Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 01:24 PM EST

PDB ID	:	4P5O
Title	:	Structure of an RBX1-UBC12 NEDD8-CUL1-DCN1 complex: a RING-E3-E 2 ubiquitin-like protein-substrate intermediate trapped in action
Authors	:	Scott, D.C.; Schulman, B.A.
Deposited on	:	2014-03-18
Resolution	:	3.11 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 (i) 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 (i)) were used in the production of this report:

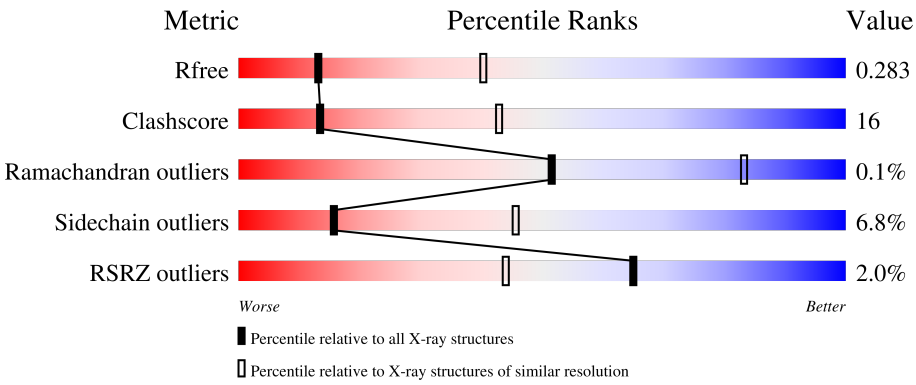
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.11 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 <=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	368	2%, 55%, 29%, •, 11%
1	C	368	2%, 59%, 25%, • •, 12%
2	B	106	2%, 51%, 17%, •, 29%
2	D	106	52%, 18%, •, 28%
3	E	200	3%, 64%, 31%, • •

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Mol	Chain	Length	Quality of chain
3	F	200	2%, 58%, 37%
4	G	189	58%, 28%, 5%, 10%
4	I	189	54%, 31%, 11%
5	H	81	%, 63%, 28%, 6%
5	K	81	7%, 64%, 26%, 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13577 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 Cullin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	327	2631	1671	447	499	14	0	0	0
1	C	322	2556	1615	436	491	14	0	0	0

- Molecule 2 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	75	619	393	112	105	9	0	0	0
2	D	76	624	397	114	104	9	0	0	0

- Molecule 3 is a protein called DCN1-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	197	1614	1039	264	302	9	0	0	0
3	F	195	1594	1027	258	300	9	0	0	0

- Molecule 4 is a protein called NEDD8-conjugating enzyme Ubc12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	I	169	1374	883	230	254	7	0	0	0
4	G	171	1384	888	231	258	7	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	AME	-	expression tag	UNP P61081
I	103	SER	ASN	engineered mutation	UNP P61081
I	111	SER	CYS	engineered mutation	UNP P61081
I	184	HIS	-	expression tag	UNP P61081
I	185	HIS	-	expression tag	UNP P61081
I	186	HIS	-	expression tag	UNP P61081
I	187	HIS	-	expression tag	UNP P61081
I	188	HIS	-	expression tag	UNP P61081
I	189	HIS	-	expression tag	UNP P61081
G	1	AME	-	expression tag	UNP P61081
G	103	SER	ASN	engineered mutation	UNP P61081
G	111	SER	CYS	engineered mutation	UNP P61081
G	184	HIS	-	expression tag	UNP P61081
G	185	HIS	-	expression tag	UNP P61081
G	186	HIS	-	expression tag	UNP P61081
G	187	HIS	-	expression tag	UNP P61081
G	188	HIS	-	expression tag	UNP P61081
G	189	HIS	-	expression tag	UNP P61081

- Molecule 5 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	K	76	591	372	102	115	2	0	0	0
			Total	C	N	O	S			
5	H	76	584	367	102	113	2	0	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

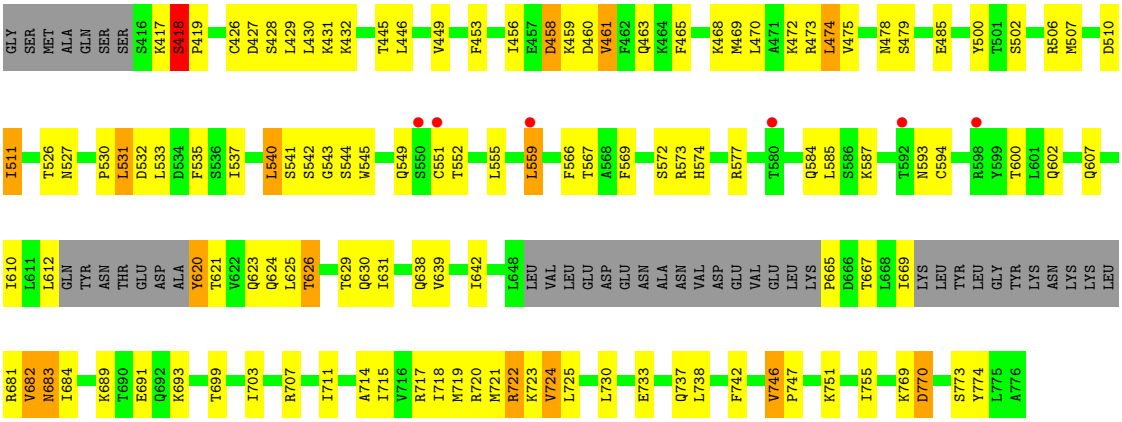
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	B	3	3	3	0	0
			Total	Zn		
6	D	3	3	3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

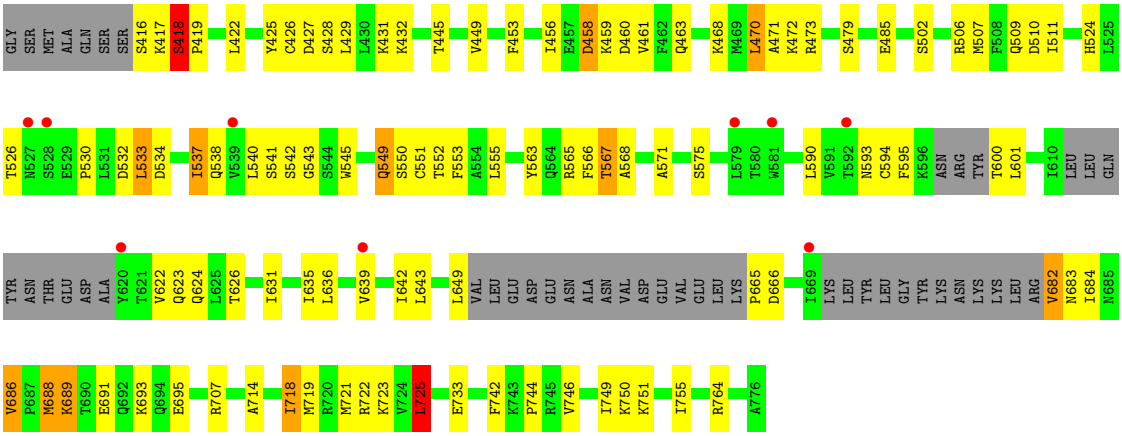
- Molecule 1: Cullin-1

Chain A:



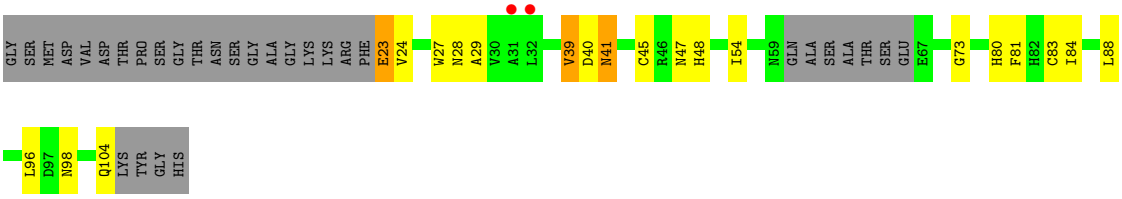
- Molecule 1: Cullin-1

Chain C:



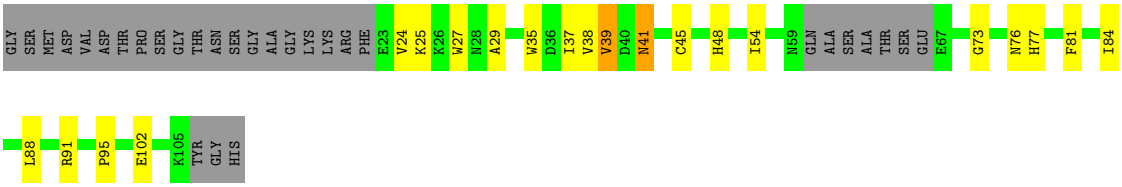
- Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain B:



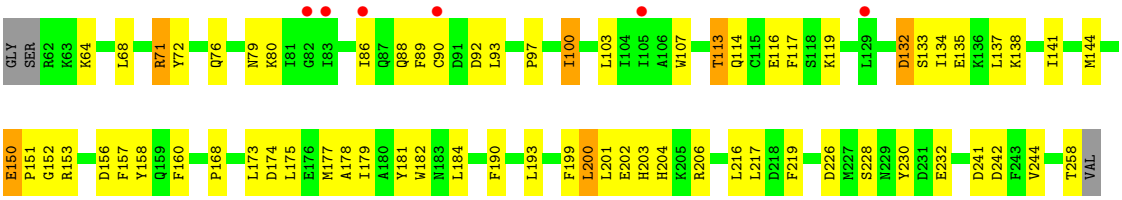
• Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain D:



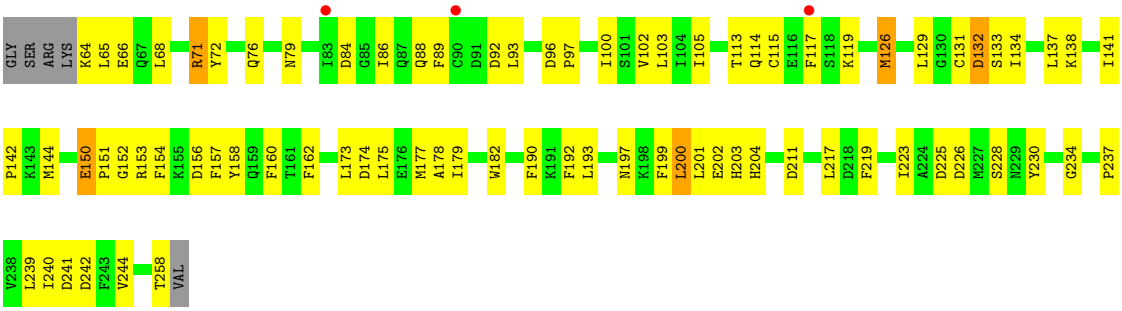
• Molecule 3: DCN1-like protein 1

Chain E:



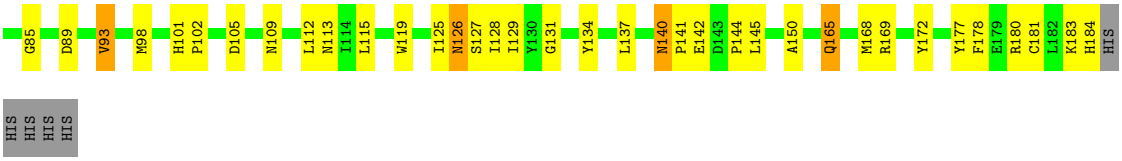
• Molecule 3: DCN1-like protein 1

Chain F:



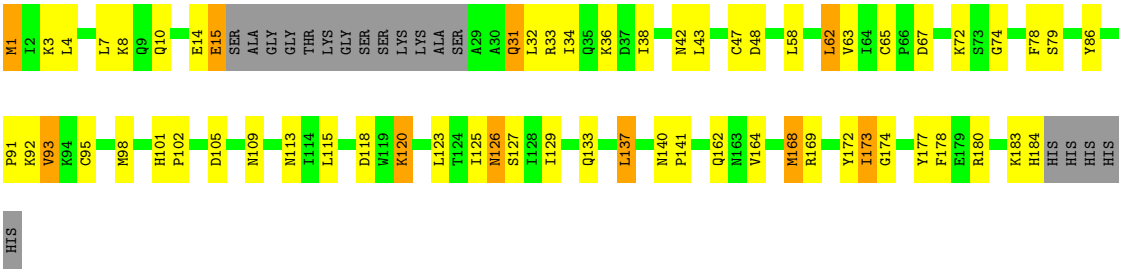
• Molecule 4: NEDD8-conjugating enzyme Ubc12

Chain I:



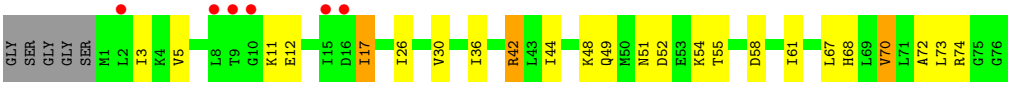
• Molecule 4: NEDD8-conjugating enzyme Ubc12

Chain G:



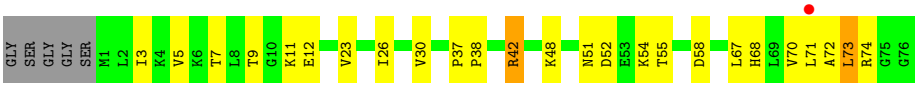
• Molecule 5: NEDD8

Chain K:



• Molecule 5: NEDD8

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.11Å 129.61Å 119.94Å 90.00° 111.79° 90.00°	Depositor
Resolution (Å)	42.13 – 3.11 42.13 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.13-3.11) 99.5 (42.13-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.227 , 0.284 0.226 , 0.283	Depositor DCC
R_{free} test set	2314 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	68.2	Xtriage
Anisotropy	0.907	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 38.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.439 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13577	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN, AME

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	0.43	0/2670	0.61	0/3587
1	C	0.43	0/2591	0.63	1/3481 (0.0%)
2	B	0.44	0/637	0.60	0/868
2	D	0.42	0/642	0.58	0/874
3	E	0.41	0/1653	0.57	1/2229 (0.0%)
3	F	0.41	0/1633	0.56	1/2204 (0.0%)
4	G	0.51	0/1404	0.65	1/1897 (0.1%)
4	I	0.55	0/1394	0.68	1/1882 (0.1%)
5	H	0.34	0/589	0.57	0/791
5	K	0.36	0/596	0.56	0/800
All	All	0.44	0/13809	0.61	5/18613 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
3	E	0	1
3	F	0	1
All	All	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	32	LEU	CA-CB-CG	6.95	131.28	115.30
3	F	200	LEU	CA-CB-CG	6.43	130.08	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	200	LEU	CA-CB-CG	5.84	128.74	115.30
1	C	725	LEU	CA-CB-CG	5.53	128.02	115.30
4	G	62	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	418	SER	Peptide
1	C	418	SER	Peptide
3	E	150	GLU	Peptide
3	F	150	GLU	Peptide

5.2 Too-close contacts (i)

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	2631	0	2660	104	0
1	C	2556	0	2547	77	0
2	B	619	0	566	17	0
2	D	624	0	575	15	0
3	E	1614	0	1570	54	1
3	F	1594	0	1544	61	0
4	G	1384	0	1361	54	1
4	I	1374	0	1364	48	0
5	H	584	0	603	15	0
5	K	591	0	616	17	0
6	B	3	0	0	0	0
6	D	3	0	0	0	0
All	All	13577	0	13406	433	1

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 16.

All (433) 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:720:ARG:NH2	1:A:774:TYR:OH	1.89	1.03
3:E:152:GLY:HA2	3:E:153:ARG:HB2	1.53	0.91
3:E:175:LEU:HD21	3:E:200:LEU:HD13	1.56	0.85
1:C:533:LEU:HD11	2:D:24:VAL:HG22	1.60	0.84
3:F:152:GLY:HA2	3:F:153:ARG:HB2	1.63	0.79
1:A:479:SER:OG	1:A:485:GLU:OE2	1.99	0.78
3:F:200:LEU:HA	3:F:204:HIS:H	1.48	0.78
4:I:142:GLU:HB3	5:K:74:ARG:HH22	1.48	0.77
3:E:71:ARG:NH2	3:E:92:ASP:OD1	2.17	0.77
5:H:42:ARG:HD3	5:H:72:ALA:HA	1.67	0.76
1:C:750:LYS:NZ	3:F:234:GLY:O	2.15	0.76
3:E:93:LEU:O	3:E:138:LYS:NZ	2.18	0.74
1:A:722:ARG:NH2	1:A:733:GLU:OE2	2.20	0.74
3:E:200:LEU:HA	3:E:204:HIS:H	1.53	0.73
4:G:173:ILE:HD12	4:G:174:GLY:H	1.53	0.73
3:F:93:LEU:HD23	3:F:138:LYS:HG2	1.70	0.73
3:F:175:LEU:HD21	3:F:200:LEU:HD13	1.69	0.72
3:E:100:ILE:HG23	3:E:184:LEU:HG	1.71	0.71
3:F:97:PRO:HB3	4:G:4:LEU:HD21	1.72	0.70
3:F:230:TYR:OH	3:F:241:ASP:OD2	2.06	0.70
2:B:41:ASN:ND2	2:B:47:ASN:O	2.24	0.70
1:A:682:VAL:HG13	1:A:683:ASN:HA	1.72	0.70
3:E:230:TYR:OH	3:E:241:ASP:OD2	2.11	0.69
3:E:93:LEU:HD23	3:E:138:LYS:HG2	1.75	0.69
3:E:230:TYR:HE2	3:E:232:GLU:HG2	1.57	0.68
2:B:96:LEU:HB3	5:K:36:ILE:HD11	1.74	0.68
1:A:526:THR:HA	1:A:530:PRO:HG3	1.76	0.68
4:G:113:ASN:HD21	5:H:73:LEU:HA	1.58	0.68
3:E:113:THR:HG21	3:E:168:PRO:HD3	1.76	0.67
5:H:3:ILE:HD12	5:H:67:LEU:HD13	1.74	0.67
3:E:93:LEU:HD21	3:E:137:LEU:HD23	1.75	0.67
3:E:79:ASN:O	3:E:119:LYS:N	2.28	0.67
1:A:720:ARG:HH21	1:A:774:TYR:HH	1.41	0.66
1:C:600:THR:O	1:C:682:VAL:N	2.28	0.66
3:F:93:LEU:HD21	3:F:137:LEU:HD23	1.77	0.66
1:C:540:LEU:HB3	1:C:545:TRP:CD1	2.31	0.66
1:A:722:ARG:HG3	1:A:725:LEU:HG	1.78	0.66
5:K:42:ARG:HD3	5:K:72:ALA:HA	1.76	0.66
3:F:84:ASP:OD1	4:G:8:LYS:NZ	2.28	0.65
1:C:526:THR:HG22	1:C:530:PRO:HG3	1.79	0.65
3:E:71:ARG:NH2	3:E:72:TYR:OH	2.30	0.64
4:G:105:ASP:OD1	4:G:109:ASN:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:764:ARG:NH1	3:F:211:ASP:OD1	2.31	0.64
3:F:71:ARG:NH2	3:F:92:ASP:OD2	2.31	0.64
4:I:105:ASP:OD1	4:I:109:ASN:N	2.30	0.64
1:A:428:SER:HA	1:A:431:LYS:NZ	2.12	0.64
1:C:510:ASP:OD2	1:C:541:SER:N	2.30	0.64
1:A:540:LEU:HG	1:A:545:TRP:CE2	2.32	0.63
1:C:549:GLN:NE2	1:C:550:SER:O	2.22	0.63
4:I:169:ARG:O	4:I:180:ARG:NH1	2.31	0.63
1:C:419:PRO:HB3	1:C:456:ILE:HD13	1.80	0.62
1:A:468:LYS:NZ	1:A:472:LYS:HE3	2.15	0.62
1:A:465:PHE:HB3	1:A:469:MET:HE3	1.82	0.62
1:C:468:LYS:HE3	1:C:695:GLU:OE2	1.99	0.62
1:C:553:PHE:HE2	1:C:555:LEU:HA	1.65	0.61
1:C:722:ARG:HG3	1:C:725:LEU:CD2	2.30	0.61
1:A:707:ARG:HG2	1:A:742:PHE:CE1	2.35	0.61
1:A:432:LYS:HD2	1:A:478:ASN:HA	1.82	0.61
1:C:553:PHE:CE2	1:C:555:LEU:HA	2.36	0.61
1:A:507:MET:HG3	1:A:545:TRP:CE2	2.36	0.61
1:C:507:MET:HG2	1:C:545:TRP:CD2	2.36	0.61
4:G:164:VAL:O	4:G:168:MET:HG2	2.01	0.60
4:G:4:LEU:HA	4:G:7:LEU:HD12	1.82	0.60
1:A:540:LEU:HB3	1:A:545:TRP:CD1	2.35	0.60
3:E:190:PHE:HB3	3:E:193:LEU:HB2	1.84	0.60
1:A:419:PRO:HB3	1:A:456:ILE:HD13	1.83	0.60
5:K:3:ILE:HG12	5:K:17:ILE:HD13	1.84	0.60
4:I:64:ILE:HG22	4:I:66:PRO:HD3	1.83	0.59
3:F:103:LEU:HB2	4:G:1:AME:HT21	1.84	0.59
4:I:98:MET:HE1	4:I:177:TYR:O	2.03	0.59
5:H:11:LYS:HG3	5:H:12:GLU:H	1.66	0.59
2:D:95:PRO:O	4:G:120:LYS:NZ	2.35	0.59
2:B:45:CYS:HB3	2:B:54:ILE:HG23	1.84	0.59
4:I:140:ASN:HD22	4:I:141:PRO:CD	2.15	0.59
1:A:715:ILE:HG13	1:A:730:LEU:HD11	1.83	0.58
2:B:80:HIS:HB2	2:B:83:CYS:SG	2.43	0.58
3:E:181:TYR:CZ	4:I:2:ILE:HG13	2.38	0.58
5:H:55:THR:OG1	5:H:58:ASP:OD1	2.21	0.58
1:A:532:ASP:OD1	1:A:533:LEU:N	2.36	0.58
1:A:717:ARG:NH1	1:A:737:GLN:OE1	2.36	0.58
3:E:141:ILE:HA	3:E:144:MET:HE2	1.85	0.58
4:I:45:LYS:NZ	4:I:67:ASP:OD2	2.36	0.58
4:I:168:MET:HG2	4:I:181:CYS:SG	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:590:LEU:O	1:C:601:LEU:N	2.25	0.58
1:A:426:CYS:SG	1:A:449:VAL:HG11	2.44	0.58
3:E:226:ASP:OD1	3:E:228:SER:OG	2.18	0.58
3:F:150:GLU:HB3	3:F:151:PRO:HD3	1.85	0.58
3:E:153:ARG:HA	3:E:156:ASP:HB3	1.86	0.57
1:A:430:LEU:HD11	1:A:446:LEU:HD21	1.85	0.57
4:G:173:ILE:HD11	4:G:178:PHE:CE2	2.39	0.57
1:A:722:ARG:HG3	1:A:725:LEU:CG	2.34	0.57
5:K:55:THR:OG1	5:K:58:ASP:OD1	2.23	0.57
4:G:62:LEU:HD11	4:G:129:ILE:HG12	1.86	0.57
1:A:531:LEU:HD23	1:A:532:ASP:H	1.71	0.56
4:I:29:ALA:O	4:I:32:LEU:HD23	2.05	0.56
3:F:226:ASP:OD1	3:F:228:SER:OG	2.20	0.56
4:I:140:ASN:HD22	4:I:141:PRO:N	2.04	0.56
4:G:172:TYR:CE2	4:G:177:TYR:HB2	2.40	0.56
3:F:88:GLN:NE2	3:F:92:ASP:OD1	2.38	0.56
4:I:172:TYR:CE2	4:I:177:TYR:HB2	2.41	0.56
1:C:682:VAL:HG13	1:C:683:ASN:HA	1.87	0.56
3:F:237:PRO:HD2	3:F:240:ILE:HD12	1.88	0.56
1:A:566:PHE:HA	1:A:569:PHE:CZ	2.41	0.56
1:A:551:CYS:SG	1:A:552:THR:N	2.77	0.56
2:D:35:TRP:O	2:D:76:ASN:ND2	2.39	0.56
5:K:54:LYS:NZ	5:K:58:ASP:OD2	2.31	0.56
1:A:537:ILE:HD12	2:B:29:ALA:H	1.70	0.55
5:K:11:LYS:HG3	5:K:12:GLU:H	1.71	0.55
3:E:199:PHE:HZ	3:E:242:ASP:HB3	1.72	0.55
5:K:5:VAL:HG22	5:K:67:LEU:HB2	1.89	0.55
1:A:691:GLU:C	1:A:693:LYS:H	2.10	0.55
4:I:140:ASN:HD22	4:I:141:PRO:HD2	1.69	0.55
1:C:429:LEU:HD13	1:C:445:THR:HG21	1.88	0.55
2:B:24:VAL:HG11	2:B:27:TRP:HB2	1.89	0.55
1:C:426:CYS:SG	1:C:449:VAL:HG11	2.46	0.55
1:C:623:GLN:O	1:C:626:THR:HB	2.07	0.55
1:A:429:LEU:HD13	1:A:445:THR:HG21	1.88	0.55
1:A:559:LEU:HD21	2:B:27:TRP:CH2	2.43	0.54
2:B:23:GLU:OE2	2:B:23:GLU:N	2.40	0.54
1:A:714:ALA:O	1:A:718:ILE:HG13	2.08	0.54
1:C:541:SER:C	1:C:543:GLY:HA3	2.28	0.54
5:H:3:ILE:HD11	5:H:26:ILE:HD11	1.90	0.54
3:F:173:LEU:HD13	3:F:178:ALA:HB2	1.89	0.54
2:D:38:VAL:O	2:D:39:VAL:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:71:ARG:HH22	3:E:92:ASP:CG	2.12	0.53
1:A:461:VAL:HA	1:A:703:ILE:HD13	1.89	0.53
1:A:541:SER:C	1:A:543:GLY:HA3	2.28	0.53
1:A:600:THR:O	1:A:681:ARG:N	2.41	0.53
1:C:537:ILE:HD12	2:D:29:ALA:HB3	1.89	0.53
1:C:707:ARG:HG2	1:C:742:PHE:CE2	2.44	0.53
3:E:86:ILE:HD11	3:E:117:PHE:CD2	2.43	0.53
4:I:43:LEU:HD13	4:I:48:ASP:HA	1.89	0.53
4:I:34:ILE:HG21	4:I:58:LEU:HD12	1.90	0.53
3:E:173:LEU:HD13	3:E:178:ALA:HB2	1.90	0.53
3:E:89:PHE:O	3:E:93:LEU:HD12	2.08	0.53
1:C:511:ILE:HD11	1:C:538:GLN:OE1	2.09	0.53
3:F:230:TYR:CZ	3:F:244:VAL:HG21	2.44	0.53
1:C:542:SER:N	1:C:543:GLY:HA3	2.24	0.53
4:G:43:LEU:HD13	4:G:48:ASP:HA	1.91	0.53
1:A:746:VAL:HG22	1:A:747:PRO:HD3	1.91	0.52
4:I:172:TYR:HE2	4:I:177:TYR:HB2	1.73	0.52
3:F:64:LYS:N	3:F:66:GLU:OE1	2.42	0.52
4:I:165:GLN:OE1	4:I:169:ARG:NH2	2.43	0.52
4:G:169:ARG:O	4:G:180:ARG:NH1	2.41	0.52
3:F:103:LEU:HB2	4:G:1:AME:CT2	2.39	0.52
2:D:37:ILE:HG22	2:D:39:VAL:H	1.75	0.52
1:A:639:VAL:O	1:A:642:ILE:HG22	2.09	0.52
1:A:566:PHE:HA	1:A:569:PHE:CE2	2.44	0.52
1:A:574:HIS:HB2	1:A:577:ARG:HH21	1.75	0.52
2:B:73:GLY:C	2:B:104:GLN:HE22	2.13	0.52
5:K:26:ILE:O	5:K:30:VAL:HG23	2.10	0.52
1:C:416:SER:O	1:C:416:SER:OG	2.25	0.52
3:F:133:SER:OG	3:F:134:ILE:N	2.42	0.52
3:E:178:ALA:O	3:E:182:TRP:CE3	2.62	0.51
3:F:132:ASP:OD2	3:F:132:ASP:N	2.43	0.51
3:E:230:TYR:CE2	3:E:232:GLU:HG2	2.41	0.51
1:C:428:SER:HA	1:C:431:LYS:NZ	2.24	0.51
3:E:132:ASP:OD2	3:E:132:ASP:N	2.43	0.51
1:C:427:ASP:C	1:C:431:LYS:HZ3	2.13	0.51
3:F:76:GLN:N	3:F:76:GLN:OE1	2.41	0.51
1:A:620:TYR:HB3	1:A:625:LEU:HG	1.92	0.51
1:A:549:GLN:N	1:A:549:GLN:OE1	2.44	0.51
4:G:34:ILE:HG21	4:G:58:LEU:HD12	1.92	0.51
1:A:542:SER:N	1:A:543:GLY:HA3	2.25	0.51
4:I:131:GLY:HA2	5:K:73:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:GLN:NE2	1:A:684:ILE:O	2.33	0.51
1:A:623:GLN:O	1:A:626:THR:HG22	2.11	0.51
2:D:37:ILE:O	2:D:39:VAL:HG13	2.11	0.51
1:C:418:SER:HB3	1:C:419:PRO:CD	2.41	0.50
3:E:150:GLU:HB3	3:E:151:PRO:CD	2.42	0.50
1:A:626:THR:OG1	1:A:631:ILE:O	2.25	0.50
3:F:199:PHE:HZ	3:F:242:ASP:HB3	1.77	0.50
4:G:125:ILE:O	4:G:129:ILE:HG13	2.11	0.50
1:A:506:ARG:HD2	1:A:544:SER:OG	2.11	0.50
1:C:563:TYR:O	1:C:567:THR:OG1	2.27	0.50
4:I:13:GLU:OE1	4:I:13:GLU:N	2.39	0.50
4:I:183:LYS:HD2	4:I:184:HIS:H	1.77	0.50
3:F:177:MET:C	3:F:179:ILE:H	2.14	0.50
1:C:764:ARG:HH12	3:F:211:ASP:CG	2.15	0.50
4:G:1:AME:HB1	4:G:4:LEU:HD23	1.94	0.50
4:G:42:ASN:H	4:G:126:ASN:HD21	1.60	0.50
1:C:684:ILE:O	1:C:686:VAL:HG12	2.12	0.50
1:A:429:LEU:HD23	1:A:430:LEU:HD12	1.94	0.49
5:K:44:ILE:HD11	5:K:70:VAL:HG12	1.92	0.49
1:C:537:ILE:HG21	1:C:566:PHE:CE1	2.46	0.49
1:A:427:ASP:C	1:A:431:LYS:HZ3	2.16	0.49
3:E:177:MET:C	3:E:179:ILE:H	2.14	0.49
1:C:507:MET:HG2	1:C:545:TRP:CE2	2.47	0.49
3:F:79:ASN:O	3:F:119:LYS:N	2.44	0.49
4:I:125:ILE:O	4:I:129:ILE:HG13	2.13	0.49
5:K:3:ILE:HD12	5:K:67:LEU:HD13	1.93	0.49
1:C:626:THR:HG23	1:C:631:ILE:O	2.13	0.49
4:I:119:TRP:CZ3	4:I:128:ILE:HD11	2.47	0.49
1:A:724:VAL:HG23	1:A:773:SER:HB2	1.95	0.49
3:F:177:MET:HG3	3:F:178:ALA:H	1.78	0.49
1:C:502:SER:O	1:C:506:ARG:HG2	2.12	0.49
1:C:593:ASN:OD1	1:C:594:CYS:N	2.46	0.49
1:C:742:PHE:HE2	1:C:744:PRO:HB3	1.78	0.49
1:C:453:PHE:CZ	1:C:459:LYS:HD3	2.47	0.49
3:F:141:ILE:HA	3:F:144:MET:HE2	1.95	0.49
4:G:62:LEU:CD1	4:G:129:ILE:HG12	2.42	0.49
3:F:93:LEU:O	3:F:138:LYS:NZ	2.38	0.48
3:E:150:GLU:HB3	3:E:151:PRO:HD3	1.93	0.48
1:C:639:VAL:O	1:C:642:ILE:HG22	2.13	0.48
1:C:744:PRO:HG2	1:C:749:ILE:HD11	1.95	0.48
3:E:76:GLN:OE1	3:E:76:GLN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:ARG:HG3	1:A:725:LEU:CD1	2.44	0.48
4:G:173:ILE:HD11	4:G:178:PHE:HE2	1.78	0.48
5:H:26:ILE:O	5:H:30:VAL:HG23	2.14	0.48
4:G:79:SER:O	4:G:93:VAL:HA	2.14	0.48
4:I:79:SER:O	4:I:93:VAL:HA	2.14	0.48
1:C:524:HIS:O	1:C:524:HIS:ND1	2.47	0.48
1:C:622:VAL:HB	1:C:665:PRO:O	2.13	0.47
3:F:152:GLY:HA3	3:F:154:PHE:H	1.79	0.47
4:G:113:ASN:CG	5:H:74:ARG:H	2.18	0.47
3:F:178:ALA:O	3:F:182:TRP:CE3	2.67	0.47
4:I:33:ARG:NH1	4:I:37:ASP:OD1	2.47	0.47
4:G:98:MET:HE1	4:G:177:TYR:O	2.14	0.47
1:A:699:THR:O	1:A:703:ILE:HG13	2.14	0.47
1:A:468:LYS:HZ1	1:A:472:LYS:HE3	1.78	0.47
3:E:230:TYR:CZ	3:E:244:VAL:HG21	2.49	0.47
3:F:162:PHE:CD1	3:F:173:LEU:HD12	2.49	0.47
1:A:602:GLN:H	1:A:683:ASN:HB2	1.80	0.47
1:A:718:ILE:HG22	1:A:722:ARG:HG2	1.96	0.47
1:A:683:ASN:HD22	1:A:683:ASN:H	1.63	0.47
1:A:769:LYS:NZ	1:A:770:ASP:OD1	2.48	0.47
4:I:33:ARG:O	4:I:36:LYS:N	2.48	0.47
4:I:66:PRO:HG2	4:I:71:TYR:O	2.15	0.47
1:A:417:LYS:HB2	1:A:418:SER:HA	1.96	0.47
1:A:418:SER:HB3	1:A:419:PRO:CD	2.44	0.47
1:C:718:ILE:H	1:C:718:ILE:HG12	1.47	0.47
3:F:157:PHE:O	3:F:160:PHE:HB3	2.14	0.46
1:A:569:PHE:O	1:A:572:SER:OG	2.18	0.46
2:D:27:TRP:CZ2	2:D:29:ALA:HB2	2.51	0.46
3:F:158:TYR:CE2	3:F:217:LEU:HB2	2.50	0.46
1:C:470:LEU:HD23	1:C:473:ARG:NH2	2.30	0.46
3:E:93:LEU:HG	3:E:134:ILE:HG23	1.98	0.46
4:I:101:HIS:CG	4:I:102:PRO:HD2	2.50	0.46
1:C:714:ALA:O	1:C:718:ILE:HG12	2.15	0.46
2:D:73:GLY:HA2	2:D:102:GLU:O	2.16	0.46
4:I:32:LEU:HD12	4:I:32:LEU:O	2.15	0.46
1:C:590:LEU:HB2	1:C:601:LEU:CD1	2.45	0.46
2:B:84:ILE:O	2:B:88:LEU:HG	2.15	0.46
5:H:37:PRO:HA	5:H:38:PRO:HD3	1.82	0.46
3:E:93:LEU:HD23	3:E:138:LYS:CG	2.46	0.46
4:I:98:MET:CE	4:I:178:PHE:HA	2.46	0.46
5:H:7:THR:OG1	5:H:9:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:ILE:HD11	2:B:29:ALA:HB3	1.98	0.46
3:F:201:LEU:HD23	3:F:201:LEU:HA	1.80	0.46
1:A:428:SER:HA	1:A:431:LYS:HZ3	1.78	0.46
5:K:61:ILE:HD13	5:K:67:LEU:HD11	1.98	0.46
1:C:468:LYS:O	1:C:471:ALA:HB3	2.16	0.46
4:G:67:ASP:C	4:G:72:LYS:HG3	2.37	0.46
3:F:200:LEU:HA	3:F:204:HIS:N	2.26	0.45
4:G:183:LYS:HD2	4:G:184:HIS:H	1.81	0.45
1:A:566:PHE:CD1	1:A:569:PHE:HZ	2.34	0.45
3:E:64:LYS:H	3:E:64:LYS:HG2	1.51	0.45
4:I:65:CYS:HA	4:I:74:GLY:O	2.16	0.45
1:C:549:GLN:HG2	1:C:550:SER:N	2.32	0.45
1:C:751:LYS:O	1:C:755:ILE:HG13	2.16	0.45
3:E:100:ILE:H	3:E:100:ILE:HG12	1.51	0.45
3:F:152:GLY:HA2	3:F:153:ARG:CB	2.40	0.45
3:E:152:GLY:HA2	3:E:153:ARG:CB	2.33	0.45
1:C:459:LYS:O	1:C:463:GLN:HG3	2.17	0.45
1:C:551:CYS:SG	1:C:552:THR:N	2.86	0.45
4:I:144:PRO:HB3	4:I:150:ALA:HB2	1.99	0.45
4:G:10:GLN:O	4:G:14:GLU:HG3	2.17	0.45
3:F:89:PHE:O	3:F:93:LEU:HD12	2.17	0.45
4:G:113:ASN:HB2	4:G:118:ASP:OD2	2.16	0.45
1:A:428:SER:HA	1:A:431:LYS:HZ1	1.81	0.45
1:A:537:ILE:CD1	2:B:29:ALA:H	2.30	0.45
1:C:422:LEU:O	1:C:425:TYR:HB3	2.17	0.45
1:C:691:GLU:C	1:C:693:LYS:H	2.19	0.45
3:F:105:ILE:HD12	3:F:137:LEU:HD11	1.99	0.45
1:C:468:LYS:HZ1	1:C:472:LYS:NZ	2.15	0.45
3:F:190:PHE:HB3	3:F:193:LEU:HB2	1.98	0.45
4:G:86:TYR:HE1	4:G:91:PRO:HD3	1.82	0.45
1:A:600:THR:O	1:A:682:VAL:HG12	2.17	0.45
1:A:629:THR:OG1	1:A:631:ILE:HG22	2.17	0.45
1:A:587:LYS:HE2	2:B:28:ASN:HD21	1.82	0.44
3:E:158:TYR:CE2	3:E:217:LEU:HB2	2.52	0.44
1:C:533:LEU:O	1:C:534:ASP:C	2.55	0.44
1:A:453:PHE:CZ	1:A:459:LYS:HD3	2.51	0.44
1:A:511:ILE:HD13	1:A:511:ILE:HA	1.81	0.44
3:E:133:SER:OG	3:E:135:GLU:OE2	2.35	0.44
2:D:84:ILE:O	2:D:88:LEU:HG	2.17	0.44
3:F:126:MET:HE2	3:F:131:CYS:HB2	2.00	0.44
3:F:179:ILE:HD11	3:F:197:ASN:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:LYS:O	1:A:463:GLN:HG3	2.17	0.44
1:A:638:GLN:OE1	1:A:691:GLU:HB2	2.18	0.44
3:E:199:PHE:O	3:E:200:LEU:HG	2.17	0.44
2:D:37:ILE:HD13	2:D:77:HIS:CD2	2.53	0.44
2:D:45:CYS:HB2	2:D:54:ILE:HG12	1.98	0.44
4:G:33:ARG:O	4:G:36:LYS:N	2.50	0.44
4:G:172:TYR:HE2	4:G:177:TYR:HB2	1.78	0.44
1:A:427:ASP:O	1:A:431:LYS:HG3	2.17	0.44
2:D:41:ASN:OD1	2:D:48:HIS:ND1	2.48	0.44
3:F:86:ILE:HD11	3:F:117:PHE:CD2	2.52	0.44
3:F:153:ARG:HA	3:F:156:ASP:HB3	2.00	0.44
3:F:230:TYR:CE1	3:F:244:VAL:HG21	2.53	0.44
4:G:133:GLN:HG2	4:G:137:LEU:CD2	2.48	0.44
2:B:27:TRP:CZ2	2:B:29:ALA:HB2	2.53	0.44
3:F:72:TYR:HE1	3:F:88:GLN:HG3	1.81	0.44
1:C:688:MET:H	1:C:688:MET:HG2	1.54	0.44
1:A:722:ARG:O	1:A:723:LYS:HB2	2.17	0.44
3:E:68:LEU:HD12	3:E:71:ARG:HE	1.83	0.44
4:I:85:GLY:O	4:I:89:ASP:N	2.27	0.44
4:I:113:ASN:CG	5:K:74:ARG:H	2.22	0.44
4:I:131:GLY:O	4:I:134:TYR:HB3	2.18	0.44
4:G:47:CYS:HA	4:G:63:VAL:O	2.17	0.44
1:A:531:LEU:HD23	1:A:532:ASP:OD1	2.18	0.44
4:G:78:PHE:HE1	4:G:95:CYS:SG	2.41	0.44
3:E:216:LEU:HD12	3:E:219:PHE:HB3	1.99	0.43
1:C:631:ILE:HD11	1:C:635:ILE:HG22	1.98	0.43
1:A:460:ASP:OD1	1:A:742:PHE:HB3	2.18	0.43
3:F:173:LEU:HD22	3:F:178:ALA:HB2	1.99	0.43
1:C:532:ASP:O	1:C:533:LEU:HB2	2.18	0.43
1:A:593:ASN:OD1	1:A:594:CYS:N	2.50	0.43
3:F:144:MET:HE2	3:F:144:MET:HB2	1.86	0.43
1:A:468:LYS:HZ3	1:A:472:LYS:HE3	1.83	0.43
4:I:31:GLN:HB3	4:I:34:ILE:HG22	1.99	0.43
1:C:479:SER:OG	1:C:485:GLU:OE1	2.17	0.43
1:C:553:PHE:CE2	1:C:555:LEU:N	2.87	0.43
1:C:722:ARG:NH2	1:C:733:GLU:OE2	2.51	0.43
3:E:90:CYS:SG	3:E:97:PRO:HA	2.58	0.43
3:E:204:HIS:CD2	3:E:206:ARG:H	2.36	0.43
4:I:31:GLN:HA	4:I:33:ARG:N	2.34	0.43
4:I:47:CYS:HA	4:I:63:VAL:O	2.18	0.43
1:A:417:LYS:N	1:A:418:SER:OG	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:177:MET:HG3	3:E:178:ALA:H	1.83	0.43
3:F:202:GLU:HG3	3:F:203:HIS:ND1	2.33	0.43
1:A:510:ASP:OD2	1:A:541:SER:N	2.45	0.43
1:C:417:LYS:N	1:C:418:SER:OG	2.52	0.43
4:G:31:GLN:CA	4:G:32:LEU:HB3	2.48	0.43
1:A:460:ASP:OD2	1:A:707:ARG:HD2	2.18	0.43
3:E:201:LEU:HD23	3:E:201:LEU:HA	1.85	0.43
4:I:61:LYS:HD3	4:I:77:VAL:HG21	2.00	0.43
1:C:428:SER:HA	1:C:431:LYS:HZ1	1.83	0.43
4:G:1:AME:HB1	4:G:4:LEU:CD2	2.49	0.43
4:I:98:MET:HE3	4:I:178:PHE:HA	1.99	0.43
1:C:460:ASP:OD1	1:C:460:ASP:N	2.42	0.43
2:D:25:LYS:HA	2:D:25:LYS:HD3	1.65	0.43
2:D:88:LEU:HA	2:D:91:ARG:O	2.19	0.43
4:G:65:CYS:HA	4:G:74:GLY:O	2.18	0.43
5:H:23:VAL:HG23	5:H:54:LYS:O	2.19	0.43
1:A:626:THR:O	1:A:630:GLN:N	2.51	0.42
3:E:202:GLU:HG3	3:E:203:HIS:ND1	2.34	0.42
1:C:460:ASP:OD1	1:C:742:PHE:HB3	2.19	0.42
1:A:621:THR:OG1	1:A:624:GLN:HG2	2.18	0.42
4:I:42:ASN:H	4:I:126:ASN:HD21	1.68	0.42
4:G:98:MET:CE	4:G:178:PHE:HA	2.50	0.42
1:C:553:PHE:CE2	1:C:555:LEU:CA	3.01	0.42
4:G:133:GLN:O	4:G:137:LEU:HD22	2.20	0.42
1:A:573:ARG:NH1	1:A:577:ARG:HH22	2.17	0.42
3:E:88:GLN:NE2	3:E:92:ASP:OD2	2.53	0.42
5:K:51:ASN:OD1	5:K:52:ASP:N	2.44	0.42
4:G:38:ILE:HD13	4:G:38:ILE:HA	1.86	0.42
4:G:115:LEU:HD23	4:G:115:LEU:HA	1.86	0.42
1:A:470:LEU:O	1:A:474:LEU:HD22	2.20	0.42
3:E:230:TYR:CE1	3:E:244:VAL:HG21	2.53	0.42
1:C:511:ILE:HD12	1:C:511:ILE:HA	1.85	0.42
4:G:15:GLU:H	4:G:15:GLU:HG2	1.49	0.42
1:C:601:LEU:HA	1:C:682:VAL:N	2.35	0.42
3:F:93:LEU:HD23	3:F:138:LYS:CG	2.45	0.42
5:H:5:VAL:HG22	5:H:67:LEU:HB2	2.02	0.42
1:A:463:GLN:HB3	1:A:500:TYR:CZ	2.54	0.42
4:I:53:ASP:HA	4:I:54:PRO:HD2	1.83	0.42
3:F:68:LEU:HD12	3:F:71:ARG:HE	1.84	0.42
3:F:204:HIS:HD1	3:F:239:LEU:HD21	1.85	0.42
4:G:113:ASN:ND2	5:H:74:ARG:H	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:51:ASN:OD1	5:H:52:ASP:N	2.43	0.42
1:A:428:SER:N	1:A:431:LYS:HZ3	2.18	0.42
1:A:507:MET:HG3	1:A:545:TRP:CD2	2.54	0.42
1:A:751:LYS:O	1:A:755:ILE:HG13	2.20	0.42
4:I:112:LEU:HD23	4:I:115:LEU:HG	2.02	0.42
3:F:115:CYS:SG	4:G:4:LEU:HB3	2.60	0.42
3:E:114:GLN:OE1	4:I:3:LYS:HG2	2.20	0.41
4:I:67:ASP:OD1	4:I:68:GLU:HG2	2.20	0.41
1:A:532:ASP:OD1	1:A:533:LEU:HG	2.20	0.41
1:A:535:PHE:HE1	2:B:27:TRP:HZ3	1.67	0.41
3:F:96:ASP:O	3:F:102:VAL:HG11	2.20	0.41
3:F:219:PHE:O	3:F:223:ILE:HG13	2.20	0.41
1:A:535:PHE:HE1	2:B:27:TRP:CZ3	2.38	0.41
1:C:689:LYS:HZ2	1:C:689:LYS:HG3	1.70	0.41
4:G:31:GLN:CA	4:G:33:ARG:H	2.33	0.41
1:A:715:ILE:CD1	1:A:730:LEU:HD21	2.51	0.41
1:A:738:LEU:HD12	1:A:738:LEU:HA	1.85	0.41
4:G:140:ASN:HA	4:G:141:PRO:HD3	1.92	0.41
1:A:693:LYS:HE3	1:A:693:LYS:HB2	1.84	0.41
1:C:590:LEU:HB2	1:C:601:LEU:HD11	2.03	0.41
3:F:192:PHE:HE2	3:F:225:ASP:O	2.04	0.41
1:A:472:LYS:HA	1:A:475:VAL:HG12	2.02	0.41
3:E:71:ARG:HH21	3:E:134:ILE:HD11	1.85	0.41
3:E:103:LEU:HD23	3:E:157:PHE:CZ	2.56	0.41
4:I:137:LEU:HD23	4:I:137:LEU:HA	1.74	0.41
1:A:458:ASP:N	1:A:458:ASP:OD2	2.53	0.41
1:C:458:ASP:N	1:C:458:ASP:OD2	2.54	0.41
1:C:666:ASP:OD1	1:C:666:ASP:N	2.49	0.41
4:G:101:HIS:CG	4:G:102:PRO:HD2	2.55	0.41
1:A:620:TYR:CD2	1:A:624:GLN:HG3	2.56	0.41
1:A:620:TYR:N	1:A:669:ILE:O	2.53	0.41
1:A:621:THR:H	1:A:624:GLN:HE21	1.68	0.41
1:A:722:ARG:HG3	1:A:725:LEU:HD11	2.02	0.41
4:I:31:GLN:CA	4:I:33:ARG:H	2.33	0.41
3:F:141:ILE:HB	3:F:142:PRO:HD3	2.02	0.41
4:G:173:ILE:HD11	4:G:178:PHE:CD2	2.56	0.41
3:E:107:TRP:HD1	3:E:160:PHE:CG	2.39	0.41
5:K:42:ARG:HG2	5:K:49:GLN:OE1	2.21	0.41
1:C:565:ARG:O	1:C:568:ALA:HB3	2.21	0.41
1:C:631:ILE:HG21	1:C:636:LEU:HD13	2.02	0.41
4:G:86:TYR:CE1	4:G:91:PRO:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:571:ALA:HA	1:C:575:SER:HA	2.03	0.41
1:C:643:LEU:HD23	1:C:643:LEU:HA	1.85	0.41
3:F:114:GLN:OE1	4:G:3:LYS:HG2	2.20	0.41
4:G:67:ASP:O	4:G:72:LYS:HG3	2.21	0.41
5:H:48:LYS:HE2	5:H:48:LYS:HB3	1.80	0.41
1:A:430:LEU:HD22	1:A:473:ARG:HH12	1.85	0.40
1:A:711:ILE:O	1:A:715:ILE:HG22	2.21	0.40
1:A:722:ARG:HA	1:A:722:ARG:HD3	1.66	0.40
3:E:103:LEU:HB2	4:I:1:AME:CT2	2.51	0.40
4:G:31:GLN:HA	4:G:33:ARG:N	2.35	0.40
4:G:98:MET:HE3	4:G:178:PHE:HA	2.03	0.40
4:G:183:LYS:HD2	4:G:184:HIS:N	2.37	0.40
1:A:623:GLN:HG2	1:A:665:PRO:O	2.20	0.40
3:E:64:LYS:HD2	3:E:132:ASP:HB3	2.03	0.40
4:I:12:LYS:H	4:I:12:LYS:HG2	1.47	0.40
5:K:48:LYS:HE3	5:K:48:LYS:HB2	1.87	0.40
3:F:129:LEU:HD23	3:F:129:LEU:HA	1.92	0.40
3:F:199:PHE:C	3:F:201:LEU:H	2.24	0.40
1:A:460:ASP:OD1	1:A:460:ASP:N	2.45	0.40
1:A:584:GLN:HG3	1:A:585:LEU:HD13	2.04	0.40
2:B:40:ASP:O	2:B:48:HIS:ND1	2.53	0.40
1:C:722:ARG:HA	1:C:722:ARG:HD3	1.45	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:258:THR:O	4:G:162:GLN:NE2[1_554]	2.14	0.06

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	319/368 (87%)	297 (93%)	22 (7%)	0	100	100
1	C	312/368 (85%)	289 (93%)	23 (7%)	0	100	100
2	B	71/106 (67%)	68 (96%)	2 (3%)	1 (1%)	11	40
2	D	72/106 (68%)	69 (96%)	2 (3%)	1 (1%)	11	40
3	E	195/200 (98%)	182 (93%)	13 (7%)	0	100	100
3	F	193/200 (96%)	179 (93%)	14 (7%)	0	100	100
4	G	167/189 (88%)	160 (96%)	7 (4%)	0	100	100
4	I	165/189 (87%)	158 (96%)	7 (4%)	0	100	100
5	H	74/81 (91%)	71 (96%)	3 (4%)	0	100	100
5	K	74/81 (91%)	71 (96%)	3 (4%)	0	100	100
All	All	1642/1888 (87%)	1544 (94%)	96 (6%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	39	VAL
2	D	39	VAL

5.3.2 Protein sidechains (i)

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	294/339 (87%)	268 (91%)	26 (9%)	10	36
1	C	282/339 (83%)	259 (92%)	23 (8%)	11	38
2	B	66/90 (73%)	61 (92%)	5 (8%)	13	41
2	D	66/90 (73%)	64 (97%)	2 (3%)	41	71
3	E	173/176 (98%)	166 (96%)	7 (4%)	31	65
3	F	171/176 (97%)	163 (95%)	8 (5%)	26	59
4	G	153/170 (90%)	142 (93%)	11 (7%)	14	44
4	I	153/170 (90%)	143 (94%)	10 (6%)	17	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	H	62/68 (91%)	57 (92%)	5 (8%)	11	39
5	K	64/68 (94%)	60 (94%)	4 (6%)	18	48
All	All	1484/1686 (88%)	1383 (93%)	101 (7%)	16	45

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	418	SER
1	A	458	ASP
1	A	461	VAL
1	A	474	LEU
1	A	502	SER
1	A	511	ILE
1	A	527	ASN
1	A	531	LEU
1	A	540	LEU
1	A	555	LEU
1	A	559	LEU
1	A	567	THR
1	A	610	ILE
1	A	612	LEU
1	A	620	TYR
1	A	626	THR
1	A	667	THR
1	A	682	VAL
1	A	683	ASN
1	A	689	LYS
1	A	719	MET
1	A	721	MET
1	A	722	ARG
1	A	724	VAL
1	A	746	VAL
1	A	770	ASP
2	B	23	GLU
2	B	39	VAL
2	B	41	ASN
2	B	81	PHE
2	B	98	ASN
3	E	71	ARG
3	E	80	LYS
3	E	100	ILE

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Mol	Chain	Res	Type
3	E	113	THR
3	E	116	GLU
3	E	132	ASP
3	E	174	ASP
4	I	2	ILE
4	I	12	LYS
4	I	31	GLN
4	I	32	LEU
4	I	93	VAL
4	I	126	ASN
4	I	127	SER
4	I	140	ASN
4	I	145	LEU
4	I	165	GLN
5	K	17	ILE
5	K	42	ARG
5	K	68	HIS
5	K	70	VAL
1	C	418	SER
1	C	432	LYS
1	C	458	ASP
1	C	461	VAL
1	C	470	LEU
1	C	509	GLN
1	C	533	LEU
1	C	537	ILE
1	C	549	GLN
1	C	567	THR
1	C	595	PHE
1	C	624	GLN
1	C	649	LEU
1	C	682	VAL
1	C	686	VAL
1	C	688	MET
1	C	689	LYS
1	C	718	ILE
1	C	719	MET
1	C	721	MET
1	C	723	LYS
1	C	725	LEU
1	C	746	VAL
2	D	41	ASN

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Mol	Chain	Res	Type
2	D	81	PHE
3	F	65	LEU
3	F	71	ARG
3	F	100	ILE
3	F	113	THR
3	F	126	MET
3	F	132	ASP
3	F	174	ASP
3	F	258	THR
4	G	15	GLU
4	G	31	GLN
4	G	92	LYS
4	G	93	VAL
4	G	120	LYS
4	G	123	LEU
4	G	126	ASN
4	G	127	SER
4	G	137	LEU
4	G	168	MET
4	G	173	ILE
5	H	42	ARG
5	H	68	HIS
5	H	70	VAL
5	H	71	LEU
5	H	73	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	463	GLN
2	B	41	ASN
4	I	140	ASN
5	K	41	GLN
1	C	436	ASN
1	C	712	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)

2 non-standard protein/DNA/RNA residues 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	AME	I	1	4	9,10,11	1.42	2 (22%)	9,11,13	1.74	2 (22%)
4	AME	G	1	4	9,10,11	1.42	2 (22%)	9,11,13	1.56	2 (22%)

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	AME	I	1	4	-	4/9/10/12	-
4	AME	G	1	4	-	2/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	AME	CA-N	-3.02	1.42	1.46
4	I	1	AME	CA-N	-2.89	1.42	1.46
4	I	1	AME	CT1-N	2.22	1.42	1.34
4	G	1	AME	CT1-N	2.14	1.41	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1	AME	CE-SD-CG	3.02	110.77	100.40
4	I	1	AME	CE-SD-CG	2.94	110.51	100.40
4	G	1	AME	C-CA-N	-2.50	105.21	109.73
4	I	1	AME	CT2-CT1-N	2.01	119.50	116.10

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	AME	C-CA-CB-CG
4	I	1	AME	N-CA-CB-CG
4	I	1	AME	O-C-CA-CB
4	G	1	AME	C-CA-CB-CG
4	G	1	AME	N-CA-CB-CG
4	I	1	AME	CA-CB-CG-SD

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	AME	1	0
4	G	1	AME	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 (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	327/368 (88%)	-0.16	6 (1%)	68	47	36, 96, 170, 195	0
1	C	322/368 (87%)	-0.14	9 (2%)	53	30	37, 93, 167, 202	0
2	B	75/106 (70%)	-0.11	2 (2%)	54	31	56, 105, 156, 160	0
2	D	76/106 (71%)	-0.17	0	100	100	54, 108, 138, 157	0
3	E	197/200 (98%)	-0.16	6 (3%)	50	27	49, 98, 155, 167	0
3	F	195/200 (97%)	-0.22	3 (1%)	73	54	60, 97, 144, 164	0
4	G	170/189 (89%)	-0.17	0	100	100	35, 63, 150, 178	0
4	I	168/189 (88%)	-0.30	0	100	100	30, 63, 132, 190	0
5	H	76/81 (93%)	-0.06	1 (1%)	77	59	75, 123, 155, 168	0
5	K	76/81 (93%)	0.16	6 (7%)	12	5	68, 119, 148, 159	0
All	All	1682/1888 (89%)	-0.16	33 (1%)	65	44	30, 92, 162, 202	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	528	SER	7.1
2	B	31	ALA	4.6
1	C	669	ILE	3.6
5	K	15	ILE	3.6
1	C	579	LEU	3.4
3	F	83	ILE	3.4
3	E	86	ILE	3.2
1	A	598	ARG	3.2
1	A	550	SER	3.0
5	K	10	GLY	3.0
1	C	592	THR	2.7
3	E	129	LEU	2.7
5	K	16	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	90	CYS	2.6
3	E	105	ILE	2.6
1	C	581	TRP	2.5
1	A	580	THR	2.5
3	E	82	GLY	2.5
1	C	620	TYR	2.4
2	B	32	LEU	2.4
1	C	539	VAL	2.3
1	A	551	CYS	2.3
5	K	8	LEU	2.2
5	K	9	THR	2.2
1	C	527	ASN	2.2
3	E	90	CYS	2.2
5	K	2	LEU	2.2
5	H	71	LEU	2.1
3	E	83	ILE	2.1
3	F	117	PHE	2.1
1	A	559	LEU	2.0
1	A	592	THR	2.0
1	C	639	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	AME	I	1	11/12	0.91	0.36	76,87,100,105	0
4	AME	G	1	11/12	0.92	0.55	74,82,97,144	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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
6	ZN	D	202	1/1	0.97	0.18	78,78,78,78	0
6	ZN	B	203	1/1	0.98	0.15	109,109,109,109	0
6	ZN	B	202	1/1	0.98	0.23	82,82,82,82	0
6	ZN	D	203	1/1	0.98	0.17	103,103,103,103	0
6	ZN	B	201	1/1	0.99	0.19	93,93,93,93	0
6	ZN	D	201	1/1	0.99	0.23	103,103,103,103	0

6.5 Other polymers (i)

There are no such residues in this entry.