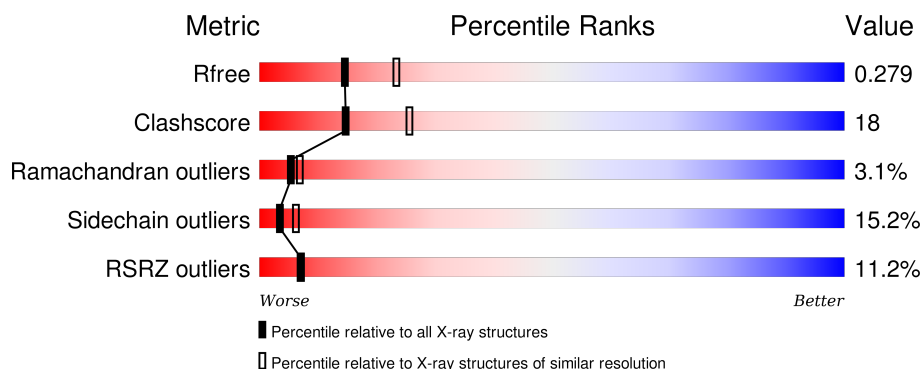
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	531	<div> <div>8%</div> <div> <div></div> <div>54%</div> <div>26%</div> <div>6% •</div> <div>13%</div> </div> </div>
1	B	531	<div> <div>5%</div> <div> <div></div> <div>55%</div> <div>24%</div> <div>7% •</div> <div>13%</div> </div> </div>
2	M	115	<div> <div>10%</div> <div> <div></div> <div>64%</div> <div>17%</div> <div>•</div> <div>15%</div> </div> </div>
2	P	115	<div> <div>10%</div> <div> <div></div> <div>53%</div> <div>23%</div> <div>6%</div> <div>18%</div> </div> </div>
3	E	160	<div> <div>6%</div> <div> <div></div> <div>54%</div> <div>31%</div> <div>8% •</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	160	<div><div></div><div>39%</div><div>54%</div><div>29%</div><div>7%</div><div>•</div><div>8%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11252 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	461	Total	C	N	O	S	0	1	0
			3622	2307	626	673	16			
1	B	463	Total	C	N	O	S	0	0	0
			3629	2312	627	674	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	EXPRESSION TAG	UNP O75473
A	31	PRO	-	EXPRESSION TAG	UNP O75473
A	558	ALA	-	EXPRESSION TAG	UNP O75473
A	559	ALA	-	EXPRESSION TAG	UNP O75473
A	560	ALA	-	EXPRESSION TAG	UNP O75473
B	30	GLY	-	EXPRESSION TAG	UNP O75473
B	31	PRO	-	EXPRESSION TAG	UNP O75473
B	558	ALA	-	EXPRESSION TAG	UNP O75473
B	559	ALA	-	EXPRESSION TAG	UNP O75473
B	560	ALA	-	EXPRESSION TAG	UNP O75473

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	98	Total	C	N	O	S	0	0	0
			750	465	131	136	18			
2	P	94	Total	C	N	O	S	0	0	0
			720	448	127	128	17			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	33	GLY	-	EXPRESSION TAG	UNP Q2MKA7
M	34	PRO	-	EXPRESSION TAG	UNP Q2MKA7

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Chain	Residue	Modelled	Actual	Comment	Reference
M	145	ALA	-	EXPRESSION TAG	UNP Q2MKA7
M	146	ALA	-	EXPRESSION TAG	UNP Q2MKA7
M	147	ALA	-	EXPRESSION TAG	UNP Q2MKA7
P	33	GLY	-	EXPRESSION TAG	UNP Q2MKA7
P	34	PRO	-	EXPRESSION TAG	UNP Q2MKA7
P	145	ALA	-	EXPRESSION TAG	UNP Q2MKA7
P	146	ALA	-	EXPRESSION TAG	UNP Q2MKA7
P	147	ALA	-	EXPRESSION TAG	UNP Q2MKA7

- Molecule 3 is a protein called E3 ubiquitin-protein ligase RNF43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	149	Total	C	N	O	S	0	0	0
			1152	734	200	212	6			
3	F	148	Total	C	N	O	S	0	0	0
			1145	729	199	211	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	42	GLY	-	EXPRESSION TAG	UNP Q68DV7
E	43	PRO	-	EXPRESSION TAG	UNP Q68DV7
E	199	ALA	-	EXPRESSION TAG	UNP Q68DV7
E	200	ALA	-	EXPRESSION TAG	UNP Q68DV7
E	201	ALA	-	EXPRESSION TAG	UNP Q68DV7
F	42	GLY	-	EXPRESSION TAG	UNP Q68DV7
F	43	PRO	-	EXPRESSION TAG	UNP Q68DV7
F	199	ALA	-	EXPRESSION TAG	UNP Q68DV7
F	200	ALA	-	EXPRESSION TAG	UNP Q68DV7
F	201	ALA	-	EXPRESSION TAG	UNP Q68DV7

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ni	0	0
			1	1		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

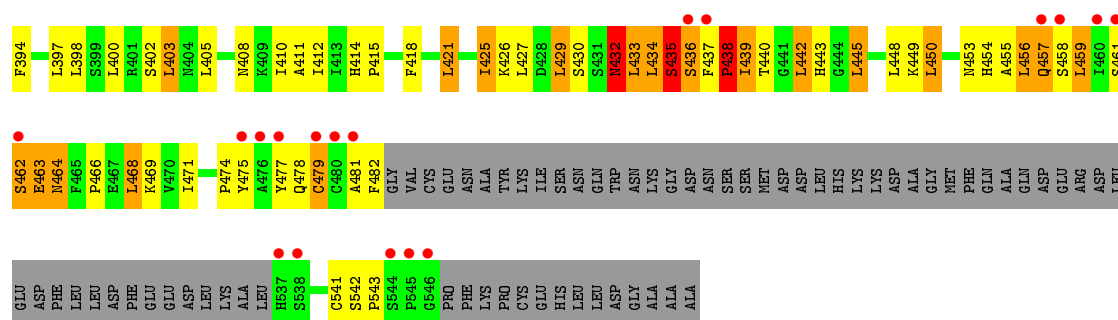


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

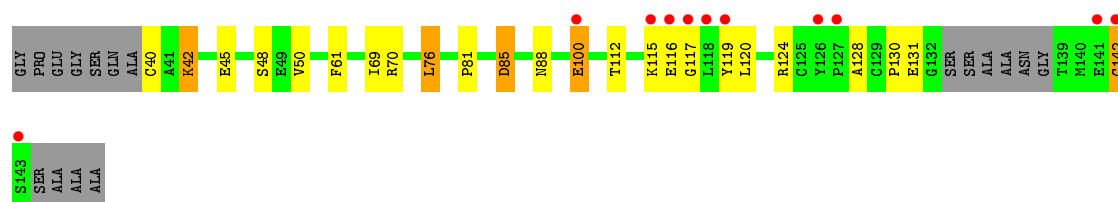
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	70	Total	O	0	0
			70	70		
6	B	85	Total	O	0	0
			85	85		
6	M	21	Total	O	0	0
			21	21		
6	P	7	Total	O	0	0
			7	7		
6	E	18	Total	O	0	0
			18	18		
6	F	4	Total	O	0	0
			4	4		

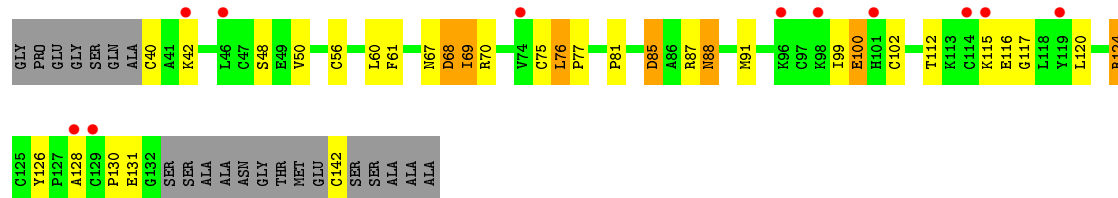




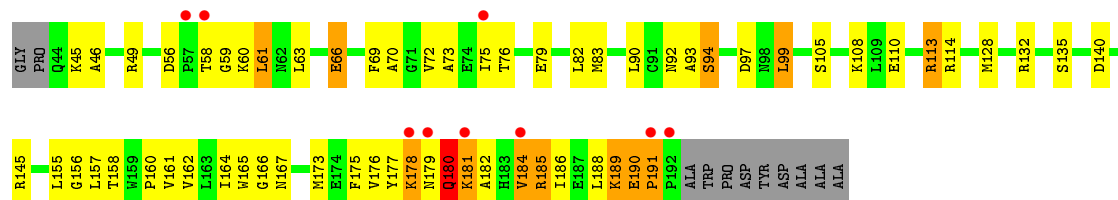
• Molecule 2: R-spondin-1



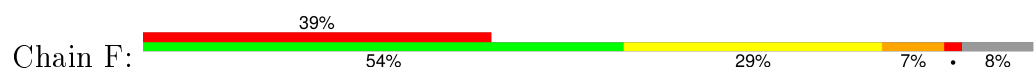
• Molecule 2: R-spondin-1



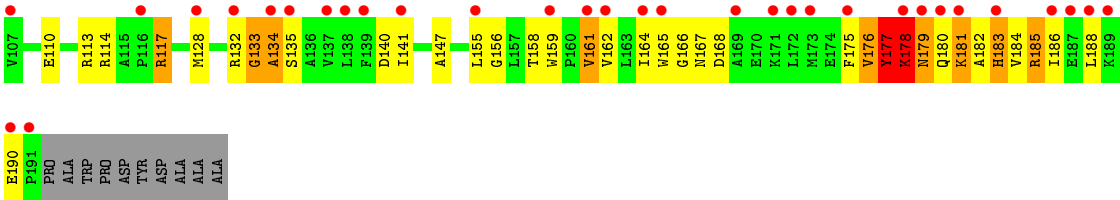
• Molecule 3: E3 ubiquitin-protein ligase RNF43



• Molecule 3: E3 ubiquitin-protein ligase RNF43







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.58Å 120.97Å 181.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.51 – 2.50 39.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (39.51-2.50) 97.1 (39.51-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.232 , 0.276 0.232 , 0.279	Depositor DCC
$R_{free}$ test set	3888 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	6 of 77914 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, 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	0.61	0/3704	0.87	9/5043 (0.2%)
1	B	0.72	1/3712 (0.0%)	0.93	8/5055 (0.2%)
2	M	0.73	0/765	0.90	0/1025
2	P	0.64	0/735	0.87	0/985
3	E	0.54	0/1175	0.80	0/1593
3	F	0.48	0/1167	0.88	2/1581 (0.1%)
All	All	0.64	1/11258 (0.0%)	0.89	19/15282 (0.1%)

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	1
1	B	0	8
2	P	0	1
3	E	0	3
3	F	0	3
All	All	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	TRP	CG-CD1	5.66	1.44	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	LEU	CA-CB-CG	-7.22	98.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	LEU	CA-CB-CG	6.30	129.79	115.30
1	B	96	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	214	VAL	CB-CA-C	-6.15	99.71	111.40
1	A	170	ASP	N-CA-CB	-6.15	99.54	110.60
1	B	214	VAL	CB-CA-C	-6.08	99.85	111.40
1	A	96	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	170	ASP	N-CA-CB	-6.00	99.81	110.60
1	A	192	THR	CB-CA-C	-5.96	95.51	111.60
1	B	192	THR	CB-CA-C	-5.83	95.85	111.60
1	B	459	LEU	CA-CB-CG	5.69	128.38	115.30
1	A	169	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	52	CYS	CA-CB-SG	-5.37	104.33	114.00
1	B	433	LEU	CB-CA-C	5.36	120.38	110.20
3	F	178	LYS	N-CA-C	5.36	125.46	111.00
1	A	168	TRP	CA-CB-CG	5.17	123.52	113.70
3	F	177	TYR	N-CA-C	-5.08	97.28	111.00
1	B	62	SER	N-CA-C	-5.03	97.41	111.00
1	A	335	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	409	LYS	Peptide
1	B	432	ASN	Peptide
1	B	434	LEU	Peptide
1	B	435	SER	Peptide
1	B	438	PRO	Peptide
1	B	466	PRO	Peptide
1	B	57	LEU	Peptide
1	B	59	GLU	Peptide
1	B	61	PRO	Peptide
3	E	180	GLN	Peptide
3	E	61	LEU	Peptide
3	E	92	ASN	Peptide
3	F	134	ALA	Peptide
3	F	177	TYR	Peptide
3	F	179	ASN	Peptide
2	P	67	ASN	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	3622	0	3626	129	0
1	B	3629	0	3634	146	0
2	M	750	0	719	17	0
2	P	720	0	692	26	0
3	E	1152	0	1182	43	0
3	F	1145	0	1175	47	0
4	B	1	0	0	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	70	0	0	8	0
6	B	85	0	0	7	0
6	E	18	0	0	4	0
6	F	4	0	0	1	0
6	M	21	0	0	2	0
6	P	7	0	0	8	0
All	All	11252	0	11054	394	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 18.

All (394) 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)
3:F:177:TYR:O	3:F:179:ASN:HA	1.44	1.17
1:B:450:LEU:HD12	1:B:453:ASN:HD22	0.98	1.15
1:B:459:LEU:HD21	1:B:478:GLN:CB	1.76	1.14
1:B:459:LEU:CD2	1:B:478:GLN:HB2	1.78	1.14
1:B:459:LEU:HD21	1:B:478:GLN:HB2	1.22	1.08
1:B:450:LEU:HD12	1:B:453:ASN:ND2	1.72	1.04
3:F:54:LYS:HA	3:F:55:MET:HB2	1.48	0.95
1:B:84:ASN:HB3	1:B:85:PRO:HA	1.48	0.93
1:B:60:LEU:HB3	1:B:61:PRO:HD3	1.50	0.91
1:A:414:HIS:HB3	1:A:415:PRO:HD2	1.52	0.91
3:F:181:LYS:HA	3:F:182:ALA:HB3	1.54	0.90
1:B:410:ILE:HB	1:B:432:ASN:OD1	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:PRO:HB2	1:B:439:ILE:HG22	1.53	0.87
3:E:173:MET:HA	3:E:176:VAL:HG12	1.58	0.85
3:E:179:ASN:N	3:E:180:GLN:HA	1.95	0.81
2:P:75:CYS:HB3	6:P:203:HOH:O	1.80	0.80
1:B:363:LEU:HD13	3:E:113:ARG:HG2	1.64	0.80
1:B:84:ASN:HB3	1:B:85:PRO:CA	2.12	0.79
1:B:192:THR:HG23	1:B:216:HIS:HB2	1.65	0.79
1:B:450:LEU:CD1	1:B:453:ASN:HD22	1.89	0.78
1:B:389:ILE:HD11	1:B:418:PHE:HE1	1.48	0.78
1:A:468:LEU:HD11	1:A:471:ILE:HG12	1.64	0.78
3:E:113:ARG:HD2	6:E:312:HOH:O	1.84	0.78
1:B:55:LEU:O	1:B:57:LEU:HG	1.85	0.77
1:B:65:SER:O	1:B:68:THR:HG22	1.86	0.76
3:E:162:VAL:HG21	3:E:188:LEU:HD11	1.68	0.76
3:F:70:ALA:HB3	3:F:161:VAL:HG22	1.68	0.76
3:F:103:PHE:O	3:F:134:ALA:CB	2.33	0.76
1:A:55:LEU:O	1:A:57:LEU:HG	1.85	0.76
1:B:394:PHE:O	1:B:421:LEU:HD11	1.86	0.76
1:B:192:THR:HG22	1:B:194:ALA:H	1.51	0.75
1:B:61:PRO:HG2	1:B:86:LEU:CD1	2.17	0.74
1:A:192:THR:HG23	1:A:216:HIS:HB2	1.69	0.74
3:E:73:ALA:HB3	6:E:311:HOH:O	1.87	0.74
1:B:459:LEU:HD21	1:B:478:GLN:HB3	1.68	0.73
2:M:61:PHE:CZ	2:M:85:ASP:HB3	2.22	0.73
1:A:435:SER:CB	1:A:456:LEU:HD12	2.17	0.73
1:A:410:ILE:HG23	1:A:432:ASN:HB2	1.69	0.73
1:B:408:ASN:O	1:B:432:ASN:HB3	1.89	0.72
2:P:60:LEU:HD12	6:P:203:HOH:O	1.90	0.72
1:A:65:SER:O	1:A:68:THR:HG22	1.89	0.72
3:F:162:VAL:HG21	3:F:188:LEU:HD11	1.70	0.72
1:B:237:GLU:OE1	2:P:124:ARG:NH2	2.24	0.71
1:B:311:THR:CG2	6:B:739:HOH:O	2.38	0.71
2:P:61:PHE:CZ	2:P:85:ASP:HB3	2.25	0.71
1:B:52:CYS:SG	1:B:60:LEU:HD11	2.32	0.70
3:F:177:TYR:C	3:F:179:ASN:HA	2.10	0.70
1:B:459:LEU:O	1:B:459:LEU:HD23	1.92	0.70
1:B:61:PRO:HG2	1:B:86:LEU:HD13	1.73	0.69
3:E:128:MET:HE3	3:E:132:ARG:CZ	2.22	0.69
1:A:468:LEU:HD21	1:A:471:ILE:HD11	1.75	0.68
1:A:218:HIS:HD2	1:A:219:ASN:HD22	1.41	0.68
1:A:192:THR:HG22	1:A:194:ALA:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ASP:OD1	1:B:221:ARG:HD3	1.94	0.67
1:B:85:PRO:O	1:B:86:LEU:HG	1.93	0.67
1:B:200:HIS:N	6:B:767:HOH:O	2.26	0.67
1:A:146:ASP:HB3	1:A:170:ASP:HB3	1.76	0.67
2:M:45:GLU:OE2	6:M:205:HOH:O	2.13	0.67
3:F:141:ILE:CG2	3:F:165:TRP:HB3	2.25	0.67
1:B:218:HIS:HD2	1:B:219:ASN:HD22	1.43	0.66
1:A:435:SER:HB2	1:A:456:LEU:HD12	1.78	0.66
1:B:433:LEU:O	1:B:433:LEU:HD12	1.95	0.66
1:A:468:LEU:O	1:A:539:VAL:HG11	1.95	0.66
1:B:468:LEU:HD21	1:B:471:ILE:HB	1.78	0.65
1:B:432:ASN:O	1:B:434:LEU:N	2.21	0.65
3:F:176:VAL:O	3:F:178:LYS:HA	1.97	0.65
1:B:442:LEU:HG	1:B:443:HIS:H	1.60	0.65
1:B:146:ASP:HB3	1:B:170:ASP:HB3	1.79	0.65
1:A:64:LEU:HD12	1:A:86:LEU:HD23	1.79	0.64
3:F:103:PHE:O	3:F:134:ALA:HB1	1.96	0.64
1:A:85:PRO:O	1:A:86:LEU:HD22	1.97	0.64
1:B:168:TRP:CZ3	6:P:204:HOH:O	2.50	0.64
3:E:190:GLU:HB2	3:E:191:PRO:CD	2.27	0.64
1:B:52:CYS:SG	1:B:60:LEU:CD1	2.86	0.64
1:B:61:PRO:HG3	1:B:64:LEU:HD13	1.78	0.64
2:P:87:ARG:CZ	6:P:201:HOH:O	2.46	0.64
2:M:48:SER:OG	3:E:110:GLU:OE2	2.11	0.64
1:A:59:GLU:HG2	1:A:83:PRO:HD2	1.80	0.64
3:F:70:ALA:HB3	3:F:161:VAL:CG2	2.28	0.63
1:B:429:LEU:O	1:B:432:ASN:ND2	2.32	0.63
3:F:141:ILE:HG22	3:F:165:TRP:HB3	1.81	0.63
1:B:471:ILE:CG2	1:B:541:CYS:SG	2.87	0.63
3:E:83:MET:O	3:E:105:SER:HA	1.99	0.62
1:B:142:SER:OG	1:B:166:HIS:HD2	1.80	0.62
2:M:70:ARG:HG2	3:E:181:LYS:HB3	1.82	0.62
3:F:83:MET:O	3:F:105:SER:HA	1.99	0.61
3:F:103:PHE:CZ	3:F:133:GLY:HA3	2.35	0.61
1:A:218:HIS:CD2	1:A:219:ASN:HD22	2.17	0.61
1:B:168:TRP:HZ3	6:P:204:HOH:O	1.83	0.61
1:B:351:LEU:N	1:B:352:PRO:CD	2.63	0.61
1:A:416:ASN:C	1:A:418:PHE:H	2.04	0.61
2:P:88:ASN:HD22	2:P:91:MET:H	1.48	0.61
1:A:199:HIS:HB2	1:A:223:HIS:CE1	2.36	0.60
1:B:335:LEU:C	1:B:335:LEU:HD23	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:HIS:CD2	1:B:219:ASN:HD22	2.20	0.60
1:A:351:LEU:N	1:A:352:PRO:CD	2.65	0.60
2:M:88:ASN:HB3	6:M:209:HOH:O	2.02	0.60
1:A:274:GLU:O	1:A:299:SER:HB2	2.02	0.60
1:A:377:GLN:HA	1:A:400:LEU:HA	1.82	0.60
1:A:315:ALA:HB3	1:A:318:ILE:HD12	1.84	0.60
3:F:184:VAL:HG12	3:F:185:ARG:N	2.16	0.60
3:F:73:ALA:HB2	3:F:161:VAL:HG13	1.82	0.60
1:B:298:ARG:NH1	6:B:758:HOH:O	2.35	0.60
3:F:54:LYS:HA	3:F:55:MET:CB	2.28	0.60
3:F:182:ALA:O	3:F:183:HIS:HB2	2.02	0.60
1:B:333:LEU:C	1:B:333:LEU:HD23	2.22	0.59
1:B:315:ALA:HB3	1:B:318:ILE:HD12	1.84	0.59
3:E:46:ALA:HB2	3:E:69:PHE:CE1	2.37	0.59
1:B:267:ASN:HB2	1:B:291:ASN:HD21	1.68	0.59
1:B:377:GLN:HA	1:B:400:LEU:HA	1.84	0.58
1:A:63:ASN:HD22	1:A:63:ASN:H	1.50	0.58
1:B:141:GLN:HB2	6:B:713:HOH:O	2.02	0.58
2:P:85:ASP:N	2:P:85:ASP:OD1	2.37	0.58
1:B:144:ARG:HG2	1:B:168:TRP:CD1	2.38	0.58
1:A:86:LEU:HD12	1:A:88:SER:OG	2.03	0.58
1:A:267:ASN:HB2	1:A:291:ASN:HD21	1.68	0.58
1:A:142:SER:OG	1:A:166:HIS:HD2	1.86	0.58
1:B:435:SER:HB3	1:B:455:ALA:HB3	1.86	0.58
1:B:389:ILE:CD1	1:B:418:PHE:HE1	2.17	0.57
1:A:387:TYR:HA	1:A:410:ILE:N	2.18	0.57
1:B:410:ILE:CB	1:B:432:ASN:OD1	2.48	0.57
1:B:459:LEU:CD2	1:B:478:GLN:CB	2.54	0.57
1:B:192:THR:HG21	6:B:779:HOH:O	2.04	0.57
1:B:200:HIS:HD2	1:B:224:SER:HB2	1.70	0.57
1:A:416:ASN:HB3	1:A:419:SER:HB3	1.87	0.57
2:M:85:ASP:N	2:M:85:ASP:OD1	2.37	0.57
3:F:90:LEU:HA	3:F:128:MET:HE2	1.86	0.57
1:B:408:ASN:O	1:B:432:ASN:CB	2.53	0.57
2:P:87:ARG:NH1	6:P:201:HOH:O	2.36	0.57
1:A:415:PRO:O	1:A:439:ILE:HD13	2.05	0.56
3:F:175:PHE:HE2	3:F:184:VAL:HG21	1.71	0.56
3:F:54:LYS:CA	3:F:55:MET:HB2	2.30	0.56
1:A:413:ILE:HG22	1:A:439:ILE:HD12	1.88	0.56
1:A:85:PRO:C	1:A:86:LEU:HD22	2.26	0.56
1:A:82:LEU:HD23	1:A:106:PRO:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:HH22	2:M:120:LEU:HD23	1.70	0.56
1:A:442:LEU:C	1:A:442:LEU:HD22	2.26	0.56
1:A:373:CYS:HB3	1:A:376:LEU:HD22	1.86	0.56
1:A:333:LEU:C	1:A:333:LEU:HD23	2.26	0.56
1:A:82:LEU:HA	1:A:84:ASN:N	2.21	0.56
3:E:82:LEU:HB3	3:E:184:VAL:HG23	1.87	0.56
3:F:175:PHE:CE2	3:F:184:VAL:HG21	2.40	0.56
3:E:73:ALA:HB2	3:E:161:VAL:HG13	1.88	0.56
2:P:128:ALA:O	2:P:130:PRO:HD3	2.05	0.56
3:E:179:ASN:N	3:E:180:GLN:CA	2.69	0.56
1:B:60:LEU:C	1:B:60:LEU:HD23	2.27	0.56
1:B:373:CYS:HB3	1:B:376:LEU:HD22	1.86	0.55
2:M:76:LEU:N	2:M:76:LEU:HD23	2.21	0.55
1:B:389:ILE:HD11	1:B:418:PHE:CE1	2.35	0.55
1:B:387:TYR:O	1:B:410:ILE:HA	2.06	0.55
3:E:70:ALA:HB2	3:E:161:VAL:HG22	1.89	0.55
2:P:76:LEU:N	2:P:76:LEU:HD23	2.22	0.55
1:A:86:LEU:HB3	1:A:89:LEU:HG	1.88	0.55
1:B:199:HIS:HB2	1:B:223:HIS:CE1	2.42	0.55
1:B:61:PRO:CG	1:B:64:LEU:HD22	2.37	0.55
3:E:162:VAL:HA	6:E:309:HOH:O	2.05	0.55
1:B:471:ILE:HG21	1:B:541:CYS:SG	2.46	0.55
1:B:61:PRO:HG2	1:B:86:LEU:HD11	1.88	0.55
1:B:438:PRO:C	1:B:439:ILE:HG22	2.27	0.54
3:F:82:LEU:HB2	3:F:186:ILE:HD13	1.89	0.54
3:F:141:ILE:HG13	3:F:147:ALA:HB3	1.89	0.54
2:M:128:ALA:O	2:M:130:PRO:HD3	2.06	0.54
1:A:254:ARG:HD3	6:A:754:HOH:O	2.06	0.54
1:A:446:THR:HA	1:A:468:LEU:HA	1.90	0.54
1:A:442:LEU:HD21	1:A:445:LEU:HD13	1.88	0.54
1:B:195:LEU:HD23	1:B:195:LEU:N	2.22	0.54
3:F:184:VAL:CG1	3:F:185:ARG:N	2.71	0.54
1:B:64:LEU:HD21	1:B:86:LEU:HD13	1.90	0.54
1:B:265:HIS:HD2	1:B:266:SER:OG	1.90	0.54
3:E:45:LYS:HB3	3:E:66:GLU:OE2	2.07	0.54
3:E:90:LEU:HA	3:E:128:MET:HE2	1.90	0.53
3:F:180:GLN:O	3:F:181:LYS:C	2.46	0.53
1:B:456:LEU:O	1:B:459:LEU:HB2	2.09	0.53
1:B:252:ALA:HB1	6:B:727:HOH:O	2.09	0.53
1:A:410:ILE:CG2	1:A:432:ASN:HB2	2.37	0.53
1:A:429:LEU:O	1:A:432:ASN:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:79:GLU:HB3	3:E:185:ARG:NH2	2.23	0.52
1:B:432:ASN:O	1:B:453:ASN:OD1	2.28	0.52
1:B:411:ALA:HB2	1:B:433:LEU:HD11	1.91	0.52
1:A:435:SER:HB3	1:A:456:LEU:HD12	1.90	0.52
1:A:58:SER:O	1:A:60:LEU:O	2.28	0.52
1:A:265:HIS:HD2	1:A:266:SER:OG	1.92	0.52
1:B:461:SER:O	1:B:461:SER:OG	2.20	0.52
1:B:336:THR:HG22	1:B:360:SER:HB3	1.91	0.52
1:A:395:GLN:O	1:A:396:GLN:HB2	2.09	0.52
1:A:468:LEU:CD2	1:A:471:ILE:HD11	2.38	0.51
1:A:411:ALA:O	1:A:434:LEU:HD23	2.09	0.51
1:A:127:ARG:CD	6:A:744:HOH:O	2.58	0.51
3:E:82:LEU:HB2	3:E:186:ILE:HD13	1.91	0.51
1:A:118:VAL:HG22	1:A:142:SER:HB2	1.92	0.51
2:M:119:TYR:HB3	2:M:142:CYS:HB2	1.92	0.51
1:A:435:SER:HB3	1:A:456:LEU:HA	1.93	0.51
3:F:65:LEU:HB2	3:F:168:ASP:HB3	1.93	0.51
1:A:414:HIS:CB	1:A:415:PRO:HD2	2.34	0.51
3:F:96:ASP:OD2	3:F:132:ARG:HG3	2.11	0.51
1:B:55:LEU:O	1:B:56:GLY:C	2.49	0.51
1:A:459:LEU:HG	1:A:478:GLN:HB2	1.92	0.51
1:B:370:PHE:O	1:B:397:LEU:HD21	2.11	0.50
1:B:448:LEU:HB3	1:B:471:ILE:HD12	1.92	0.50
1:B:242:ASN:ND2	1:B:265:HIS:H	2.10	0.50
1:A:418:PHE:HA	1:A:421:LEU:HD23	1.92	0.50
2:M:61:PHE:CE2	2:M:85:ASP:HB3	2.47	0.50
1:A:59:GLU:HG2	1:A:83:PRO:CD	2.41	0.50
1:A:442:LEU:HD21	1:A:445:LEU:HD22	1.92	0.50
3:F:135:SER:HB3	3:F:159:TRP:HB3	1.93	0.50
1:B:201:ILE:HG22	1:B:229:CYS:HB2	1.93	0.50
3:E:58:THR:O	3:E:60:LYS:N	2.45	0.50
1:B:462:SER:O	1:B:464:ASN:N	2.41	0.50
1:A:311:THR:HB	1:A:334:THR:HB	1.93	0.50
3:F:185:ARG:HD3	3:F:186:ILE:N	2.27	0.49
1:B:60:LEU:HB3	1:B:61:PRO:CD	2.34	0.49
1:A:370:PHE:O	1:A:397:LEU:HD21	2.12	0.49
1:A:63:ASN:ND2	1:A:63:ASN:H	2.09	0.49
1:B:82:LEU:HG	1:B:106:PRO:HG3	1.94	0.49
2:P:56:CYS:HB3	6:P:203:HOH:O	2.13	0.48
1:B:311:THR:HB	1:B:334:THR:HB	1.94	0.48
1:B:242:ASN:HD22	1:B:265:HIS:H	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:69:ILE:CG2	3:F:82:LEU:O	2.62	0.48
1:A:432:ASN:OD1	1:A:453:ASN:HB3	2.14	0.48
2:P:61:PHE:CE2	2:P:85:ASP:HB3	2.47	0.48
1:A:247:ASP:HB2	6:A:721:HOH:O	2.13	0.48
3:E:190:GLU:O	3:E:191:PRO:O	2.30	0.48
1:A:59:GLU:HG2	1:A:83:PRO:HG2	1.96	0.48
1:A:201:ILE:HG22	1:A:229:CYS:HB2	1.94	0.48
1:A:59:GLU:O	1:A:60:LEU:C	2.51	0.48
1:B:450:LEU:CD1	1:B:453:ASN:ND2	2.61	0.48
3:F:52:PRO:C	3:F:54:LYS:H	2.16	0.48
2:P:75:CYS:CB	6:P:203:HOH:O	2.52	0.48
1:A:96:ARG:HA	1:A:120:MET:HB2	1.95	0.48
1:A:269:ILE:H	1:A:291:ASN:HD22	1.62	0.48
1:A:403:LEU:C	1:A:403:LEU:CD1	2.82	0.48
1:A:360:SER:HB3	1:A:361:TYR:CD1	2.48	0.48
1:B:459:LEU:HD13	1:B:475:TYR:HB2	1.95	0.48
1:B:403:LEU:CD1	1:B:403:LEU:C	2.82	0.48
1:A:171:ASP:HA	1:A:195:LEU:O	2.14	0.48
1:A:322:PRO:HB3	6:A:733:HOH:O	2.12	0.47
1:A:59:GLU:CG	1:A:83:PRO:HG2	2.44	0.47
3:E:97:ASP:HB3	3:E:99:LEU:CD1	2.44	0.47
1:B:403:LEU:HD11	1:B:405:LEU:HG	1.96	0.47
1:B:457:GLN:O	1:B:459:LEU:N	2.40	0.47
3:F:181:LYS:HA	3:F:182:ALA:CB	2.32	0.47
2:M:69:ILE:HB	3:E:181:LYS:HB2	1.97	0.47
1:A:459:LEU:CD2	1:A:475:TYR:HD1	2.28	0.47
1:B:204:TYR:OH	1:B:228:LYS:HE2	2.15	0.47
2:P:120:LEU:O	2:P:142:CYS:HA	2.14	0.47
1:B:436:SER:HA	1:B:437:PHE:HA	1.80	0.47
3:E:175:PHE:CZ	3:E:182:ALA:HB3	2.50	0.47
3:E:70:ALA:N	6:E:309:HOH:O	2.48	0.47
1:A:55:LEU:O	1:A:56:GLY:C	2.51	0.47
1:B:400:LEU:C	1:B:400:LEU:HD23	2.35	0.47
3:E:182:ALA:O	3:E:184:VAL:HG22	2.15	0.47
1:A:127:ARG:HD3	6:A:744:HOH:O	2.13	0.47
1:B:122:GLN:HG3	1:B:144:ARG:HB3	1.97	0.47
3:F:90:LEU:HA	3:F:128:MET:CE	2.45	0.47
1:B:275:LYS:O	1:B:278:VAL:HG22	2.14	0.46
3:E:189:LYS:O	3:E:190:GLU:O	2.33	0.46
1:A:242:ASN:ND2	1:A:265:HIS:H	2.13	0.46
3:E:140:ASP:OD1	3:E:140:ASP:C	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ILE:HG22	1:B:426:LYS:HG2	1.98	0.46
1:A:122:GLN:HG3	1:A:144:ARG:HB3	1.98	0.46
3:E:70:ALA:CB	3:E:161:VAL:HG22	2.45	0.46
1:A:146:ASP:CB	1:A:170:ASP:HB3	2.44	0.46
1:B:298:ARG:HE	1:B:320:GLU:HG2	1.81	0.46
3:F:48:ILE:HB	3:F:65:LEU:HD22	1.96	0.46
1:B:96:ARG:HA	1:B:120:MET:HB2	1.98	0.46
3:E:49:ARG:NH1	3:E:61:LEU:HB3	2.29	0.46
3:E:90:LEU:HA	3:E:128:MET:CE	2.46	0.46
1:B:143:LEU:O	1:B:168:TRP:HD1	1.97	0.46
1:B:269:ILE:H	1:B:291:ASN:HD22	1.64	0.46
1:B:61:PRO:HB3	1:B:62:SER:C	2.35	0.46
1:A:457:GLN:O	1:A:459:LEU:N	2.44	0.46
1:A:336:THR:HG22	1:A:360:SER:HB2	1.98	0.46
2:P:48:SER:OG	3:F:110:GLU:OE2	2.23	0.46
3:F:177:TYR:C	3:F:177:TYR:CD1	2.90	0.46
2:P:69:ILE:N	2:P:69:ILE:HD13	2.31	0.46
1:A:459:LEU:HD23	1:A:475:TYR:HD1	1.81	0.46
3:E:135:SER:O	3:E:160:PRO:HD2	2.16	0.46
3:F:140:ASP:OD1	3:F:140:ASP:C	2.54	0.46
1:A:416:ASN:ND2	1:A:441:GLY:HA3	2.31	0.46
1:A:410:ILE:HG23	1:A:433:LEU:H	1.81	0.46
1:B:168:TRP:CD1	1:B:168:TRP:N	2.84	0.46
2:P:99:ILE:HG23	2:P:102:CYS:CB	2.46	0.46
1:B:154:PRO:HA	1:B:155:PRO:HD3	1.83	0.45
2:P:68:ASP:OD2	3:F:178:LYS:HB3	2.16	0.45
2:M:70:ARG:CG	3:E:181:LYS:HB3	2.45	0.45
1:A:200:HIS:HB3	6:A:712:HOH:O	2.15	0.45
1:A:51:ASP:OD1	1:A:53:SER:HB3	2.17	0.45
3:E:93:ALA:O	3:E:94:SER:O	2.34	0.45
1:A:425:ILE:HG22	1:A:426:LYS:HG2	1.98	0.45
1:A:275:LYS:O	1:A:278:VAL:HG22	2.15	0.45
1:B:478:GLN:HA	1:B:481:ALA:HB3	1.98	0.45
1:A:413:ILE:HG21	1:A:418:PHE:HE2	1.82	0.45
1:A:416:ASN:C	1:A:418:PHE:N	2.69	0.45
3:F:184:VAL:CG1	3:F:185:ARG:H	2.30	0.45
3:E:72:VAL:HG12	3:E:157:LEU:HD12	1.98	0.45
1:A:411:ALA:HA	1:A:433:LEU:O	2.17	0.45
3:F:117:ARG:CZ	3:F:117:ARG:HB3	2.47	0.45
1:A:413:ILE:HG21	1:A:418:PHE:CE2	2.52	0.45
1:A:448:LEU:HB3	1:A:471:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:N	1:B:83:PRO:CD	2.80	0.45
3:E:190:GLU:HB2	3:E:191:PRO:HD3	1.98	0.45
1:A:199:HIS:HB2	1:A:223:HIS:HE1	1.78	0.45
1:B:85:PRO:C	1:B:86:LEU:HG	2.33	0.44
1:A:471:ILE:CG2	1:A:472:GLU:N	2.80	0.44
1:A:403:LEU:HD11	1:A:405:LEU:HG	1.98	0.44
1:A:459:LEU:HD22	1:A:474:PRO:HG2	2.00	0.44
1:B:106:PRO:HD2	1:B:109:ALA:HB2	1.99	0.44
1:A:341:SER:HA	1:A:363:LEU:O	2.17	0.44
2:M:50:VAL:HG11	3:E:108:LYS:HB2	1.99	0.44
1:A:469:LYS:C	1:A:539:VAL:HG13	2.38	0.44
1:B:242:ASN:HD22	1:B:265:HIS:N	2.16	0.44
1:B:456:LEU:HD23	1:B:474:PRO:HG2	1.99	0.43
3:F:54:LYS:CA	3:F:55:MET:CB	2.94	0.43
1:B:61:PRO:HB3	1:B:62:SER:CA	2.48	0.43
1:B:84:ASN:ND2	1:B:85:PRO:O	2.50	0.43
3:F:56:ASP:N	3:F:56:ASP:OD1	2.50	0.43
1:B:118:VAL:HG22	1:B:142:SER:HB2	2.00	0.43
3:E:175:PHE:CE2	3:E:182:ALA:HB3	2.53	0.43
1:B:351:LEU:N	1:B:352:PRO:HD2	2.34	0.43
2:P:88:ASN:HB3	2:P:91:MET:O	2.18	0.43
2:M:50:VAL:HG11	3:E:108:LYS:CB	2.49	0.43
1:A:388:GLU:HB3	6:A:738:HOH:O	2.17	0.43
1:B:459:LEU:HD12	1:B:474:PRO:HG2	1.99	0.43
1:A:442:LEU:CD2	1:A:445:LEU:HD13	2.48	0.43
1:B:171:ASP:HA	1:B:195:LEU:O	2.19	0.43
1:B:414:HIS:CG	1:B:415:PRO:HD2	2.54	0.43
1:B:52:CYS:HB2	1:B:73:LEU:HD12	2.00	0.43
1:A:413:ILE:CG2	1:A:439:ILE:HD12	2.48	0.43
1:B:418:PHE:N	1:B:418:PHE:HD1	2.17	0.43
1:B:335:LEU:O	1:B:335:LEU:HD23	2.19	0.43
3:F:177:TYR:HD1	3:F:177:TYR:C	2.22	0.42
2:P:99:ILE:HG23	2:P:102:CYS:HB2	2.01	0.42
1:B:442:LEU:HD11	1:B:445:LEU:CD2	2.49	0.42
1:B:146:ASP:CB	1:B:170:ASP:HB3	2.48	0.42
1:A:343:LEU:C	6:A:735:HOH:O	2.57	0.42
1:B:84:ASN:ND2	1:B:86:LEU:HD11	2.34	0.42
1:B:435:SER:CB	1:B:455:ALA:HB3	2.50	0.42
1:B:51:ASP:C	1:B:51:ASP:OD1	2.56	0.42
1:B:442:LEU:HD11	1:B:445:LEU:HD22	2.01	0.42
1:B:371:SER:N	6:B:745:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:CYS:HB2	1:A:73:LEU:HD12	2.01	0.42
2:P:69:ILE:HG22	3:F:83:MET:HA	2.01	0.42
1:B:75:MET:HA	1:B:75:MET:CE	2.49	0.42
1:A:351:LEU:N	1:A:352:PRO:HD2	2.35	0.42
1:B:403:LEU:C	1:B:403:LEU:HD12	2.40	0.42
2:P:124:ARG:HG3	2:P:126:TYR:CZ	2.55	0.42
1:B:265:HIS:HB2	1:B:289:TYR:O	2.20	0.42
1:A:265:HIS:HB2	1:A:289:TYR:O	2.20	0.42
1:A:266:SER:HA	1:A:290:ASP:O	2.20	0.42
3:F:175:PHE:HA	3:F:179:ASN:HD21	1.84	0.42
1:B:438:PRO:CB	1:B:439:ILE:HG22	2.36	0.42
1:A:459:LEU:HD11	1:A:473:MET:CE	2.50	0.42
1:A:82:LEU:HD13	1:A:84:ASN:HB2	2.02	0.41
2:M:42:LYS:HB3	2:M:42:LYS:HE2	1.74	0.41
1:B:457:GLN:C	1:B:459:LEU:N	2.73	0.41
1:A:123:ASN:HA	1:A:147:ALA:O	2.20	0.41
1:A:394:PHE:O	1:A:421:LEU:HD11	2.19	0.41
1:B:418:PHE:N	1:B:418:PHE:CD1	2.87	0.41
1:A:400:LEU:C	1:A:400:LEU:HD23	2.40	0.41
1:B:479:CYS:SG	1:B:542:SER:N	2.93	0.41
1:A:390:LYS:HA	1:A:414:HIS:CG	2.54	0.41
2:P:60:LEU:HD22	2:P:77:PRO:HA	2.02	0.41
1:A:373:CYS:O	1:A:376:LEU:HB2	2.20	0.41
1:A:459:LEU:HD23	1:A:475:TYR:CD1	2.55	0.41
1:B:299:SER:O	1:B:300:ALA:C	2.57	0.41
1:A:409:LYS:HA	6:F:301:HOH:O	2.20	0.41
2:P:116:GLU:HA	2:P:117:GLY:HA2	1.76	0.41
1:B:61:PRO:CB	1:B:62:SER:CA	2.98	0.41
1:B:341:SER:HA	1:B:363:LEU:O	2.20	0.41
1:A:403:LEU:HD12	1:A:403:LEU:C	2.41	0.41
3:E:177:TYR:O	3:E:178:LYS:C	2.58	0.41
1:A:154:PRO:HA	1:A:155:PRO:HD3	1.83	0.41
3:F:178:LYS:O	3:F:182:ALA:HB2	2.21	0.41
1:A:410:ILE:O	1:A:410:ILE:HG23	2.21	0.41
1:B:61:PRO:CG	1:B:64:LEU:HD13	2.49	0.41
1:A:415:PRO:O	1:A:439:ILE:CD1	2.69	0.41
1:A:144:ARG:HG2	1:A:168:TRP:CE3	2.55	0.41
1:A:414:HIS:HB3	1:A:415:PRO:CD	2.35	0.41
1:A:468:LEU:HD21	1:A:471:ILE:CD1	2.48	0.41
1:B:333:LEU:C	1:B:333:LEU:CD2	2.88	0.41
1:B:373:CYS:O	1:B:376:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:LYS:HG3	1:B:402:SER:HB3	2.02	0.41
2:M:116:GLU:HA	2:M:117:GLY:HA2	1.78	0.41
1:B:459:LEU:HD22	1:B:477:TYR:CE1	2.56	0.40
1:A:63:ASN:N	1:A:63:ASN:ND2	2.69	0.40
1:B:266:SER:HA	1:B:290:ASP:O	2.21	0.40
1:B:192:THR:CG2	1:B:216:HIS:HB2	2.44	0.40
1:A:461:SER:O	1:A:478:GLN:NE2	2.54	0.40
1:A:145:LEU:HB2	1:A:169:LEU:HD13	2.04	0.40
3:E:69:PHE:CZ	3:E:188:LEU:HD21	2.56	0.40
1:A:82:LEU:HD13	1:A:84:ASN:CB	2.52	0.40
2:P:50:VAL:O	2:P:70:ARG:NH1	2.52	0.40
1:A:134:LEU:O	1:A:161:LEU:HD21	2.21	0.40
1:B:340:ILE:H	1:B:362:ASN:HD22	1.70	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	458/531 (86%)	389 (85%)	58 (13%)	11 (2%)	7	11
1	B	459/531 (86%)	392 (85%)	56 (12%)	11 (2%)	7	11
2	M	94/115 (82%)	82 (87%)	10 (11%)	2 (2%)	9	14
2	P	91/115 (79%)	80 (88%)	8 (9%)	3 (3%)	5	6
3	E	147/160 (92%)	120 (82%)	19 (13%)	8 (5%)	2	2
3	F	146/160 (91%)	119 (82%)	19 (13%)	8 (6%)	2	2
All	All	1395/1612 (86%)	1182 (85%)	170 (12%)	43 (3%)	5	7

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	ILE
1	A	430	SER
1	B	84	ASN
1	B	430	SER
1	B	438	PRO
2	M	142	CYS
3	E	94	SER
3	E	166	GLY
3	E	190	GLU
3	F	55	MET
3	F	166	GLY
1	A	53	SER
1	A	170	ASP
1	B	458	SER
3	E	59	GLY
3	E	75	ILE
3	F	181	LYS
1	A	31	PRO
1	A	417	ALA
1	A	458	SER
1	B	170	ASP
1	B	435	SER
1	B	463	GLU
2	P	100	GLU
3	E	191	PRO
1	A	83	PRO
1	A	437	PHE
1	A	451	THR
1	B	543	PRO
2	M	100	GLU
2	P	68	ASP
3	E	178	LYS
3	F	133	GLY
1	A	415	PRO
1	B	37	HIS
2	P	42	LYS
3	F	53	LEU
3	F	60	LYS
3	F	178	LYS
1	B	85	PRO
1	B	439	ILE
3	F	156	GLY
3	E	156	GLY



### 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	418/476 (88%)	356 (85%)	62 (15%)	4	7
1	B	419/476 (88%)	354 (84%)	65 (16%)	3	6
2	M	87/95 (92%)	77 (88%)	10 (12%)	7	13
2	P	83/95 (87%)	72 (87%)	11 (13%)	5	9
3	E	124/130 (95%)	106 (86%)	18 (14%)	4	7
3	F	123/130 (95%)	98 (80%)	25 (20%)	1	2
All	All	1254/1402 (89%)	1063 (85%)	191 (15%)	3	6

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	34	CYS
1	A	37	HIS
1	A	45	ARG
1	A	53	SER
1	A	55	LEU
1	A	58	SER
1	A	63	ASN
1	A	73	LEU
1	A	81	LEU
1	A	82	LEU
1	A	113	LEU
1	A	122	GLN
1	A	127	ARG
1	A	146	ASP
1	A	169	LEU
1	A	176	GLU
1	A	192	THR
1	A	221	ARG
1	A	235	SER
1	A	246	LEU
1	A	247	ASP

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Mol	Chain	Res	Type
1	A	251	THR
1	A	255	THR
1	A	256	LEU
1	A	278	VAL
1	A	285	THR
1	A	299	SER
1	A	304	LEU
1	A	307	LEU
1	A	310	LEU
1	A	311	THR
1	A	313	ASN
1	A	316	SER
1	A	319	THR
1	A	330	LEU
1	A	335	LEU
1	A	365	GLU
1	A	367	LEU
1	A	389	ILE
1	A	390	LYS
1	A	392	ASP
1	A	398	LEU
1	A	403	LEU
1	A	425	ILE
1	A	427	LEU
1	A	429	LEU
1	A	435	SER
1	A	442	LEU
1	A	443	HIS
1	A	445	LEU
1	A	448	LEU
1	A	449	LYS
1	A	454	HIS
1	A	456	LEU
1	A	457	GLN
1	A	459	LEU
1	A	463	GLU
1	A	464	ASN
1	A	468	LEU
1	A	479	CYS
1	A	541	CYS
1	B	55	LEU
1	B	59	GLU

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Mol	Chain	Res	Type
1	B	62	SER
1	B	64	LEU
1	B	73	LEU
1	B	75	MET
1	B	77	ASN
1	B	81	LEU
1	B	86	LEU
1	B	92	LEU
1	B	113	LEU
1	B	122	GLN
1	B	127	ARG
1	B	146	ASP
1	B	168	TRP
1	B	192	THR
1	B	195	LEU
1	B	221	ARG
1	B	227	LYS
1	B	228	LYS
1	B	235	SER
1	B	246	LEU
1	B	251	THR
1	B	255	THR
1	B	256	LEU
1	B	266	SER
1	B	278	VAL
1	B	285	THR
1	B	304	LEU
1	B	307	LEU
1	B	310	LEU
1	B	311	THR
1	B	316	SER
1	B	319	THR
1	B	330	LEU
1	B	363	LEU
1	B	367	LEU
1	B	389	ILE
1	B	390	LYS
1	B	391	VAL
1	B	392	ASP
1	B	398	LEU
1	B	403	LEU
1	B	412	ILE

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Mol	Chain	Res	Type
1	B	421	LEU
1	B	425	ILE
1	B	427	LEU
1	B	429	LEU
1	B	432	ASN
1	B	436	SER
1	B	440	THR
1	B	442	LEU
1	B	445	LEU
1	B	449	LYS
1	B	450	LEU
1	B	454	HIS
1	B	456	LEU
1	B	457	GLN
1	B	462	SER
1	B	463	GLU
1	B	464	ASN
1	B	468	LEU
1	B	469	LYS
1	B	479	CYS
1	B	482	PHE
2	M	40	CYS
2	M	42	LYS
2	M	76	LEU
2	M	81	PRO
2	M	85	ASP
2	M	100	GLU
2	M	112	THR
2	M	115	LYS
2	M	124	ARG
2	M	131	GLU
2	P	40	CYS
2	P	69	ILE
2	P	76	LEU
2	P	81	PRO
2	P	85	ASP
2	P	88	ASN
2	P	100	GLU
2	P	112	THR
2	P	115	LYS
2	P	124	ARG
2	P	131	GLU

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Mol	Chain	Res	Type
3	E	56	ASP
3	E	63	LEU
3	E	66	GLU
3	E	76	THR
3	E	99	LEU
3	E	113	ARG
3	E	114	ARG
3	E	145	ARG
3	E	155	LEU
3	E	158	THR
3	E	164	ILE
3	E	165	TRP
3	E	167	ASN
3	E	180	GLN
3	E	181	LYS
3	E	184	VAL
3	E	185	ARG
3	E	189	LYS
3	F	44	GLN
3	F	55	MET
3	F	56	ASP
3	F	61	LEU
3	F	63	LEU
3	F	65	LEU
3	F	66	GLU
3	F	72	VAL
3	F	84	GLN
3	F	92	ASN
3	F	99	LEU
3	F	113	ARG
3	F	114	ARG
3	F	117	ARG
3	F	155	LEU
3	F	158	THR
3	F	161	VAL
3	F	164	ILE
3	F	167	ASN
3	F	176	VAL
3	F	177	TYR
3	F	178	LYS
3	F	183	HIS
3	F	185	ARG

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Mol	Chain	Res	Type
3	F	190	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	76	ASN
1	A	141	GLN
1	A	166	HIS
1	A	200	HIS
1	A	218	HIS
1	A	223	HIS
1	A	242	ASN
1	A	258	ASN
1	A	265	HIS
1	A	291	ASN
1	A	302	GLN
1	A	350	GLN
1	A	355	GLN
1	A	362	ASN
1	A	478	GLN
1	B	84	ASN
1	B	141	GLN
1	B	166	HIS
1	B	199	HIS
1	B	200	HIS
1	B	218	HIS
1	B	223	HIS
1	B	242	ASN
1	B	258	ASN
1	B	265	HIS
1	B	291	ASN
1	B	302	GLN
1	B	313	ASN
1	B	350	GLN
1	B	355	GLN
1	B	362	ASN
1	B	416	ASN
1	B	540	GLN
2	M	51	ASN
2	P	51	ASN
2	P	88	ASN

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Mol	Chain	Res	Type
3	E	167	ASN
3	F	179	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	A	601	1	14,14,15	0.76	1 (7%)	15,19,21	1.94	3 (20%)
5	NAG	B	602	1	14,14,15	0.84	0	15,19,21	1.97	3 (20%)

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	A	601	1	-	0/6/23/26	0/1/1/1
5	NAG	B	602	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)
5	A	601	NAG	C1-C2	2.29	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	NAG	C4-C3-C2	-5.16	103.20	111.23
5	B	602	NAG	C1-O5-C5	-5.02	105.87	112.25
5	A	601	NAG	O3-C3-C2	2.34	113.74	109.11
5	B	602	NAG	O5-C5-C6	2.76	113.32	107.35
5	B	602	NAG	C6-C5-C4	2.88	120.11	113.02
5	A	601	NAG	C1-O5-C5	3.82	117.10	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	461/531 (86%)	0.39	40 (8%)	13 13	25, 66, 145, 192	0
1	B	463/531 (87%)	0.19	25 (5%)	29 33	23, 52, 120, 159	0
2	M	98/115 (85%)	0.27	11 (11%)	7 7	32, 59, 110, 123	0
2	P	94/115 (81%)	0.52	11 (11%)	6 6	31, 83, 113, 125	0
3	E	149/160 (93%)	0.34	9 (6%)	25 28	40, 79, 132, 151	0
3	F	148/160 (92%)	2.10	62 (41%)	0 0	78, 133, 169, 200	0
All	All	1413/1612 (87%)	0.50	158 (11%)	7 7	23, 68, 148, 200	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	480	CYS	12.8
3	F	191	PRO	11.6
1	A	481	ALA	9.3
1	A	539	VAL	9.1
1	B	480	CYS	8.3
3	F	61	LEU	8.2
3	F	190	GLU	8.2
1	B	82	LEU	8.2
3	F	175	PHE	7.6
3	F	69	PHE	7.4
3	F	51	ILE	7.4
1	B	458	SER	7.3
3	F	74	GLU	7.1
3	F	99	LEU	7.0
3	E	179	ASN	6.8
3	F	58	THR	6.8
1	B	462	SER	6.6
1	B	546	GLY	6.4
1	A	537	HIS	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	437	PHE	6.0
3	F	101	PRO	5.9
3	F	180	GLN	5.9
3	F	47	ILE	5.9
1	A	483	GLY	5.9
1	B	437	PHE	5.7
3	F	55	MET	5.7
3	E	192	PRO	5.7
3	F	189	LYS	5.5
1	B	81	LEU	5.5
1	B	84	ASN	5.3
3	F	138	LEU	5.2
1	A	482	PHE	5.2
3	F	137	VAL	5.0
2	P	119	TYR	5.0
1	A	477	TYR	5.0
1	B	436	SER	4.9
3	F	159	TRP	4.8
3	F	135	SER	4.8
1	A	457	GLN	4.7
1	A	540	GLN	4.7
1	A	470	VAL	4.7
3	F	132	ARG	4.7
2	P	42	LYS	4.6
3	F	63	LEU	4.6
1	A	418	PHE	4.5
1	A	469	LYS	4.4
1	A	460	ILE	4.4
3	F	75	ILE	4.4
3	F	60	LYS	4.4
3	F	44	GLN	4.3
3	F	79	GLU	4.3
1	B	538	SER	4.2
1	B	460	ILE	4.2
3	F	183	HIS	4.2
1	A	455	ALA	4.2
3	F	134	ALA	4.2
2	M	116	GLU	4.2
1	A	538	SER	4.2
3	F	80	GLY	4.1
1	A	446	THR	4.0
1	B	537	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
3	F	102	GLY	3.9
3	F	62	ASN	3.8
3	F	186	ILE	3.8
1	B	481	ALA	3.7
3	F	164	ILE	3.6
1	B	545	PRO	3.5
2	M	117	GLY	3.5
3	F	90	LEU	3.5
3	F	50	VAL	3.5
3	F	49	ARG	3.4
2	M	100	GLU	3.4
1	A	453	ASN	3.4
1	A	394	PHE	3.4
3	F	56	ASP	3.4
3	F	172	LEU	3.4
1	A	465	PHE	3.3
1	B	457	GLN	3.3
3	F	179	ASN	3.3
3	F	46	ALA	3.2
2	M	143	SER	3.2
3	F	178	LYS	3.2
2	P	98	LYS	3.2
3	F	128	MET	3.2
2	P	96	LYS	3.1
2	M	126	TYR	3.1
3	F	181	LYS	3.1
1	A	370	PHE	3.1
3	F	139	PHE	3.1
1	B	461	SER	3.1
3	F	100	GLU	3.1
2	P	115	LYS	3.1
2	M	115	LYS	3.1
3	F	77	PRO	3.1
3	F	188	LEU	3.0
1	A	45	ARG	3.0
1	A	343	LEU	3.0
2	P	128	ALA	3.0
1	B	479	CYS	3.0
3	E	191	PRO	3.0
1	A	541	CYS	2.9
1	A	414	HIS	2.9
1	A	456	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	475	TYR	2.9
3	F	161	VAL	2.8
1	A	467	GLU	2.8
3	F	169	ALA	2.8
3	F	98	ASN	2.8
1	A	59	GLU	2.7
3	E	58	THR	2.7
2	M	141	GLU	2.7
3	F	155	LEU	2.7
2	M	127	PRO	2.7
1	A	60	LEU	2.6
1	B	61	PRO	2.6
1	B	476	ALA	2.6
1	A	454	HIS	2.6
1	A	462	SER	2.6
2	P	74	VAL	2.6
3	F	85	SER	2.6
1	B	60	LEU	2.6
3	F	187	GLU	2.6
1	A	479	CYS	2.6
3	E	178	LYS	2.5
1	A	389	ILE	2.5
1	A	413	ILE	2.5
3	F	57	PRO	2.4
1	A	412	ILE	2.4
2	M	118	LEU	2.4
1	B	59	GLU	2.4
1	B	544	SER	2.3
1	A	447	HIS	2.3
2	P	46	LEU	2.3
3	F	141	ILE	2.3
1	A	543	PRO	2.3
3	F	95	ASP	2.3
3	F	165	TRP	2.3
2	P	129	CYS	2.3
3	F	173	MET	2.3
2	M	119	TYR	2.3
3	F	45	LYS	2.3
1	B	168	TRP	2.3
2	P	101	HIS	2.2
1	B	477	TYR	2.2
2	P	114	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	162	VAL	2.2
3	F	171	LYS	2.2
3	E	75	ILE	2.2
1	A	86	LEU	2.2
3	E	57	PRO	2.2
3	E	184	VAL	2.1
3	E	181	LYS	2.1
2	M	142	CYS	2.1
1	A	464	ASN	2.1
1	A	478	GLN	2.1
3	F	107	VAL	2.0
3	F	116	PRO	2.0
3	F	105	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NI	B	601	1/1	0.99	0.12	-	44,44,44,44	0
5	NAG	A	601	14/15	0.90	0.31	-	66,82,88,95	0
5	NAG	B	602	14/15	0.93	0.28	-	54,60,66,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.