



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:04 AM GMT

PDB ID : 2FFL
Title : Crystal Structure of Dicer from Giardia intestinalis
Authors : Doudna, J.A.; MacRae, I.J.; Adams, P.D.
Deposited on : 2005-12-19
Resolution : 3.33 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

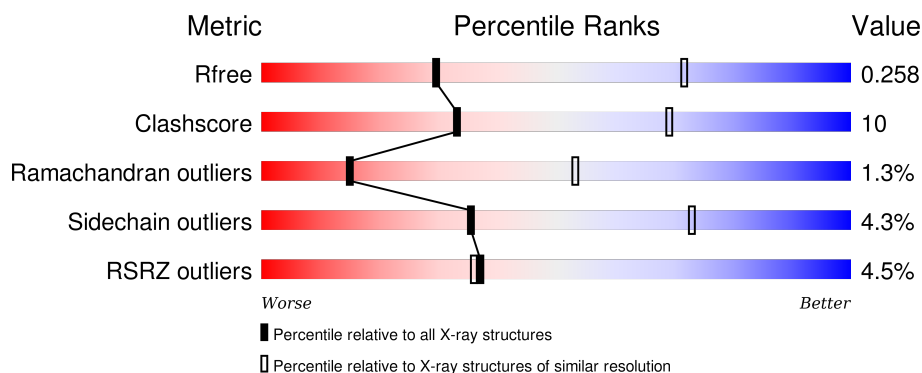
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.33 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	1004 (3.40-3.28)
Clashscore	102246	1072 (3.40-3.28)
Ramachandran outliers	100387	1055 (3.40-3.28)
Sidechain outliers	100360	1054 (3.40-3.28)
RSRZ outliers	91569	1009 (3.40-3.28)

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	756	<div> <div></div> <div>71%23%••</div> </div>
1	B	756	<div> <div>3%</div> <div>72%22%••</div> </div>
1	C	756	<div> <div>7%</div> <div>74%20%•5%</div> </div>
1	D	756	<div> <div>6%</div> <div>70%23%•5%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MN	A	5034	-	-	-	X
2	MN	C	5032	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22426 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 Dicer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	732	Total	C	N	O	S	0	0	0
			5630	3614	957	1029	30			
1	B	726	Total	C	N	O	S	0	0	0
			5590	3589	950	1021	30			
1	C	718	Total	C	N	O	S	0	0	0
			5539	3560	941	1008	30			
1	D	720	Total	C	N	O	S	0	0	0
			5574	3586	942	1016	30			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	GB 71078474
A	0	ALA	-	CLONING ARTIFACT	GB 71078474
B	-1	GLY	-	CLONING ARTIFACT	GB 71078474
B	0	ALA	-	CLONING ARTIFACT	GB 71078474
C	-1	GLY	-	CLONING ARTIFACT	GB 71078474
C	0	ALA	-	CLONING ARTIFACT	GB 71078474
D	-1	GLY	-	CLONING ARTIFACT	GB 71078474
D	0	ALA	-	CLONING ARTIFACT	GB 71078474

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	9	Total	Mn	0	0
			9	9		
2	A	12	Total	Mn	0	0
			12	12		
2	D	8	Total	Mn	0	0
			8	8		
2	C	10	Total	Mn	0	0
			10	10		

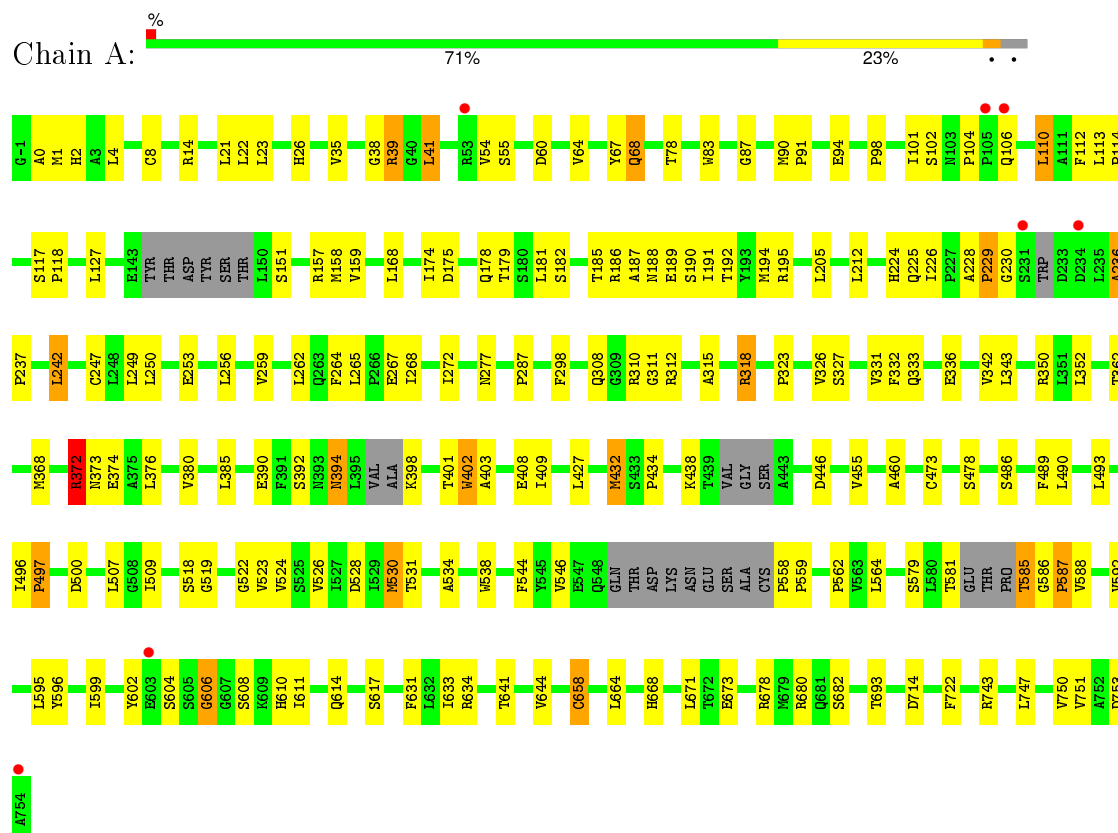
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	21	Total	O	0	0
			21	21		
3	C	7	Total	O	0	0
			7	7		
3	D	9	Total	O	0	0
			9	9		

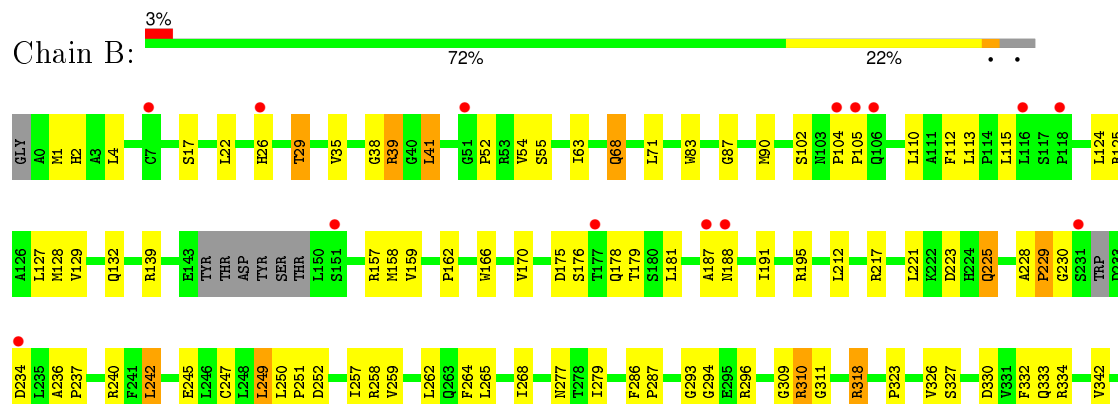
3 Residue-property plots

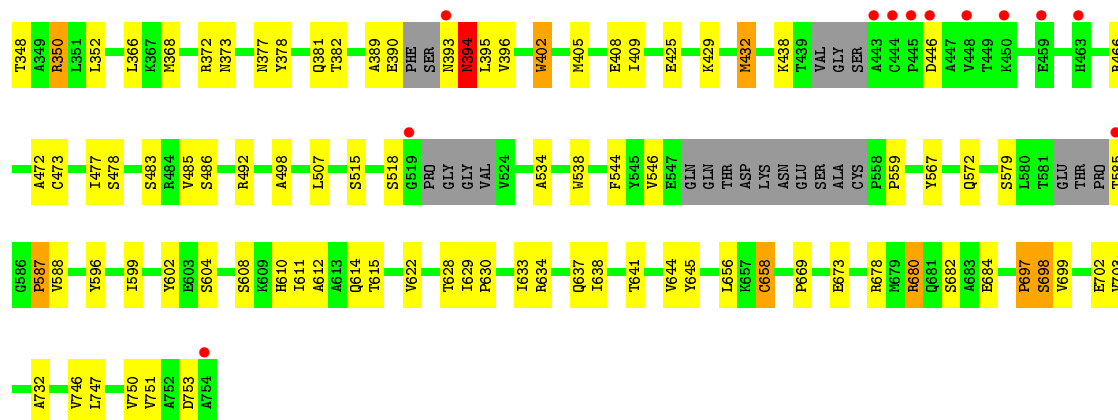
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: Dicer

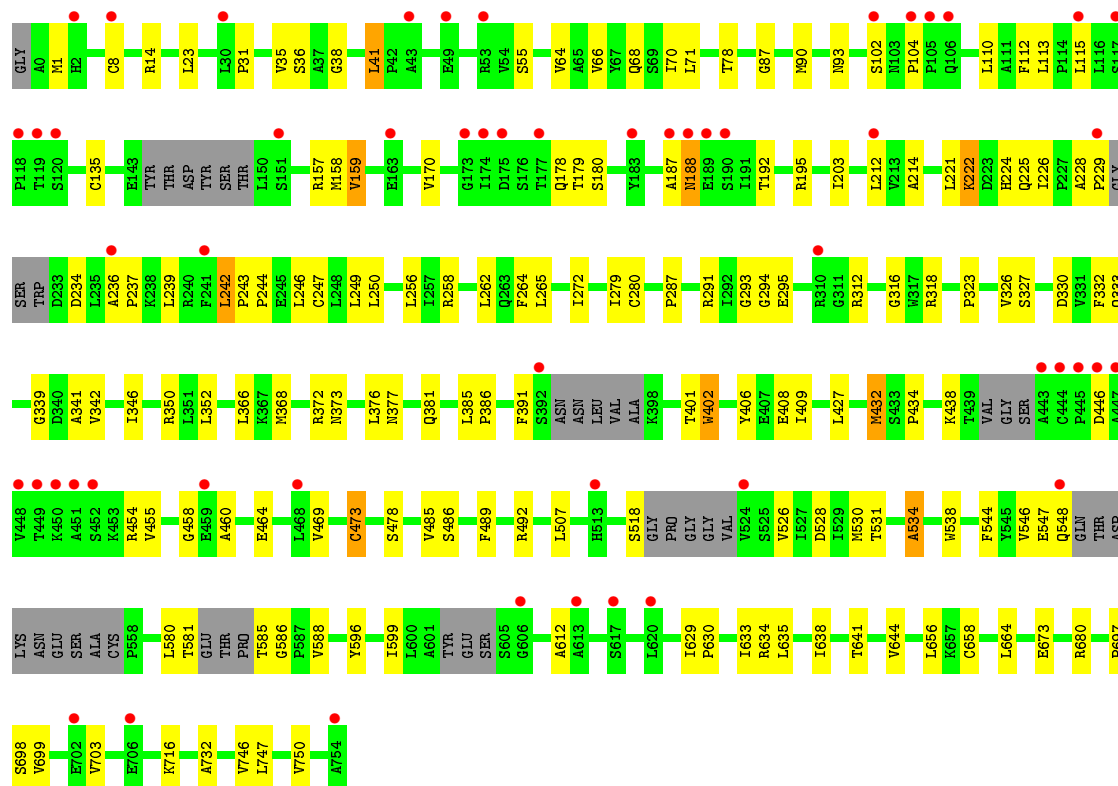
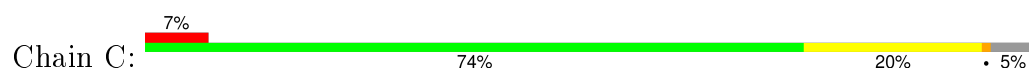


• Molecule 1: Dicer

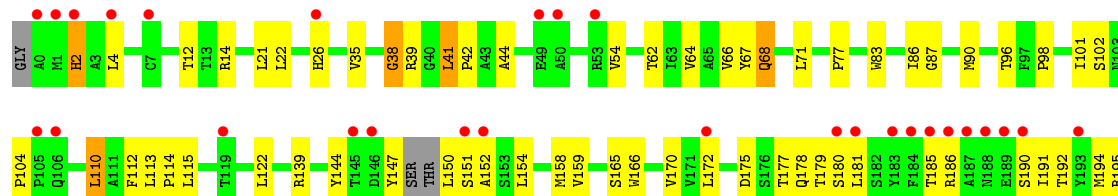


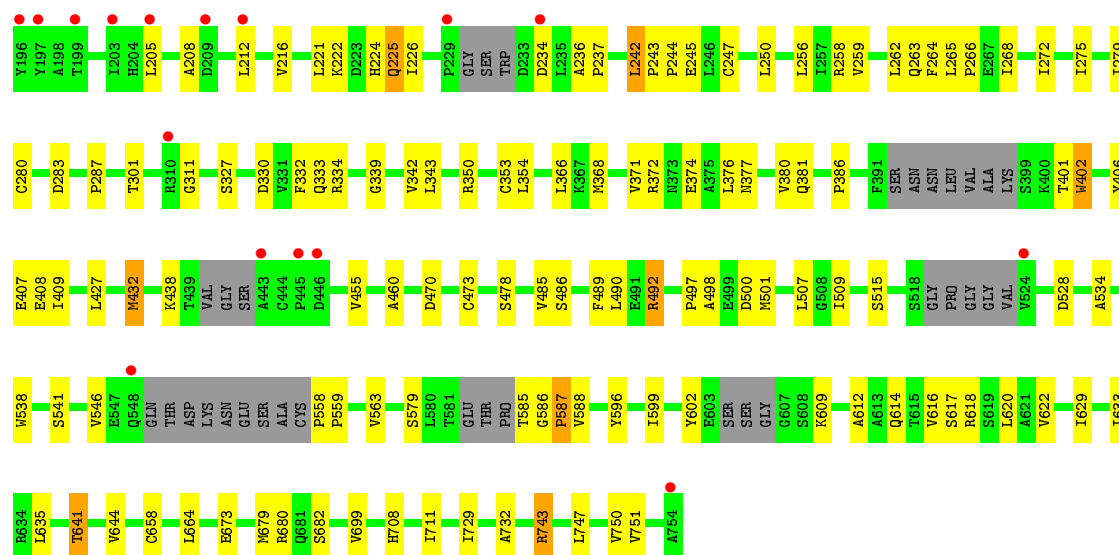


• Molecule 1: Dicer



• Molecule 1: Dicer





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	155.51Å 174.10Å 152.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.33 49.68 – 3.33	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-3.33) 98.6 (49.68-3.33)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.243 , 0.275 0.221 , 0.258	Depositor DCC
R_{free} test set	2991 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.0	EDS
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 60689 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22426	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/5761	0.59	1/7836 (0.0%)
1	B	0.48	0/5718	0.60	1/7777 (0.0%)
1	C	0.42	0/5666	0.55	1/7704 (0.0%)
1	D	0.44	0/5704	0.56	1/7759 (0.0%)
All	All	0.46	0/22849	0.58	4/31076 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	LEU	CA-CB-CG	5.36	127.62	115.30
1	C	242	LEU	CA-CB-CG	5.24	127.34	115.30
1	B	242	LEU	CA-CB-CG	5.09	127.01	115.30
1	D	38	GLY	N-CA-C	5.03	125.69	113.10

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	5630	0	5674	130	0
1	B	5590	0	5640	121	1
1	C	5539	0	5592	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	5574	0	5611	123	1
2	A	12	0	0	0	0
2	B	9	0	0	0	0
2	C	10	0	0	0	0
2	D	8	0	0	0	0
3	A	17	0	0	1	0
3	B	21	0	0	0	0
3	C	7	0	0	0	0
3	D	9	0	0	0	0
All	All	22426	0	22517	462	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 10.

All (462) 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:C:455:VAL:HA	1:C:460:ALA:HB2	1.37	1.03
1:A:38:GLY:HA3	1:A:41:LEU:HD12	1.48	0.96
1:D:342:VAL:HG12	1:D:658:CYS:SG	2.09	0.92
1:C:432:MET:CE	1:C:538:TRP:HB2	2.04	0.88
1:D:38:GLY:HA3	1:D:41:LEU:HD12	1.57	0.87
1:B:38:GLY:HA3	1:B:41:LEU:HD12	1.57	0.84
1:B:1:MET:HG3	1:B:55:SER:HB2	1.56	0.84
1:C:747:LEU:O	1:C:750:VAL:HG12	1.81	0.81
1:A:159:VAL:HG21	1:A:247:CYS:HB3	1.63	0.81
1:D:226:ILE:HD11	1:D:256:LEU:HD22	1.64	0.80
1:C:115:LEU:H	1:C:258:ARG:HH22	1.28	0.79
1:A:368:MET:O	1:A:372:ARG:HB2	1.83	0.79
1:D:144:TYR:CE2	1:D:244:PRO:HB3	2.17	0.79
1:B:113:LEU:HD22	1:B:127:LEU:HD11	1.64	0.78
1:A:91:PRO:HG2	1:A:94:GLU:HG3	1.64	0.78
1:D:368:MET:O	1:D:372:ARG:HB2	1.83	0.78
1:B:368:MET:O	1:B:372:ARG:HB2	1.84	0.77
1:C:432:MET:HE3	1:C:538:TRP:HB2	1.67	0.75
1:B:393:ASN:O	1:B:394:ASN:HB3	1.86	0.75
1:A:228:ALA:HB1	1:A:229:PRO:HD2	1.68	0.75
1:A:68:GLN:HE21	1:A:83:TRP:HE1	1.32	0.74
1:D:455:VAL:HA	1:D:460:ALA:HB2	1.68	0.74
1:D:68:GLN:HE21	1:D:83:TRP:HE1	1.36	0.73
1:C:656:LEU:HD11	1:C:746:VAL:HG11	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:GLN:HG2	1:C:673:GLU:HB2	1.70	0.73
1:A:226:ILE:HD11	1:A:256:LEU:HD22	1.69	0.72
1:C:287:PRO:HG2	1:C:409:ILE:HD13	1.71	0.72
1:B:381:GLN:HE21	1:B:402:TRP:HD1	1.37	0.72
1:C:368:MET:O	1:C:372:ARG:HB2	1.90	0.71
1:B:287:PRO:HG2	1:B:409:ILE:HD13	1.72	0.71
1:A:310:ARG:HH11	1:A:310:ARG:HB2	1.54	0.71
1:D:432:MET:HE2	1:D:534:ALA:HB1	1.73	0.71
1:A:64:VAL:HG13	1:A:113:LEU:HD21	1.70	0.71
1:B:228:ALA:HB1	1:B:229:PRO:HD2	1.71	0.71
1:B:326:VAL:HG12	1:B:330:ASP:HB2	1.73	0.71
1:A:581:THR:H	1:A:585:THR:HG23	1.55	0.70
1:A:401:THR:HG22	1:A:403:ALA:H	1.56	0.70
1:A:432:MET:CE	1:A:538:TRP:HB2	2.21	0.70
1:D:104:PRO:HB3	1:D:280:CYS:SG	2.32	0.70
1:C:434:PRO:HD3	1:C:531:THR:HG21	1.74	0.70
1:D:185:THR:HG22	1:D:190:SER:HB3	1.72	0.69
1:B:333:GLN:HG2	1:B:673:GLU:HB2	1.74	0.69
1:D:747:LEU:O	1:D:750:VAL:HG12	1.92	0.69
1:D:42:PRO:HB3	1:D:222:LYS:O	1.92	0.69
1:A:287:PRO:HG2	1:A:409:ILE:HD13	1.73	0.69
1:B:38:GLY:HA3	1:B:41:LEU:O	1.93	0.68
1:D:159:VAL:HG21	1:D:247:CYS:HB3	1.76	0.68
1:D:178:GLN:HG3	1:D:212:LEU:HD12	1.75	0.68
1:B:175:ASP:OD2	1:B:178:GLN:HG2	1.94	0.68
1:C:432:MET:HE1	1:C:538:TRP:HB2	1.75	0.67
1:A:35:VAL:HG21	1:A:264:PHE:CE2	2.30	0.67
1:A:606:GLY:HA2	1:A:610:HIS:HB2	1.74	0.67
1:A:432:MET:HE2	1:A:534:ALA:HB1	1.76	0.66
1:B:139:ARG:NH2	1:B:162:PRO:HG2	2.11	0.66
1:A:21:LEU:HD21	1:A:272:ILE:HD11	1.75	0.66
1:C:104:PRO:HB3	1:C:280:CYS:SG	2.35	0.66
1:D:144:TYR:HE2	1:D:244:PRO:HB3	1.59	0.66
1:C:38:GLY:HA3	1:C:41:LEU:HD12	1.76	0.66
1:D:170:VAL:HG11	1:D:221:LEU:HD22	1.78	0.66
1:C:68:GLN:NE2	1:C:112:PHE:H	1.94	0.66
1:A:68:GLN:NE2	1:A:112:PHE:H	1.95	0.65
1:B:604:SER:HB3	1:B:637:GLN:HE22	1.62	0.65
1:D:558:PRO:N	1:D:602:TYR:HH	1.94	0.65
1:D:682:SER:HB2	1:D:751:VAL:HG12	1.79	0.64
1:A:310:ARG:NH1	1:A:310:ARG:HB2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ARG:HD3	1:C:538:TRP:O	1.97	0.64
1:B:507:LEU:HD22	1:B:588:VAL:HG21	1.79	0.63
1:A:102:SER:O	1:A:104:PRO:HD3	1.98	0.63
1:D:629:ILE:O	1:D:633:ILE:HG12	1.99	0.63
1:A:373:ASN:HD21	1:A:401:THR:HG21	1.64	0.63
1:B:39:ARG:HD3	1:B:39:ARG:H	1.64	0.62
1:A:68:GLN:HE22	1:A:112:PHE:H	1.45	0.62
1:C:327:SER:HB3	1:C:330:ASP:OD2	1.99	0.62
1:A:157:ARG:HH21	1:A:249:LEU:HD21	1.64	0.62
1:D:67:TYR:OH	1:D:114:PRO:HG3	1.99	0.62
1:D:332:PHE:CD1	1:D:408:GLU:HG3	2.35	0.62
1:A:159:VAL:CG2	1:A:247:CYS:HB3	2.29	0.62
1:C:342:VAL:HG12	1:C:658:CYS:SG	2.40	0.62
1:B:342:VAL:HG12	1:B:658:CYS:SG	2.40	0.61
1:B:747:LEU:O	1:B:747:LEU:HD23	2.01	0.61
1:A:432:MET:HE1	1:A:538:TRP:HB2	1.81	0.61
1:D:150:LEU:HG	1:D:154:LEU:HG	1.82	0.61
1:A:523:VAL:HG11	1:D:618:ARG:HB2	1.83	0.60
1:B:191:ILE:HG22	1:B:195:ARG:HB3	1.82	0.60
1:B:178:GLN:HG3	1:B:212:LEU:HD12	1.82	0.60
1:B:68:GLN:HE22	1:B:112:PHE:H	1.49	0.60
1:B:191:ILE:HG23	1:B:195:ARG:HD3	1.84	0.60
1:B:102:SER:O	1:B:104:PRO:HD3	2.02	0.60
1:A:606:GLY:HA2	1:A:610:HIS:CB	2.31	0.60
1:A:87:GLY:O	1:A:90:MET:HG3	2.01	0.59
1:D:287:PRO:HG2	1:D:409:ILE:HD13	1.84	0.59
1:D:354:LEU:O	1:D:492:ARG:HD3	2.03	0.59
1:A:390:GLU:HA	1:A:390:GLU:OE1	2.00	0.59
1:D:35:VAL:HG21	1:D:264:PHE:CD2	2.38	0.59
1:A:14:ARG:NH2	1:A:224:HIS:O	2.35	0.59
1:A:179:THR:HG22	1:A:181:LEU:H	1.67	0.59
1:A:310:ARG:NH2	1:A:392:SER:HB3	2.18	0.59
1:D:507:LEU:HD22	1:D:588:VAL:HG21	1.84	0.59
1:B:425:GLU:HG2	1:B:429:LYS:HE3	1.84	0.59
1:C:546:VAL:HB	1:C:644:VAL:HG13	1.85	0.59
1:C:352:LEU:O	1:C:544:PHE:HB3	2.03	0.59
1:B:170:VAL:HG11	1:B:221:LEU:HD22	1.85	0.59
1:C:612:ALA:HB2	1:C:703:VAL:HG21	1.85	0.59
1:D:158:MET:HB3	1:D:250:LEU:HD12	1.85	0.58
1:C:455:VAL:HA	1:C:460:ALA:CB	2.25	0.58
1:D:596:TYR:O	1:D:599:ILE:HG22	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:TYR:O	1:A:634:ARG:NH1	2.36	0.58
1:D:432:MET:CE	1:D:538:TRP:HB2	2.34	0.58
1:C:236:ALA:N	1:C:237:PRO:HD2	2.17	0.58
1:D:609:LYS:HZ2	1:D:641:THR:HB	1.68	0.58
1:D:102:SER:O	1:D:104:PRO:HD3	2.04	0.58
1:B:602:TYR:O	1:B:634:ARG:NH1	2.37	0.58
1:A:60:ASP:OD2	3:A:5051:HOH:O	2.17	0.58
1:B:35:VAL:HG21	1:B:264:PHE:CE2	2.40	0.57
1:A:4:LEU:HD21	1:A:26:HIS:ND1	2.20	0.57
1:A:668:HIS:HB3	1:A:671:LEU:HG	1.86	0.57
1:A:333:GLN:HG2	1:A:673:GLU:HB2	1.86	0.57
1:D:343:LEU:HD13	1:D:427:LEU:HD21	1.85	0.57
1:D:455:VAL:CA	1:D:460:ALA:HB2	2.35	0.57
1:D:159:VAL:CG2	1:D:247:CYS:HB3	2.35	0.57
1:C:71:LEU:HD22	1:C:262:LEU:HD13	1.87	0.57
1:B:395:LEU:HD21	1:B:402:TRP:HB2	1.87	0.57
1:B:366:LEU:HD22	1:B:485:VAL:HG22	1.86	0.57
1:B:394:ASN:OD1	1:B:396:VAL:HG12	2.05	0.56
1:B:638:ILE:HG23	1:B:644:VAL:HG12	1.86	0.56
1:C:64:VAL:HG13	1:C:113:LEU:HD21	1.85	0.56
1:D:35:VAL:HG21	1:D:264:PHE:CE2	2.41	0.56
1:A:526:VAL:O	1:A:530:MET:HB2	2.05	0.56
1:B:373:ASN:O	1:B:377:ASN:HB2	2.06	0.56
1:A:519:GLY:HA3	1:D:699:VAL:HG22	1.87	0.56
1:B:279:ILE:CD1	1:B:293:GLY:HA2	2.35	0.56
1:B:68:GLN:NE2	1:B:112:PHE:H	2.03	0.56
1:B:381:GLN:NE2	1:B:402:TRP:HD1	2.03	0.56
1:A:350:ARG:HD3	1:A:538:TRP:O	2.05	0.56
1:D:147:TYR:CG	1:D:150:LEU:HB2	2.40	0.56
1:B:567:TYR:HA	1:B:572:GLN:HE22	1.70	0.56
1:B:159:VAL:HG21	1:B:247:CYS:HB3	1.88	0.55
1:A:432:MET:HE3	1:A:538:TRP:HB2	1.88	0.55
1:A:158:MET:HB3	1:A:250:LEU:HD12	1.88	0.55
1:D:333:GLN:HG2	1:D:673:GLU:HB2	1.87	0.55
1:A:35:VAL:HG21	1:A:264:PHE:CD2	2.41	0.55
1:C:102:SER:O	1:C:104:PRO:HD3	2.06	0.55
1:A:39:ARG:H	1:A:39:ARG:CD	2.20	0.55
1:C:179:THR:HG22	1:C:180:SER:N	2.21	0.55
1:B:604:SER:CB	1:B:637:GLN:HE22	2.20	0.54
1:A:546:VAL:HB	1:A:644:VAL:HG13	1.88	0.54
1:D:236:ALA:N	1:D:237:PRO:CD	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:MET:HB3	1:B:250:LEU:HD12	1.90	0.54
1:D:115:LEU:H	1:D:258:ARG:HH22	1.56	0.54
1:C:332:PHE:CD1	1:C:408:GLU:HG3	2.43	0.54
1:B:682:SER:HB2	1:B:751:VAL:HG12	1.88	0.54
1:D:21:LEU:HD21	1:D:272:ILE:HD11	1.90	0.53
1:D:350:ARG:HD3	1:D:538:TRP:O	2.08	0.53
1:B:432:MET:HE1	1:B:534:ALA:O	2.08	0.53
1:C:170:VAL:HG11	1:C:221:LEU:HD22	1.91	0.53
1:D:614:GLN:O	1:D:617:SER:HB3	2.08	0.53
1:B:402:TRP:HA	1:B:402:TRP:CE3	2.44	0.53
1:C:68:GLN:HE22	1:C:112:PHE:H	1.55	0.53
1:D:587:PRO:HD2	1:D:588:VAL:H	1.73	0.53
1:D:265:LEU:HD23	1:D:268:ILE:HD12	1.91	0.53
1:A:682:SER:HB2	1:A:751:VAL:HG12	1.90	0.53
1:A:39:ARG:H	1:A:39:ARG:HD3	1.74	0.53
1:A:102:SER:H	1:A:277:ASN:HD21	1.57	0.53
1:A:402:TRP:CE3	1:A:402:TRP:HA	2.44	0.53
1:B:587:PRO:HD2	1:B:588:VAL:H	1.73	0.53
1:B:236:ALA:N	1:B:237:PRO:HD2	2.24	0.53
1:B:236:ALA:N	1:B:237:PRO:CD	2.72	0.53
1:D:478:SER:HB2	1:D:486:SER:OG	2.09	0.52
1:B:432:MET:CE	1:B:538:TRP:HB2	2.40	0.52
1:B:596:TYR:O	1:B:599:ILE:HG22	2.09	0.52
1:A:228:ALA:O	1:A:230:GLY:N	2.43	0.52
1:D:172:LEU:HD11	1:D:216:VAL:HG23	1.92	0.52
1:C:469:VAL:O	1:C:473:CYS:HB2	2.09	0.52
1:B:432:MET:HE2	1:B:534:ALA:HB1	1.91	0.51
1:C:236:ALA:N	1:C:237:PRO:CD	2.72	0.51
1:D:87:GLY:O	1:D:90:MET:HG3	2.11	0.51
1:D:498:ALA:HA	1:D:501:MET:HG3	1.91	0.51
1:C:630:PRO:O	1:C:634:ARG:HG2	2.10	0.51
1:B:90:MET:HE1	1:B:318:ARG:HH22	1.75	0.51
1:D:432:MET:HE1	1:D:538:TRP:HB2	1.92	0.51
1:D:139:ARG:HG2	1:D:245:GLU:O	2.10	0.51
1:D:339:GLY:HA3	1:D:407:GLU:O	2.10	0.51
1:B:330:ASP:O	1:B:334:ARG:HG2	2.11	0.51
1:C:226:ILE:HD11	1:C:256:LEU:HD22	1.92	0.51
1:A:1:MET:HG3	1:A:55:SER:HB2	1.93	0.51
1:A:104:PRO:HB2	1:A:106:GLN:O	2.10	0.51
1:B:697:PRO:O	1:B:699:VAL:N	2.44	0.51
1:B:124:LEU:HD23	1:B:127:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ARG:HD3	1:B:538:TRP:O	2.10	0.50
1:C:547:GLU:HG2	1:C:548:GLN:H	1.76	0.50
1:B:4:LEU:HD21	1:B:26:HIS:ND1	2.26	0.50
1:D:455:VAL:HA	1:D:460:ALA:CB	2.38	0.50
1:D:185:THR:HG22	1:D:190:SER:CB	2.41	0.50
1:A:376:LEU:O	1:A:380:VAL:HG23	2.11	0.50
1:C:664:LEU:HD12	1:C:680:ARG:HB3	1.93	0.50
1:B:332:PHE:CD1	1:B:408:GLU:HG3	2.47	0.50
1:B:747:LEU:O	1:B:750:VAL:HG12	2.11	0.50
1:D:259:VAL:O	1:D:262:LEU:HB3	2.11	0.50
1:C:115:LEU:H	1:C:258:ARG:NH2	2.04	0.50
1:B:396:VAL:O	1:B:396:VAL:HG13	2.11	0.50
1:A:191:ILE:HG23	1:A:195:ARG:HD3	1.94	0.50
1:B:393:ASN:N	1:B:402:TRP:HZ2	2.10	0.50
1:B:610:HIS:CD2	1:B:614:GLN:HE21	2.30	0.50
1:D:609:LYS:HZ2	1:D:641:THR:CG2	2.24	0.50
1:D:192:THR:OG1	1:D:195:ARG:HB2	2.12	0.50
1:D:682:SER:HB2	1:D:751:VAL:CG1	2.42	0.49
1:B:39:ARG:H	1:B:39:ARG:CD	2.24	0.49
1:B:629:ILE:O	1:B:633:ILE:HG12	2.12	0.49
1:B:381:GLN:NE2	1:B:402:TRP:CD1	2.80	0.49
1:B:682:SER:CB	1:B:751:VAL:HG12	2.43	0.49
1:C:23:LEU:HD21	1:C:272:ILE:HD13	1.93	0.49
1:C:35:VAL:HG21	1:C:264:PHE:CE2	2.47	0.49
1:D:98:PRO:HA	1:D:101:ILE:HD11	1.95	0.49
1:A:4:LEU:HD21	1:A:26:HIS:CE1	2.47	0.49
1:A:599:ILE:HG21	1:A:631:PHE:CE1	2.48	0.49
1:A:113:LEU:HD22	1:A:127:LEU:HD11	1.93	0.49
1:A:194:MET:HA	1:A:205:LEU:HD12	1.95	0.49
1:A:22:LEU:O	1:A:110:LEU:HA	2.13	0.49
1:A:398:LYS:O	1:B:395:LEU:HD12	2.12	0.49
1:C:192:THR:OG1	1:C:195:ARG:HB2	2.12	0.49
1:A:374:GLU:CD	1:A:374:GLU:H	2.15	0.49
1:D:71:LEU:HD22	1:D:262:LEU:HD13	1.94	0.49
1:D:14:ARG:NH2	1:D:224:HIS:O	2.45	0.49
1:D:179:THR:HG22	1:D:181:LEU:H	1.77	0.49
1:D:546:VAL:HB	1:D:644:VAL:HG13	1.94	0.49
1:B:228:ALA:O	1:B:230:GLY:N	2.46	0.49
1:D:191:ILE:HG23	1:D:195:ARG:HD3	1.95	0.49
1:D:96:THR:HG21	1:D:301:THR:HG23	1.95	0.49
1:B:352:LEU:O	1:B:544:PHE:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:ASP:O	1:D:334:ARG:HG2	2.13	0.49
1:C:31:PRO:HD3	1:C:294:GLY:CA	2.43	0.49
1:A:23:LEU:HD21	1:A:272:ILE:HD13	1.95	0.48
1:A:189:GLU:OE2	1:A:191:ILE:HD11	2.13	0.48
1:A:175:ASP:OD2	1:A:178:GLN:HG2	2.14	0.48
1:C:638:ILE:HG23	1:C:644:VAL:CG1	2.43	0.48
1:A:315:ALA:O	1:A:318:ARG:HG3	2.14	0.48
1:B:279:ILE:HD11	1:B:293:GLY:HA2	1.96	0.48
1:A:8:CYS:SG	1:A:268:ILE:HD13	2.54	0.48
1:B:478:SER:HA	1:B:486:SER:HB3	1.96	0.48
1:C:635:LEU:HD12	1:C:732:ALA:HB2	1.95	0.48
1:B:432:MET:HE3	1:B:538:TRP:HB2	1.95	0.48
1:B:697:PRO:C	1:B:699:VAL:H	2.17	0.48
1:C:159:VAL:HG21	1:C:247:CYS:HB3	1.95	0.48
1:A:747:LEU:HD23	1:A:747:LEU:O	2.14	0.48
1:B:68:GLN:HE21	1:B:83:TRP:HE1	1.61	0.47
1:B:546:VAL:HB	1:B:644:VAL:HG13	1.96	0.47
1:A:608:SER:HA	1:A:611:ILE:HD12	1.96	0.47
1:A:581:THR:H	1:A:585:THR:CG2	2.25	0.47
1:B:389:ALA:O	1:B:390:GLU:HB2	2.13	0.47
1:C:112:PHE:CD1	1:C:265:LEU:HD22	2.50	0.47
1:D:158:MET:HG3	1:D:259:VAL:HG21	1.95	0.47
1:B:559:PRO:HG2	1:B:599:ILE:HG13	1.95	0.47
1:D:113:LEU:HD13	1:D:122:LEU:CD1	2.45	0.47
1:C:90:MET:CE	1:C:318:ARG:HH22	2.28	0.47
1:A:587:PRO:HD2	1:A:588:VAL:H	1.78	0.47
1:A:599:ILE:HG21	1:A:631:PHE:HE1	1.79	0.47
1:C:455:VAL:CA	1:C:460:ALA:HB2	2.27	0.47
1:D:68:GLN:NE2	1:D:112:PHE:H	2.13	0.47
1:C:638:ILE:HG23	1:C:644:VAL:HG12	1.97	0.47
1:A:434:PRO:HD3	1:A:531:THR:HG21	1.97	0.47
1:B:378:TYR:O	1:B:382:THR:HG23	2.15	0.47
1:B:225:GLN:CD	1:B:225:GLN:H	2.18	0.47
1:B:432:MET:HE1	1:B:534:ALA:C	2.35	0.47
1:A:98:PRO:HA	1:A:101:ILE:HD11	1.97	0.47
1:A:178:GLN:HG3	1:A:212:LEU:HD12	1.97	0.47
1:A:186:ARG:O	1:A:187:ALA:C	2.54	0.47
1:D:402:TRP:CE3	1:D:402:TRP:HA	2.49	0.46
1:C:279:ILE:CD1	1:C:293:GLY:HA2	2.45	0.46
1:D:64:VAL:HG13	1:D:113:LEU:HD21	1.97	0.46
1:C:373:ASN:HD21	1:C:401:THR:HG21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ARG:HH21	1:B:249:LEU:HD21	1.80	0.46
1:C:366:LEU:HD22	1:C:485:VAL:HG22	1.96	0.46
1:B:698:SER:O	1:B:702:GLU:HG3	2.16	0.46
1:D:68:GLN:HE22	1:D:112:PHE:H	1.63	0.46
1:B:217:ARG:HD3	1:B:240:ARG:NH1	2.30	0.46
1:B:125:ARG:O	1:B:129:VAL:HG23	2.14	0.46
1:D:165:SER:O	1:D:166:TRP:HB2	2.16	0.46
1:B:656:LEU:HD11	1:B:746:VAL:HG11	1.97	0.46
1:D:620:LEU:HD22	1:D:729:ILE:HD11	1.98	0.46
1:C:489:PHE:CZ	1:C:534:ALA:HA	2.51	0.46
1:A:473:CYS:HA	1:A:490:LEU:HD13	1.98	0.46
1:B:587:PRO:CD	1:B:588:VAL:H	2.29	0.46
1:A:102:SER:N	1:A:277:ASN:HD21	2.13	0.46
1:B:157:ARG:HH12	1:B:252:ASP:HA	1.81	0.46
1:C:596:TYR:O	1:C:599:ILE:HG22	2.16	0.46
1:A:151:SER:HB2	1:A:174:ILE:H	1.80	0.46
1:D:175:ASP:OD2	1:D:177:THR:HB	2.15	0.46
1:B:326:VAL:CG1	1:B:330:ASP:HB2	2.45	0.46
1:A:680:ARG:HG3	1:A:680:ARG:NH1	2.31	0.46
1:C:478:SER:HA	1:C:486:SER:HB3	1.96	0.46
1:B:394:ASN:O	1:B:395:LEU:HB2	2.16	0.46
1:B:87:GLY:O	1:B:90:MET:HG3	2.16	0.46
1:A:372:ARG:HG2	1:A:374:GLU:OE1	2.16	0.45
1:A:310:ARG:O	1:A:312:ARG:HG2	2.16	0.45
1:C:339:GLY:HA2	1:C:342:VAL:HG22	1.97	0.45
1:D:262:LEU:HD12	1:D:265:LEU:HD12	1.98	0.45
1:D:353:CYS:SG	1:D:563:VAL:HG21	2.55	0.45
1:D:371:VAL:O	1:D:371:VAL:HG12	2.17	0.45
1:A:332:PHE:CD1	1:A:408:GLU:HG3	2.51	0.45
1:D:372:ARG:HG2	1:D:374:GLU:OE1	2.17	0.45
1:D:67:TYR:CZ	1:D:114:PRO:HG3	2.52	0.45
1:B:348:THR:O	1:B:352:LEU:HB2	2.16	0.45
1:A:507:LEU:HD22	1:A:588:VAL:HG21	1.98	0.45
1:B:472:ALA:HA	1:B:477:ILE:HD12	1.98	0.45
1:B:680:ARG:NH1	1:B:684:GLU:OE1	2.49	0.45
1:D:380:VAL:HG12	1:D:386:PRO:HD3	1.98	0.45
1:D:21:LEU:HD13	1:D:112:PHE:CE1	2.52	0.45
1:B:405:MET:O	1:B:409:ILE:HG13	2.16	0.45
1:B:191:ILE:CG2	1:B:195:ARG:HB3	2.46	0.45
1:C:243:PRO:HA	1:C:244:PRO:HD3	1.81	0.45
1:A:385:LEU:HD11	1:A:409:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:ARG:NH2	1:B:753:ASP:OD1	2.44	0.45
1:C:291:ARG:HD3	1:C:295:GLU:HB3	1.99	0.45
1:A:682:SER:CB	1:A:751:VAL:HG12	2.47	0.45
1:D:473:CYS:HA	1:D:490:LEU:HD13	1.98	0.45
1:A:509:ILE:HD11	1:A:522:GLY:N	2.32	0.45
1:D:366:LEU:HD22	1:D:485:VAL:HG22	1.98	0.45
1:C:323:PRO:O	1:C:326:VAL:HG23	2.16	0.45
1:C:158:MET:HB3	1:C:250:LEU:HD12	1.99	0.45
1:A:496:ILE:HA	1:A:497:PRO:HD2	1.70	0.45
1:A:236:ALA:N	1:A:237:PRO:CD	2.80	0.45
1:C:458:GLY:C	1:C:460:ALA:H	2.19	0.44
1:A:39:ARG:HH22	1:A:267:GLU:CD	2.20	0.44
1:A:617:SER:HB2	1:A:633:ILE:HD13	1.99	0.44
1:B:38:GLY:CA	1:B:41:LEU:HD12	2.39	0.44
1:C:368:MET:HG3	1:D:368:MET:HG3	1.98	0.44
1:B:608:SER:HA	1:B:611:ILE:HD12	2.00	0.44
1:D:62:THR:O	1:D:66:VAL:HG23	2.17	0.44
1:C:402:TRP:HA	1:C:402:TRP:CE3	2.52	0.44
1:A:562:PRO:HB3	1:A:595:LEU:HB2	1.99	0.44
1:D:612:ALA:O	1:D:616:VAL:HG23	2.18	0.44
1:C:385:LEU:N	1:C:386:PRO:CD	2.81	0.44
1:B:38:GLY:CA	1:B:41:LEU:O	2.65	0.44
1:B:630:PRO:O	1:B:634:ARG:HG2	2.17	0.44
1:A:191:ILE:HG22	1:A:192:THR:N	2.33	0.44
1:C:90:MET:HE3	1:C:318:ARG:HH22	1.82	0.44
1:B:323:PRO:O	1:B:326:VAL:HG23	2.18	0.44
1:D:478:SER:HA	1:D:486:SER:HB3	1.99	0.44
1:C:381:GLN:NE2	1:C:402:TRP:HD1	2.14	0.44
1:A:455:VAL:HA	1:A:460:ALA:CB	2.48	0.44
1:B:286:PHE:O	1:B:296:ARG:NH2	2.44	0.44
1:D:225:GLN:H	1:D:225:GLN:CD	2.20	0.44
1:D:279:ILE:O	1:D:283:ASP:HB2	2.17	0.44
1:D:191:ILE:HG22	1:D:192:THR:O	2.18	0.44
1:A:185:THR:HG22	1:A:190:SER:HB3	1.98	0.44
1:C:178:GLN:HG3	1:C:212:LEU:HD12	1.99	0.44
1:A:478:SER:HA	1:A:486:SER:HB3	1.99	0.44
1:B:29:THR:O	1:B:294:GLY:HA3	2.18	0.44
1:B:115:LEU:H	1:B:258:ARG:HH22	1.66	0.44
1:B:162:PRO:HB3	1:B:166:TRP:CE2	2.53	0.44
1:A:497:PRO:HG2	1:A:500:ASP:OD2	2.18	0.44
1:C:346:ILE:HG21	1:C:427:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ARG:NH2	1:C:224:HIS:O	2.50	0.43
1:A:310:ARG:CB	1:A:310:ARG:HH11	2.28	0.43
1:D:150:LEU:C	1:D:152:ALA:H	2.21	0.43
1:C:203:ILE:HG21	1:C:246:LEU:HD21	2.00	0.43
1:A:564:LEU:HB3	1:A:592:VAL:HG11	1.99	0.43
1:C:1:MET:HG3	1:C:55:SER:HB2	2.00	0.43
1:D:743:ARG:HA	1:D:747:LEU:HB2	1.99	0.43
1:A:308:GLN:H	1:A:308:GLN:HG2	1.70	0.43
1:B:129:VAL:O	1:B:132:GLN:HB2	2.18	0.43
1:A:664:LEU:CD1	1:A:680:ARG:HB3	2.48	0.43
1:C:228:ALA:HB1	1:C:229:PRO:HD2	2.00	0.43
1:D:489:PHE:CZ	1:D:534:ALA:HA	2.54	0.43
1:A:747:LEU:O	1:A:750:VAL:HG12	2.19	0.43
1:A:352:LEU:O	1:A:544:PHE:HB3	2.19	0.43
1:D:243:PRO:HA	1:D:244:PRO:HD3	1.77	0.43
1:C:454:ARG:HE	1:C:464:GLU:HG2	1.83	0.43
1:B:612:ALA:HB2	1:B:703:VAL:HG21	2.00	0.43
1:A:342:VAL:HG12	1:A:658:CYS:SG	2.59	0.43
1:C:580:LEU:O	1:C:581:THR:OG1	2.29	0.43
1:A:489:PHE:CZ	1:A:534:ALA:HA	2.54	0.42
1:C:341:ALA:HB1	1:C:658:CYS:HA	2.00	0.42
1:D:343:LEU:HD13	1:D:427:LEU:CD2	2.49	0.42
1:C:526:VAL:O	1:C:530:MET:HB2	2.19	0.42
1:A:678:ARG:NH2	1:A:753:ASP:OD1	2.34	0.42
1:A:117:SER:HB2	1:A:118:PRO:HD2	2.01	0.42
1:D:376:LEU:HD22	1:D:406:TYR:CD2	2.54	0.42
1:A:664:LEU:HD12	1:A:680:ARG:HB3	2.02	0.42
1:B:187:ALA:O	1:B:188:ASN:HB2	2.20	0.42
1:C:222:LYS:HE2	1:C:222:LYS:HB2	1.64	0.42
1:C:66:VAL:O	1:C:70:ILE:HG12	2.19	0.42
1:D:4:LEU:HD21	1:D:26:HIS:ND1	2.35	0.42
1:C:747:LEU:O	1:C:747:LEU:HD23	2.19	0.42
1:D:113:LEU:HD13	1:D:122:LEU:HD13	2.01	0.42
1:D:194:MET:HG3	1:D:205:LEU:HB2	2.01	0.42
1:B:179:THR:HG22	1:B:181:LEU:H	1.85	0.42
1:A:67:TYR:OH	1:A:114:PRO:HG3	2.18	0.42
1:A:298:PHE:HE2	1:A:331:VAL:HG21	1.84	0.42
1:D:242:LEU:HA	1:D:243:PRO:HD3	1.91	0.42
1:D:609:LYS:HZ2	1:D:641:THR:CB	2.31	0.42
1:D:77:PRO:HD3	1:D:165:SER:O	2.19	0.42
1:C:376:LEU:HD22	1:C:406:TYR:CD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:664:LEU:HD22	1:D:679:MET:HE1	2.01	0.42
1:A:228:ALA:C	1:A:230:GLY:N	2.73	0.42
1:A:392:SER:C	1:A:394:ASN:H	2.23	0.42
1:D:609:LYS:NZ	1:D:641:THR:CG2	2.83	0.42
1:C:664:LEU:CD1	1:C:680:ARG:HB3	2.49	0.42
1:D:12:THR:HG22	1:D:44:ALA:HB2	2.01	0.42
1:D:682:SER:CB	1:D:751:VAL:HG12	2.46	0.42
1:D:147:TYR:CZ	1:D:150:LEU:N	2.88	0.42
1:D:401:THR:HG22	1:D:402:TRP:N	2.34	0.42
1:C:377:ASN:O	1:C:381:GLN:HG2	2.20	0.42
1:D:4:LEU:HD21	1:D:26:HIS:CE1	2.55	0.42
1:C:391:PHE:CE2	1:C:402:TRP:HH2	2.38	0.42
1:A:168:LEU:HD13	1:A:259:VAL:CG1	2.50	0.42
1:D:708:HIS:HB3	1:D:711:ILE:HG21	2.00	0.42
1:B:228:ALA:HB1	1:B:229:PRO:CD	2.46	0.42
1:D:497:PRO:HG2	1:D:500:ASP:OD2	2.20	0.42
1:C:87:GLY:O	1:C:90:MET:HG3	2.20	0.41
1:C:157:ARG:HH21	1:C:249:LEU:HD21	1.84	0.41
1:B:310:ARG:HB2	1:B:310:ARG:HH11	1.84	0.41
1:B:334:ARG:NH2	1:B:669:PRO:HA	2.34	0.41
1:A:179:THR:O	1:A:182:SER:N	2.39	0.41
1:D:664:LEU:HD12	1:D:680:ARG:HB3	2.02	0.41
1:C:187:ALA:O	1:C:188:ASN:HB2	2.20	0.41
1:D:587:PRO:CD	1:D:588:VAL:H	2.33	0.41
1:A:693:THR:OG1	1:A:722:PHE:HB2	2.20	0.41
1:B:63:ILE:HG12	1:B:128:MET:SD	2.61	0.41
1:A:604:SER:C	1:A:606:GLY:H	2.23	0.41
1:B:158:MET:HG3	1:B:259:VAL:HG21	2.00	0.41
1:A:187:ALA:O	1:A:188:ASN:HB2	2.20	0.41
1:A:262:LEU:HD12	1:A:265:LEU:HD12	2.02	0.41
1:A:323:PRO:O	1:A:326:VAL:HG23	2.20	0.41
1:A:402:TRP:HA	1:A:402:TRP:HE3	1.83	0.41
1:A:606:GLY:CA	1:A:610:HIS:CB	2.98	0.41
1:C:31:PRO:HD3	1:C:294:GLY:HA3	2.01	0.41
1:B:17:SER:HB2	1:B:257:ILE:HG22	2.02	0.41
1:B:402:TRP:HE3	1:B:402:TRP:HA	1.85	0.41
1:D:83:TRP:CE3	1:D:86:ILE:HD12	2.56	0.41
1:B:221:LEU:O	1:B:221:LEU:HG	2.21	0.41
1:C:547:GLU:HG2	1:C:548:GLN:N	2.35	0.41
1:C:629:ILE:O	1:C:633:ILE:HG12	2.21	0.41
1:B:628:THR:OG1	1:B:732:ALA:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:THR:HG22	1:A:402:TRP:N	2.35	0.41
1:B:102:SER:H	1:B:277:ASN:HD21	1.69	0.41
1:B:466:ARG:NH1	1:B:498:ALA:CB	2.84	0.41
1:D:272:ILE:HA	1:D:275:ILE:HD12	2.03	0.41
1:D:381:GLN:NE2	1:D:402:TRP:HD1	2.19	0.41
1:A:336:GLU:HA	1:A:408:GLU:HA	2.03	0.41
1:A:455:VAL:HA	1:A:460:ALA:HB2	2.03	0.41
1:C:697:PRO:O	1:C:699:VAL:N	2.54	0.41
1:C:507:LEU:HD22	1:C:588:VAL:HG21	2.02	0.41
1:C:214:ALA:HB1	1:C:239:LEU:HD11	2.01	0.41
1:D:180:SER:HB2	1:D:208:ALA:O	2.21	0.41
1:D:263:GLN:O	1:D:266:PRO:HD2	2.19	0.41
1:A:614:GLN:O	1:A:617:SER:HB3	2.21	0.40
1:A:343:LEU:HD13	1:A:427:LEU:CD2	2.51	0.40
1:A:596:TYR:O	1:A:599:ILE:HG22	2.21	0.40
1:A:680:ARG:HH11	1:A:680:ARG:HG3	1.86	0.40
1:C:312:ARG:HH21	1:C:316:GLY:HA2	1.85	0.40
1:D:635:LEU:HD12	1:D:732:ALA:HB2	2.02	0.40
1:B:645:TYR:C	1:B:645:TYR:CD1	2.94	0.40
1:D:22:LEU:O	1:D:110:LEU:HA	2.22	0.40
1:A:38:GLY:HA3	1:A:41:LEU:O	2.21	0.40
1:A:228:ALA:C	1:A:230:GLY:H	2.25	0.40
1:C:333:GLN:HE21	1:C:673:GLU:HB3	1.86	0.40
1:D:620:LEU:HD22	1:D:729:ILE:CD1	2.52	0.40
1:B:71:LEU:HD22	1:B:262:LEU:HD13	2.03	0.40
1:B:265:LEU:HD23	1:B:268:ILE:HD12	2.02	0.40
1:B:22:LEU:HD22	1:B:54:VAL:HG11	2.04	0.40
1:A:493:LEU:HD23	1:A:493:LEU:HA	1.90	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)
1:B:466:ARG:NH1	1:D:470:ASP:OD2[4_455]	2.07	0.13

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	718/756 (95%)	656 (91%)	50 (7%)	12 (2%)	11	47
1	B	710/756 (94%)	661 (93%)	38 (5%)	11 (2%)	13	50
1	C	700/756 (93%)	644 (92%)	50 (7%)	6 (1%)	21	62
1	D	702/756 (93%)	638 (91%)	55 (8%)	9 (1%)	15	53
All	All	2830/3024 (94%)	2599 (92%)	193 (7%)	38 (1%)	15	53

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	ALA
1	A	54	VAL
1	A	229	PRO
1	A	586	GLY
1	A	606	GLY
1	B	229	PRO
1	B	394	ASN
1	D	54	VAL
1	A	2	HIS
1	B	2	HIS
1	B	309	GLY
1	B	587	PRO
1	B	698	SER
1	C	586	GLY
1	D	2	HIS
1	D	234	ASP
1	D	586	GLY
1	C	234	ASP
1	D	39	ARG
1	A	372	ARG
1	A	559	PRO
1	A	587	PRO

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Mol	Chain	Res	Type
1	C	698	SER
1	D	151	SER
1	D	311	GLY
1	D	587	PRO
1	A	524	VAL
1	B	52	PRO
1	B	223	ASP
1	D	559	PRO
1	A	311	GLY
1	C	93	ASN
1	C	188	ASN
1	C	534	ALA
1	B	251	PRO
1	A	236	ALA
1	B	311	GLY
1	B	105	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	611/632 (97%)	583 (95%)	28 (5%)	33	72
1	B	607/632 (96%)	574 (95%)	33 (5%)	27	66
1	C	602/632 (95%)	581 (96%)	21 (4%)	43	78
1	D	605/632 (96%)	583 (96%)	22 (4%)	42	77
All	All	2425/2528 (96%)	2321 (96%)	104 (4%)	35	73

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	41	LEU
1	A	68	GLN
1	A	78	THR
1	A	110	LEU

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Mol	Chain	Res	Type
1	A	225	GLN
1	A	242	LEU
1	A	253	GLU
1	A	318	ARG
1	A	327	SER
1	A	362	THR
1	A	372	ARG
1	A	394	ASN
1	A	402	TRP
1	A	432	MET
1	A	438	LYS
1	A	446	ASP
1	A	497	PRO
1	A	518	SER
1	A	528	ASP
1	A	530	MET
1	A	558	PRO
1	A	579	SER
1	A	585	THR
1	A	641	THR
1	A	658	CYS
1	A	714	ASP
1	A	743	ARG
1	B	29	THR
1	B	39	ARG
1	B	41	LEU
1	B	68	GLN
1	B	110	LEU
1	B	176	SER
1	B	225	GLN
1	B	234	ASP
1	B	242	LEU
1	B	245	GLU
1	B	249	LEU
1	B	310	ARG
1	B	318	ARG
1	B	327	SER
1	B	350	ARG
1	B	394	ASN
1	B	402	TRP
1	B	432	MET
1	B	438	LYS

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Mol	Chain	Res	Type
1	B	446	ASP
1	B	473	CYS
1	B	483	SER
1	B	492	ARG
1	B	515	SER
1	B	518	SER
1	B	579	SER
1	B	585	THR
1	B	615	THR
1	B	622	VAL
1	B	641	THR
1	B	658	CYS
1	B	680	ARG
1	B	697	PRO
1	C	8	CYS
1	C	36	SER
1	C	41	LEU
1	C	78	THR
1	C	110	LEU
1	C	135	CYS
1	C	159	VAL
1	C	222	LYS
1	C	225	GLN
1	C	242	LEU
1	C	402	TRP
1	C	432	MET
1	C	438	LYS
1	C	446	ASP
1	C	473	CYS
1	C	492	ARG
1	C	518	SER
1	C	528	ASP
1	C	585	THR
1	C	641	THR
1	C	716	LYS
1	D	2	HIS
1	D	41	LEU
1	D	68	GLN
1	D	110	LEU
1	D	186	ARG
1	D	225	GLN
1	D	242	LEU

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Mol	Chain	Res	Type
1	D	327	SER
1	D	377	ASN
1	D	402	TRP
1	D	432	MET
1	D	438	LYS
1	D	492	ARG
1	D	509	ILE
1	D	515	SER
1	D	528	ASP
1	D	541	SER
1	D	579	SER
1	D	585	THR
1	D	622	VAL
1	D	641	THR
1	D	743	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	178	GLN
1	A	202	ASN
1	A	277	ASN
1	A	333	GLN
1	A	373	ASN
1	A	381	GLN
1	A	436	HIS
1	A	548	GLN
1	A	637	GLN
1	B	68	GLN
1	B	178	GLN
1	B	202	ASN
1	B	333	GLN
1	B	373	ASN
1	B	381	GLN
1	B	393	ASN
1	B	436	HIS
1	B	572	GLN
1	B	614	GLN
1	B	637	GLN
1	C	68	GLN
1	C	178	GLN

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Mol	Chain	Res	Type
1	C	333	GLN
1	C	373	ASN
1	C	381	GLN
1	C	436	HIS
1	C	614	GLN
1	C	668	HIS
1	C	708	HIS
1	C	749	GLN
1	D	68	GLN
1	D	333	GLN
1	D	373	ASN
1	D	377	ASN
1	D	381	GLN
1	D	532	HIS
1	D	548	GLN
1	D	572	GLN
1	D	637	GLN
1	D	749	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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 39 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

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	732/756 (96%)	0.02	7 (0%) 84 85	21, 37, 67, 94	1 (0%)
1	B	726/756 (96%)	0.12	26 (3%) 46 45	22, 37, 69, 95	1 (0%)
1	C	718/756 (94%)	0.44	54 (7%) 17 17	20, 38, 69, 94	1 (0%)
1	D	720/756 (95%)	0.31	44 (6%) 25 24	22, 37, 68, 94	1 (0%)
All	All	2896/3024 (95%)	0.22	131 (4%) 37 36	20, 38, 68, 95	4 (0%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	190	SER	6.0
1	C	188	ASN	6.0
1	D	187	ALA	5.4
1	D	185	THR	5.4
1	D	180	SER	5.2
1	D	188	ASN	5.2
1	B	446	ASP	4.6
1	D	189	GLU	4.5
1	D	152	ALA	4.3
1	A	234	ASP	4.2
1	C	448	VAL	4.1
1	C	173	GLY	4.0
1	D	184	PHE	3.9
1	B	443	ALA	3.9
1	A	231	SER	3.9
1	C	446	ASP	3.8
1	C	151	SER	3.6
1	C	445	PRO	3.6
1	D	146	ASP	3.6
1	C	105	PRO	3.6
1	B	177	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	183	TYR	3.5
1	C	447	ALA	3.5
1	D	151	SER	3.5
1	C	189	GLU	3.5
1	C	451	ALA	3.4
1	D	199	THR	3.4
1	B	459	GLU	3.4
1	B	105	PRO	3.4
1	C	212	LEU	3.4
1	D	181	LEU	3.4
1	C	310	ARG	3.3
1	D	229	PRO	3.3
1	B	106	GLN	3.3
1	A	53	ARG	3.2
1	C	450	LYS	3.2
1	D	186	ARG	3.2
1	C	452	SER	3.2
1	D	754	ALA	3.1
1	D	212	LEU	3.1
1	C	102	SER	3.1
1	D	234	ASP	3.0
1	C	187	ALA	3.0
1	B	393	ASN	2.9
1	B	754	ALA	2.9
1	B	234	ASP	2.9
1	C	706	GLU	2.9
1	D	0	ALA	2.9
1	B	463	HIS	2.9
1	B	151	SER	2.9
1	D	203	ILE	2.9
1	C	174	ILE	2.8
1	B	188	ASN	2.8
1	D	548	GLN	2.8
1	C	392	SER	2.8
1	B	118	PRO	2.8
1	C	236	ALA	2.8
1	C	49	GLU	2.8
1	D	26	HIS	2.8
1	C	241	PHE	2.8
1	C	617	SER	2.8
1	C	449	THR	2.8
1	C	443	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	193	TYR	2.7
1	D	7	CYS	2.7
1	C	8	CYS	2.7
1	C	104	PRO	2.6
1	C	444	CYS	2.6
1	D	446	ASP	2.6
1	B	231	SER	2.6
1	C	754	ALA	2.6
1	C	524	VAL	2.6
1	C	183	TYR	2.5
1	D	196	TYR	2.5
1	C	117	SER	2.5
1	C	115	LEU	2.5
1	C	106	GLN	2.5
1	B	51	GLY	2.5
1	D	205	LEU	2.5
1	C	43	ALA	2.4
1	C	613	ALA	2.4
1	C	229	PRO	2.4
1	D	197	TYR	2.4
1	D	172	LEU	2.4
1	B	187	ALA	2.4
1	C	190	SER	2.4
1	D	53	ARG	2.4
1	C	620	LEU	2.4
1	B	519	GLY	2.4
1	B	445	PRO	2.3
1	B	116	LEU	2.3
1	C	177	THR	2.3
1	D	145	THR	2.3
1	D	106	GLN	2.3
1	C	513	HIS	2.3
1	B	444	CYS	2.3
1	C	606	GLY	2.3
1	C	468	LEU	2.3
1	D	209	ASP	2.3
1	C	2	HIS	2.3
1	B	585	THR	2.3
1	A	754	ALA	2.2
1	D	105	PRO	2.2
1	D	443	ALA	2.2
1	D	119	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	105	PRO	2.2
1	C	175	ASP	2.2
1	C	120	SER	2.2
1	B	104	PRO	2.2
1	C	119	THR	2.2
1	D	1	MET	2.2
1	B	450	LYS	2.2
1	D	310	ARG	2.2
1	D	49	GLU	2.2
1	D	2	HIS	2.2
1	B	7	CYS	2.1
1	C	459	GLU	2.1
1	C	163	GLU	2.1
1	D	445	PRO	2.1
1	D	4	LEU	2.1
1	C	118	PRO	2.1
1	A	603	GLU	2.1
1	C	548	GLN	2.1
1	B	448	VAL	2.1
1	A	106	GLN	2.1
1	D	524	VAL	2.1
1	C	702	GLU	2.1
1	B	26	HIS	2.0
1	D	50	ALA	2.0
1	C	53	ARG	2.0
1	C	30	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](#)

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, 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
2	MN	A	5034	1/1	0.85	0.27	3.40	85,85,85,85	0
2	MN	C	5032	1/1	0.93	0.32	3.29	95,95,95,95	0
2	MN	B	5007	1/1	0.96	0.24	0.23	40,40,40,40	0
2	MN	D	5020	1/1	0.99	0.16	-1.82	41,41,41,41	0
2	MN	B	5037	1/1	0.95	0.15	-2.61	78,78,78,78	0
2	MN	C	5014	1/1	0.94	0.10	-3.21	50,50,50,50	0
2	MN	C	5019	1/1	0.87	0.10	-3.28	94,94,94,94	0
2	MN	D	5022	1/1	0.90	0.33	-	72,72,72,72	0
2	MN	A	5006	1/1	0.96	0.11	-	36,36,36,36	0
2	MN	C	5018	1/1	0.78	0.19	-	115,115,115,115	0
2	MN	B	5039	1/1	0.92	0.13	-	50,50,50,50	0
2	MN	A	5033	1/1	0.47	0.18	-	97,97,97,97	0
2	MN	A	5003	1/1	0.71	0.21	-	79,79,79,79	0
2	MN	D	5021	1/1	0.97	0.19	-	36,36,36,36	0
2	MN	B	5008	1/1	0.98	0.22	-	27,27,27,27	0
2	MN	B	5028	1/1	0.94	0.06	-	63,63,63,63	0
2	MN	C	5025	1/1	0.86	0.13	-	109,109,109,109	0
2	MN	D	5038	1/1	0.95	0.10	-	88,88,88,88	0
2	MN	D	5035	1/1	0.88	0.09	-	116,116,116,116	0
2	MN	A	5013	1/1	0.80	0.14	-	74,74,74,74	0
2	MN	A	5004	1/1	0.87	0.34	-	70,70,70,70	0
2	MN	A	5001	1/1	0.90	0.09	-	34,34,34,34	0
2	MN	D	5023	1/1	0.63	0.46	-	101,101,101,101	0
2	MN	C	5036	1/1	0.96	0.10	-	116,116,116,116	0
2	MN	C	5015	1/1	0.96	0.23	-	40,40,40,40	0
2	MN	B	5012	1/1	0.91	0.06	-	51,51,51,51	0
2	MN	A	5026	1/1	0.88	0.07	-	64,64,64,64	0
2	MN	D	5031	1/1	0.80	0.18	-	83,83,83,83	0
2	MN	C	5017	1/1	0.66	0.32	-	86,86,86,86	0
2	MN	C	5016	1/1	0.86	0.29	-	101,101,101,101	0
2	MN	A	5002	1/1	0.99	0.18	-	21,21,21,21	0
2	MN	A	5027	1/1	0.88	0.12	-	52,52,52,52	0
2	MN	B	5010	1/1	0.76	0.40	-	99,99,99,99	0
2	MN	C	5030	1/1	0.88	0.23	-	80,80,80,80	0
2	MN	A	5005	1/1	0.95	0.09	-	51,51,51,51	0
2	MN	A	5029	1/1	0.86	0.28	-	67,67,67,67	0
2	MN	D	5024	1/1	0.75	0.08	-	109,109,109,109	0
2	MN	B	5009	1/1	0.67	0.30	-	80,80,80,80	0
2	MN	B	5011	1/1	0.93	0.06	-	51,51,51,51	0

6.5 Other polymers ⓘ

There are no such residues in this entry.