



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:45 PM UTC

PDB ID : 2FFL / pdb_00002ffl
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

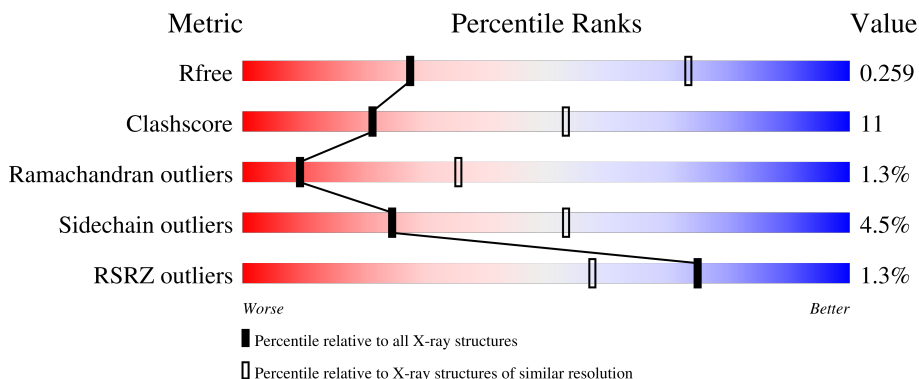
1 Overall quality at a glance i

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}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	756	
1	B	756	
1	C	756	
1	D	756	

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

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 (CCD ID: MN) (formula: Mn).

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

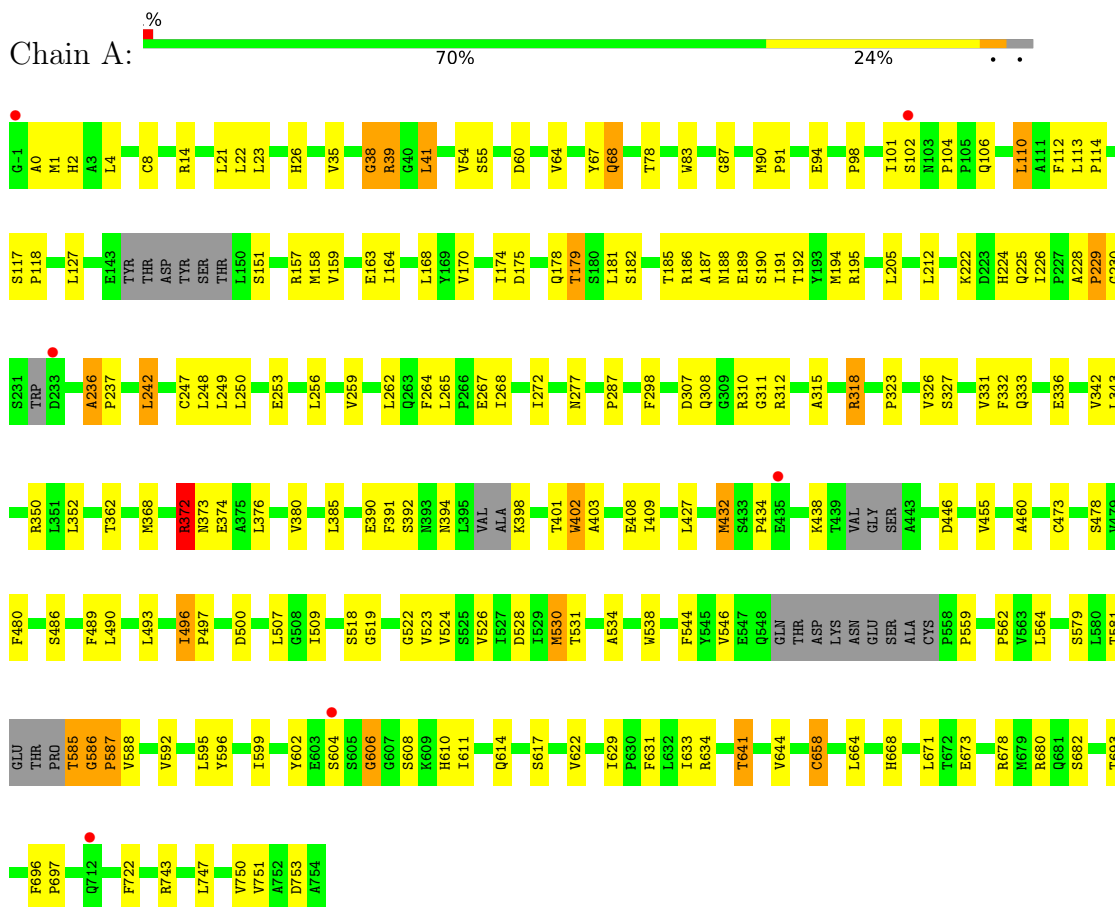
- Molecule 3 is water.

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

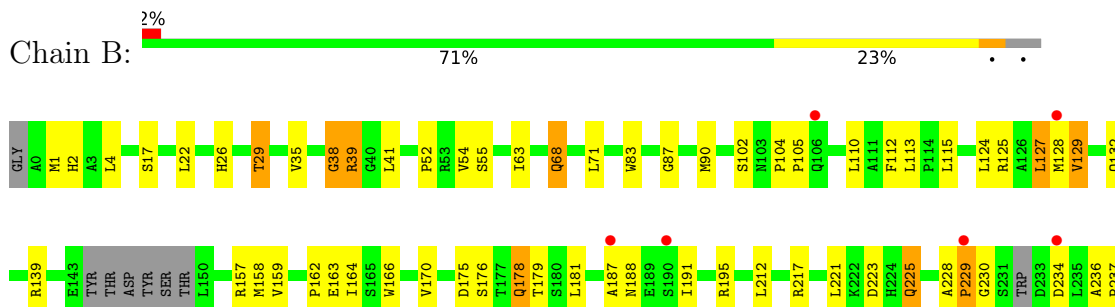
3 Residue-property plots [i](#)

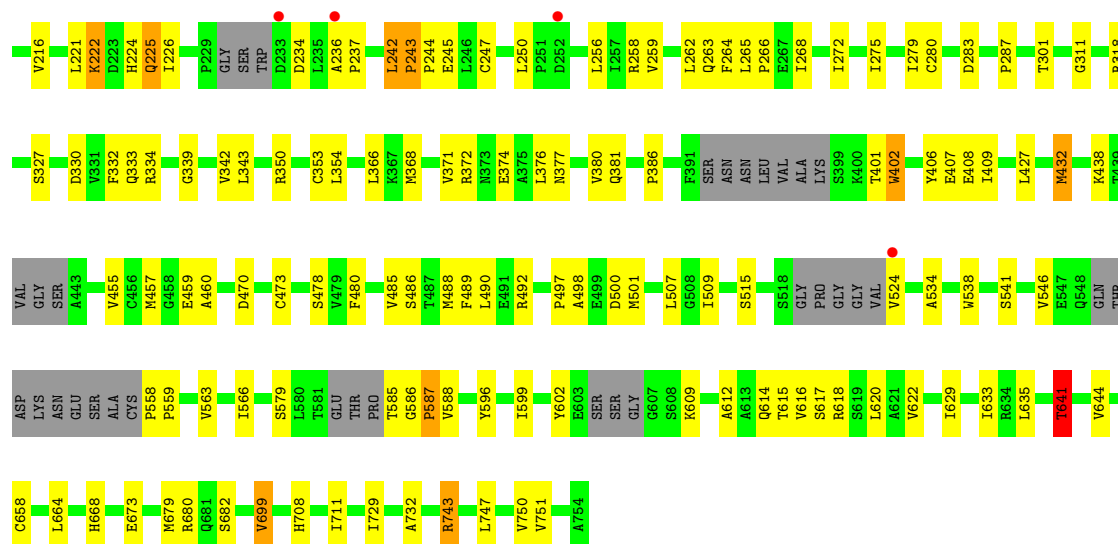
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dicer



- Molecule 1: Dicer





4 Data and refinement statistics i

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 20.00 – 3.33	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-3.33) 98.2 (20.00-3.33)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 3.33Å)	Xtrriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.243 , 0.275 0.222 , 0.259	Depositor DCC
R_{free} test set	3003 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtrriage
Anisotropy	0.158	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.011 for l,-k,h	Xtrriage
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

Xtrriage'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, 0.333 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: 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	0.59	1/5761 (0.0%)	0.92	10/7836 (0.1%)
1	B	0.60	2/5718 (0.0%)	0.91	9/7777 (0.1%)
1	C	0.51	0/5666	0.88	7/7704 (0.1%)
1	D	0.53	0/5704	0.87	5/7759 (0.1%)
All	All	0.56	3/22849 (0.0%)	0.90	31/31076 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	127	LEU	C-N	8.05	1.44	1.33
1	B	129	VAL	C-N	7.65	1.43	1.33
1	A	629	ILE	CA-CB	6.11	1.57	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	641	THR	CA-C-N	8.12	127.42	118.97
1	A	641	THR	C-N-CA	8.12	127.42	118.97
1	D	38	GLY	N-CA-C	8.11	125.69	111.57
1	D	641	THR	CA-C-N	7.58	129.31	119.84
1	D	641	THR	C-N-CA	7.58	129.31	119.84
1	D	243	PRO	CA-C-N	7.55	127.92	119.32
1	D	243	PRO	C-N-CA	7.55	127.92	119.32
1	B	641	THR	CA-C-N	6.94	126.46	119.24
1	B	641	THR	C-N-CA	6.94	126.46	119.24
1	C	641	THR	CA-C-N	6.81	128.35	119.84
1	C	641	THR	C-N-CA	6.81	128.35	119.84
1	C	38	GLY	N-CA-C	6.59	124.11	112.64
1	B	38	GLY	N-CA-C	6.52	123.66	112.51
1	C	541	SER	CA-C-N	6.44	126.36	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	541	SER	C-N-CA	6.44	126.36	119.28
1	A	38	GLY	N-CA-C	6.23	123.16	112.51
1	C	243	PRO	CA-C-N	6.03	125.92	119.28
1	C	243	PRO	C-N-CA	6.03	125.92	119.28
1	A	242	LEU	CA-C-N	5.97	126.53	120.38
1	A	242	LEU	C-N-CA	5.97	126.53	120.38
1	A	586	GLY	CA-C-N	5.93	127.26	119.84
1	A	586	GLY	C-N-CA	5.93	127.26	119.84
1	B	242	LEU	CA-C-N	5.71	126.26	120.38
1	B	242	LEU	C-N-CA	5.71	126.26	120.38
1	B	178	GLN	N-CA-C	5.66	118.02	109.41
1	A	586	GLY	N-CA-C	5.57	123.70	112.34
1	B	243	PRO	CA-C-N	5.44	125.27	119.28
1	B	243	PRO	C-N-CA	5.44	125.27	119.28
1	B	343	LEU	N-CA-C	-5.20	105.53	111.14
1	A	496	ILE	CA-C-N	5.10	126.22	119.84
1	A	496	ILE	C-N-CA	5.10	126.22	119.84

There are no chirality outliers.

There are no planarity outliers.

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	5630	0	5674	138	0
1	B	5590	0	5640	129	1
1	C	5539	0	5592	97	0
1	D	5574	0	5611	130	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22426	0	22517	490	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 11.

All (490) 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:432:MET:HE1	1:C:538:TRP:HB2	1.11	1.09
1:A:432:MET:HE1	1:A:538:TRP:HB2	1.36	1.05
1:C:455:VAL:HA	1:C:460:ALA:HB2	1.37	1.03
1:D:432:MET:HE1	1:D:538:TRP:HB2	1.43	0.97
1:A:38:GLY:HA3	1:A:41:LEU:HD12	1.48	0.96
1:C:432:MET:HE1	1:C:538:TRP:CB	1.98	0.94
1:D:342:VAL:HG12	1:D:658:CYS:SG	2.09	0.92
1:B:432:MET:HE1	1:B:538:TRP:HB2	1.51	0.91
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:C:432:MET:CE	1:C:538:TRP:HB2	2.04	0.80
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:A:432:MET:HE1	1:A:538:TRP:CB	2.13	0.78
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:B:432:MET:HE3	1:B:480:PHE:CZ	2.20	0.76
1:C:90:MET:HE1	1:C:318:ARG:HH22	1.49	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:310:ARG:HH11	1:A:310:ARG:HB2	1.54	0.71
1:B:287:PRO:HG2	1:B:409:ILE:HD13	1.72	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:401:THR:HG22	1:A:403:ALA:H	1.56	0.70
1:A:581:THR:H	1:A:585:THR:HG23	1.55	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:B:333:GLN:HG2	1:B:673:GLU:HB2	1.74	0.69
1:D:185:THR:HG22	1:D:190:SER:HB3	1.72	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:A:35:VAL:HG21	1:A:264:PHE:CE2	2.30	0.67
1:B:158:MET:HE1	1:B:170:VAL:HB	1.76	0.67
1:A:606:GLY:HA2	1:A:610:HIS:HB2	1.74	0.67
1:A:21:LEU:HD21	1:A:272:ILE:HD11	1.75	0.66
1:B:139:ARG:NH2	1:B:162:PRO:HG2	2.11	0.66
1:A:432:MET:CE	1:A:538:TRP:HB2	2.21	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:C:68:GLN:NE2	1:C:112:PHE:H	1.94	0.66
1:D:170:VAL:HG11	1:D:221:LEU:HD22	1.78	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:682:SER:HB2	1:D:751:VAL:HG12	1.79	0.64
1:A:310:ARG:HB2	1:A:310:ARG:NH1	2.12	0.64
1:C:350:ARG:HD3	1:C:538:TRP:O	1.97	0.64
1:C:432:MET:HE3	1:C:480:PHE:CZ	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ASN:HD21	1:A:401:THR:HG21	1.64	0.63
1:B:39:ARG:H	1:B:39:ARG:HD3	1.64	0.62
1:A:68:GLN:HE22	1:A:112:PHE:H	1.45	0.62
1:A:158:MET:HE1	1:A:170:VAL:HB	1.79	0.62
1:A:157:ARG:HH21	1:A:249:LEU:HD21	1.64	0.62
1:C:327:SER:HB3	1:C:330:ASP:OD2	1.99	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:HD23	1:B:747:LEU:O	2.01	0.61
1:D:558:PRO:N	1:D:602:TYR:HH	1.98	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:68:GLN:HE22	1:B:112:PHE:H	1.49	0.60
1:B:178:GLN:HG3	1:B:212:LEU:HD12	1.82	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:A:390:GLU:OE1	1:A:390:GLU:HA	2.00	0.59
1:D:354:LEU:O	1:D:492:ARG:HD3	2.03	0.59
1:D:609:LYS:HZ2	1:D:641:THR:HB	1.67	0.59
1:A:14:ARG:NH2	1:A:224:HIS:O	2.35	0.59
1:D:35:VAL:HG21	1:D:264:PHE:CD2	2.38	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:B:425:GLU:HG2	1:B:429:LYS:HE3	1.84	0.59
1:C:352:LEU:O	1:C:544:PHE:HB3	2.03	0.59
1:C:546:VAL:HB	1:C:644:VAL:HG13	1.85	0.59
1:D:507:LEU:HD22	1:D:588:VAL:HG21	1.84	0.59
1:B:170:VAL:HG11	1:B:221:LEU:HD22	1.85	0.59
1:B:432:MET:HE2	1:B:534:ALA:HB1	1.85	0.59
1:C:612:ALA:HB2	1:C:703:VAL:HG21	1.85	0.59
1:D:432:MET:HE1	1:D:538:TRP:CB	2.25	0.58
1:D:158:MET:HB3	1:D:250:LEU:HD12	1.85	0.58
1:A:602:TYR:O	1:A:634:ARG:NH1	2.36	0.58
1:C:455:VAL:HA	1:C:460:ALA:CB	2.25	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:596:TYR:O	1:D:599:ILE:HG22	2.02	0.58
1:C:236:ALA:N	1:C:237:PRO:HD2	2.17	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:333:GLN:HG2	1:A:673:GLU:HB2	1.86	0.57
1:A:668:HIS:HB3	1:A:671:LEU:HG	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:C:71:LEU:HD22	1:C:262:LEU:HD13	1.87	0.57
1:D:159:VAL:CG2	1:D:247:CYS:HB3	2.35	0.57
1:D:432:MET:HE3	1:D:480:PHE:CZ	2.38	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:A:432:MET:HE2	1:A:534:ALA:HB1	1.87	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:D:35:VAL:HG21	1:D:264:PHE:CE2	2.41	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:381:GLN:HE21	1:B:402:TRP:CD1	2.23	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: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:A:39:ARG:CD	1:A:39:ARG:H	2.20	0.55
1:C:102:SER:O	1:C:104:PRO:HD3	2.06	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:432:MET:HE3	1:A:480:PHE:CZ	2.43	0.54
1:A:546:VAL:HB	1:A:644:VAL:HG13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:ALA:N	1:D:237:PRO:CD	2.71	0.54
1:B:158:MET:HB3	1:B:250:LEU:HD12	1.90	0.54
1:C:332:PHE:CD1	1:C:408:GLU:HG3	2.43	0.54
1:D:115:LEU:H	1:D:258:ARG:HH22	1.56	0.54
1:B:682:SER:HB2	1:B:751:VAL:HG12	1.88	0.54
1:A:374:GLU:CD	1:A:374:GLU:H	2.15	0.53
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: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:A:682:SER:HB2	1:A:751:VAL:HG12	1.90	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:265:LEU:HD23	1:D:268:ILE:HD12	1.91	0.53
1:D:587:PRO:HD2	1:D:588:VAL:H	1.73	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:HA	1:A:402:TRP:CE3	2.44	0.53
1:B:236:ALA:N	1:B:237:PRO:HD2	2.24	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:CD	2.72	0.53
1:D:478:SER:HB2	1:D:486:SER:OG	2.09	0.52
1:B:697:PRO:C	1:B:699:VAL:H	2.17	0.52
1:D:432:MET:HE2	1:D:534:ALA:HB1	1.91	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:225:GLN:CD	1:B:225:GLN:H	2.18	0.51
1:B:432:MET:HE1	1:B:538:TRP:CB	2.30	0.51
1:A:186:ARG:O	1:A:187:ALA:C	2.54	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:C:630:PRO:O	1:C:634:ARG:HG2	2.10	0.51
1:D:498:ALA:HA	1:D:501:MET:HG3	1.91	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:A:1:MET:HG3	1:A:55:SER:HB2	1.93	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:104:PRO:HB2	1:A:106:GLN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:PRO:O	1:B:699:VAL:N	2.44	0.51
1:B:4:LEU:HD21	1:B:26:HIS:ND1	2.26	0.50
1:B:124:LEU:HD23	1:B:127:LEU:HD12	1.93	0.50
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:A:376:LEU:O	1:A:380:VAL:HG23	2.11	0.50
1:B:332:PHE:CD1	1:B:408:GLU:HG3	2.47	0.50
1:C:664:LEU:HD12	1:C:680:ARG:HB3	1.93	0.50
1:D:185:THR:HG22	1:D:190:SER:CB	2.41	0.50
1:D:455:VAL:HA	1:D:460:ALA:CB	2.38	0.50
1:B:747:LEU:O	1:B:750:VAL:HG12	2.11	0.50
1:C:458:GLY:C	1:C:460:ALA:H	2.19	0.50
1:D:259:VAL:O	1:D:262:LEU:HB3	2.11	0.50
1:B:396:VAL:O	1:B:396:VAL:HG13	2.11	0.50
1:C:115:LEU:H	1:C:258:ARG:NH2	2.04	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:192:THR:OG1	1:D:195:ARG:HB2	2.12	0.50
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:D:682:SER:HB2	1:D:751:VAL:CG1	2.42	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:39:ARG:HH22	1:A:267:GLU:CD	2.20	0.49
1:A:599:ILE:HG21	1:A:631:PHE:CE1	2.48	0.49
1:A:22:LEU:O	1:A:110:LEU:HA	2.13	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: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:D:14:ARG:NH2	1:D:224:HIS:O	2.45	0.49
1:D:71:LEU:HD22	1:D:262:LEU:HD13	1.94	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: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:C:31:PRO:HD3	1:C:294:GLY:CA	2.43	0.49
1:D:96:THR:HG21	1:D:301:THR:HG23	1.95	0.49
1:D:191:ILE:HG23	1:D:195:ARG:HD3	1.95	0.49
1:D:330:ASP:O	1:D:334:ARG:HG2	2.13	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:A:315:ALA:O	1:A:318:ARG:HG3	2.14	0.48
1:C:638:ILE:HG23	1:C:644:VAL:CG1	2.43	0.48
1:D:150:LEU:C	1:D:152:ALA:H	2.21	0.48
1:A:8:CYS:SG	1:A:268:ILE:HD13	2.54	0.48
1:B:279:ILE:HD11	1:B:293:GLY:HA2	1.96	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:D:225:GLN:CD	1:D:225:GLN:H	2.20	0.48
1:A:747:LEU:O	1:A:747:LEU:HD23	2.14	0.48
1:C:159:VAL:HG21	1:C:247:CYS:HB3	1.95	0.48
1:A:608:SER:HA	1:A:611:ILE:HD12	1.96	0.47
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:392:SER:C	1:A:394:ASN:H	2.23	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:A:587:PRO:HD2	1:A:588:VAL:H	1.78	0.47
1:B:559:PRO:HG2	1:B:599:ILE:HG13	1.95	0.47
1:C:112:PHE:CD1	1:C:265:LEU:HD22	2.50	0.47
1:D:113:LEU:HD13	1:D:122:LEU:CD1	2.45	0.47
1:D:158:MET:HG3	1:D:259:VAL:HG21	1.95	0.47
1:A:599:ILE:HG21	1:A:631:PHE:HE1	1.79	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:C:455:VAL:CA	1:C:460:ALA:HB2	2.27	0.47
1:C:638:ILE:HG23	1:C:644:VAL:HG12	1.97	0.47
1:D:68:GLN:NE2	1:D:112:PHE:H	2.13	0.47
1:A:228:ALA:C	1:A:230:GLY:N	2.73	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:D:90:MET:HE1	1:D:318:ARG:HH22	1.79	0.47
1:A:158:MET:HE1	1:A:170:VAL:CB	2.45	0.46
1:C:279:ILE:CD1	1:C:293:GLY:HA2	2.45	0.46
1:D:402:TRP:CE3	1:D:402:TRP:HA	2.49	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:B:698:SER:O	1:B:702:GLU:HG3	2.16	0.46
1:C:366:LEU:HD22	1:C:485:VAL:HG22	1.96	0.46
1:C:373:ASN:HD21	1:C:401:THR:HG21	1.80	0.46
1:C:432:MET:HE2	1:C:534:ALA:C	2.40	0.46
1:D:64:VAL:HG13	1:D:113:LEU:HD21	1.97	0.46
1:B:90:MET:HE1	1:B:318:ARG:HH22	1.79	0.46
1:B:125:ARG:O	1:B:129:VAL:HG23	2.14	0.46
1:B:217:ARG:HD3	1:B:240:ARG:NH1	2.30	0.46
1:D:68:GLN:HE22	1:D:112:PHE:H	1.63	0.46
1:B:656:LEU:HD11	1:B:746:VAL:HG11	1.97	0.46
1:C:489:PHE:CZ	1:C:534:ALA:HA	2.51	0.46
1:D:165:SER:O	1:D:166:TRP:HB2	2.16	0.46
1:D:620:LEU:HD22	1:D:729:ILE:HD11	1.98	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:A:151:SER:HB2	1:A:174:ILE:H	1.80	0.46
1:C:596:TYR:O	1:C:599:ILE:HG22	2.16	0.46
1:D:175:ASP:OD2	1:D:177:THR:HB	2.15	0.46
1:A:680:ARG:NH1	1:A:680:ARG:HG3	2.31	0.46
1:B:326:VAL:CG1	1:B:330:ASP:HB2	2.45	0.46
1:C:478:SER:HA	1:C:486:SER:HB3	1.96	0.46
1:B:87:GLY:O	1:B:90:MET:HG3	2.16	0.46
1:B:394:ASN:O	1:B:395:LEU:HB2	2.16	0.46
1:D:609:LYS:HZ2	1:D:641:THR:CG2	2.28	0.45
1:A:310:ARG:O	1:A:312:ARG:HG2	2.16	0.45
1:A:372:ARG:HG2	1:A:374:GLU:OE1	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:A:332:PHE:CD1	1:A:408:GLU:HG3	2.51	0.45
1:B:645:TYR:CD1	1:B:645:TYR:C	2.94	0.45
1:A:507:LEU:HD22	1:A:588:VAL:HG21	1.98	0.45
1:B:348:THR:O	1:B:352:LEU:HB2	2.16	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:67:TYR:CZ	1:D:114:PRO:HG3	2.52	0.45
1:D:372:ARG:HG2	1:D:374:GLU:OE1	2.17	0.45
1:D:380:VAL:HG12	1:D:386:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ALA:C	1:A:230:GLY:H	2.25	0.45
1:B:191:ILE:CG2	1:B:195:ARG:HB3	2.46	0.45
1:B:405:MET:O	1:B:409:ILE:HG13	2.16	0.45
1:C:243:PRO:HA	1:C:244:PRO:HD3	1.81	0.45
1:D:21:LEU:HD13	1:D:112:PHE:CE1	2.52	0.45
1:A:163:GLU:C	1:A:164:ILE:HG13	2.42	0.45
1:A:385:LEU:HD11	1:A:409:ILE:HD11	1.99	0.45
1:A:604:SER:C	1:A:606:GLY:H	2.23	0.45
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:509:ILE:HD11	1:A:522:GLY:N	2.32	0.45
1:A:682:SER:CB	1:A:751:VAL:HG12	2.47	0.45
1:C:225:GLN:CD	1:C:225:GLN:H	2.25	0.45
1:D:366:LEU:HD22	1:D:485:VAL:HG22	1.98	0.45
1:D:473:CYS:HA	1:D:490:LEU:HD13	1.98	0.45
1:A:236:ALA:N	1:A:237:PRO:CD	2.80	0.45
1:A:496:ILE:HA	1:A:497:PRO:HD2	1.70	0.45
1:A:696:PHE:O	1:A:697:PRO:C	2.59	0.45
1:C:158:MET:HB3	1:C:250:LEU:HD12	1.99	0.45
1:C:323:PRO:O	1:C:326:VAL:HG23	2.16	0.45
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:B:608:SER:HA	1:B:611:ILE:HD12	2.00	0.44
1:C:368:MET:HG3	1:D:368:MET:HG3	1.98	0.44
1:D:62:THR:O	1:D:66:VAL:HG23	2.17	0.44
1:D:488:MET:HE2	1:D:488:MET:HB3	1.81	0.44
1:A:562:PRO:HB3	1:A:595:LEU:HB2	1.99	0.44
1:C:385:LEU:N	1:C:386:PRO:CD	2.81	0.44
1:C:402:TRP:HA	1:C:402:TRP:CE3	2.52	0.44
1:D:612:ALA:O	1:D:616:VAL:HG23	2.18	0.44
1:A:191:ILE:HG22	1:A:192:THR:N	2.33	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: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:B:323:PRO:O	1:B:326:VAL:HG23	2.18	0.44
1:C:381:GLN:NE2	1:C:402:TRP:HD1	2.14	0.44
1:D:279:ILE:O	1:D:283:ASP:HB2	2.17	0.44
1:D:478:SER:HA	1:D:486:SER:HB3	1.99	0.44
1:B:228:ALA:C	1:B:230:GLY:H	2.25	0.44
1:A:185:THR:HG22	1:A:190:SER:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:178:GLN:HG3	1:C:212:LEU:HD12	1.99	0.44
1:D:191:ILE:HG22	1:D:192:THR:O	2.18	0.44
1:B:115:LEU:H	1:B:258:ARG:HH22	1.66	0.44
1:D:371:VAL:O	1:D:371:VAL:HG12	2.17	0.44
1:A:497:PRO:HG2	1:A:500:ASP:OD2	2.18	0.44
1:B:162:PRO:HB3	1:B:166:TRP:CE2	2.53	0.44
1:C:14:ARG:NH2	1:C:224:HIS:O	2.50	0.43
1:C:346:ILE:HG21	1:C:427:LEU:HD12	2.00	0.43
1:A:310:ARG:HH11	1:A:310:ARG:CB	2.28	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:A:308:GLN:H	1:A:308:GLN:HG2	1.70	0.43
1:D:743:ARG:HA	1:D:747:LEU:HB2	1.99	0.43
1:A:664:LEU:CD1	1:A:680:ARG:HB3	2.48	0.43
1:B:129:VAL:O	1:B:132:GLN:HB2	2.18	0.43
1:B:432:MET:HE2	1:B:534:ALA:C	2.44	0.43
1:C:228:ALA:HB1	1:C:229:PRO:HD2	2.00	0.43
1:A:747:LEU:O	1:A:750:VAL:HG12	2.19	0.43
1:D:489:PHE:CZ	1:D:534:ALA:HA	2.54	0.43
1:A:352:LEU:O	1:A:544:PHE:HB3	2.19	0.43
1:D:668:HIS:NE2	1:D:679:MET:HE1	2.34	0.43
1:A:342:VAL:HG12	1:A:658:CYS:SG	2.59	0.43
1:B:612:ALA:HB2	1:B:703:VAL:HG21	2.00	0.43
1:C:454:ARG:HE	1:C:464:GLU:HG2	1.83	0.43
1:C:580:LEU:O	1:C:581:THR:OG1	2.29	0.43
1:D:243:PRO:HA	1:D:244:PRO:HD3	1.77	0.43
1:A:117:SER:HB2	1:A:118:PRO:HD2	2.01	0.42
1:A:489:PHE:CZ	1:A:534:ALA:HA	2.54	0.42
1:A:678:ARG:NH2	1:A:753:ASP:OD1	2.34	0.42
1:C:341:ALA:HB1	1:C:658:CYS:HA	2.00	0.42
1:C:526:VAL:O	1:C:530:MET:HB2	2.19	0.42
1:D:343:LEU:HD13	1:D:427:LEU:CD2	2.49	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:66:VAL:O	1:C:70:ILE:HG12	2.19	0.42
1:C:222:LYS:HE2	1:C:222:LYS:HB2	1.64	0.42
1:D:4:LEU:HD21	1:D:26:HIS:ND1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:MET:C	1:D:459:GLU:H	2.27	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:B:179:THR:HG22	1:B:181:LEU:H	1.85	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:432:MET:HE3	1:B:480:PHE:HZ	1.79	0.42
1:C:376:LEU:HD22	1:C:406:TYR:CD2	2.53	0.42
1:D:77:PRO:HD3	1:D:165:SER:O	2.19	0.42
1:D:242:LEU:HA	1:D:243:PRO:HD3	1.91	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:609:LYS:NZ	1:D:641:THR:CG2	2.83	0.42
1:B:409:ILE:O	1:B:410:VAL:C	2.62	0.42
1:D:668:HIS:CD2	1:D:679:MET:HE1	2.54	0.42
1:D:682:SER:CB	1:D:751:VAL:HG12	2.46	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:D:147:TYR:CZ	1:D:150:LEU:N	2.88	0.42
1:D:158:MET:HE1	1:D:170:VAL:HG23	2.01	0.42
1:D:401:THR:HG22	1:D:402:TRP:N	2.34	0.42
1:D:609:LYS:HZ2	1:D:641:THR:CB	2.32	0.42
1:A:168:LEU:HD13	1:A:259:VAL:CG1	2.50	0.42
1:C:391:PHE:CE2	1:C:402:TRP:HH2	2.38	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:B:310:ARG:HB2	1:B:310:ARG:HH11	1.84	0.41
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:A:179:THR:O	1:A:182:SER:N	2.39	0.41
1:A:307:ASP:CG	1:A:391:PHE:HA	2.45	0.41
1:B:334:ARG:NH2	1:B:669:PRO:HA	2.34	0.41
1:C:187:ALA:O	1:C:188:ASN:HB2	2.20	0.41
1:D:664:LEU:HD12	1:D:680:ARG:HB3	2.02	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:B:697:PRO:C	1:B:699:VAL:N	2.78	0.41
1:D:587:PRO:CD	1:D:588:VAL:H	2.33	0.41
1:A:187:ALA:O	1:A:188:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:158:MET:HG3	1:B:259:VAL:HG21	2.00	0.41
1:C:696:PHE:O	1:C:697:PRO:C	2.62	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:B:17:SER:HB2	1:B:257:ILE:HG22	2.02	0.41
1:B:228:ALA:C	1:B:230:GLY:N	2.78	0.41
1:C:31:PRO:HD3	1:C:294:GLY:HA3	2.01	0.41
1:C:697:PRO:C	1:C:699:VAL:H	2.29	0.41
1:B:221:LEU:O	1:B:221:LEU:HG	2.21	0.41
1:B:402:TRP:HA	1:B:402:TRP:HE3	1.85	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:D:83:TRP:CE3	1:D:86:ILE:HD12	2.56	0.41
1:B:628:THR:OG1	1:B:732:ALA:O	2.39	0.41
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: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:B:163:GLU:C	1:B:164:ILE:HG13	2.45	0.41
1:C:214:ALA:HB1	1:C:239:LEU:HD11	2.01	0.41
1:C:507:LEU:HD22	1:C:588:VAL:HG21	2.02	0.41
1:C:626:SER:C	1:C:628:THR:H	2.29	0.41
1:C:697:PRO:O	1:C:699:VAL:N	2.54	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: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:343:LEU:HD13	1:A:427:LEU:CD2	2.51	0.40
1:A:614:GLN:O	1:A:617:SER:HB3	2.21	0.40
1:A:596:TYR:O	1:A:599:ILE:HG22	2.21	0.40
1:A:680:ARG:HG3	1:A:680:ARG:HH11	1.86	0.40
1:C:312:ARG:HH21	1:C:316:GLY:HA2	1.85	0.40
1:D:22:LEU:O	1:D:110:LEU:HA	2.22	0.40
1:D:635:LEU:HD12	1:D:732:ALA:HB2	2.02	0.40
1:A:38:GLY:HA3	1:A:41:LEU:O	2.21	0.40
1:A:248:LEU:HD23	1:A:248:LEU:C	2.47	0.40
1:A:432:MET:HE2	1:A:534:ALA:C	2.47	0.40
1:D:87:GLY:C	1:D:89:THR:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:LEU:HD23	1:A:493:LEU:HA	1.90	0.40
1:B:22:LEU:HD22	1:B:54:VAL:HG11	2.04	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: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

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 [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	718/756 (95%)	656 (91%)	50 (7%)	12 (2%)	7	30
1	B	710/756 (94%)	661 (93%)	38 (5%)	11 (2%)	8	33
1	C	700/756 (93%)	644 (92%)	50 (7%)	6 (1%)	14	43
1	D	702/756 (93%)	638 (91%)	55 (8%)	9 (1%)	9	35
All	All	2830/3024 (94%)	2599 (92%)	193 (7%)	38 (1%)	9	35

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

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Mol	Chain	Res	Type
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
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 [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	611/632 (97%)	584 (96%)	27 (4%)	25	53
1	B	607/632 (96%)	575 (95%)	32 (5%)	20	49
1	C	602/632 (95%)	578 (96%)	24 (4%)	28	55
1	D	605/632 (96%)	580 (96%)	25 (4%)	27	55
All	All	2425/2528 (96%)	2317 (96%)	108 (4%)	24	53

All (108) 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
1	A	179	THR
1	A	222	LYS
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	402	TRP
1	A	432	MET
1	A	438	LYS
1	A	446	ASP
1	A	518	SER
1	A	528	ASP
1	A	530	MET
1	A	579	SER
1	A	585	THR
1	A	622	VAL
1	A	641	THR
1	A	658	CYS
1	A	743	ARG
1	B	29	THR
1	B	39	ARG
1	B	68	GLN
1	B	110	LEU
1	B	176	SER
1	B	225	GLN

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Mol	Chain	Res	Type
1	B	234	ASP
1	B	242	LEU
1	B	245	GLU
1	B	249	LEU
1	B	292	ILE
1	B	310	ARG
1	B	318	ARG
1	B	327	SER
1	B	394	ASN
1	B	402	TRP
1	B	432	MET
1	B	438	LYS
1	B	446	ASP
1	B	473	CYS
1	B	483	SER
1	B	515	SER
1	B	518	SER
1	B	524	VAL
1	B	526	VAL
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	C	36	SER
1	C	39	ARG
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	372	ARG
1	C	402	TRP
1	C	430	THR
1	C	432	MET
1	C	438	LYS
1	C	473	CYS

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Mol	Chain	Res	Type
1	C	499	GLU
1	C	518	SER
1	C	526	VAL
1	C	585	THR
1	C	628	THR
1	C	641	THR
1	C	716	LYS
1	C	730	LEU
1	D	41	LEU
1	D	78	THR
1	D	110	LEU
1	D	179	THR
1	D	186	ARG
1	D	222	LYS
1	D	225	GLN
1	D	242	LEU
1	D	327	SER
1	D	377	ASN
1	D	402	TRP
1	D	432	MET
1	D	438	LYS
1	D	509	ILE
1	D	515	SER
1	D	524	VAL
1	D	541	SER
1	D	566	ILE
1	D	579	SER
1	D	585	THR
1	D	615	THR
1	D	622	VAL
1	D	641	THR
1	D	699	VAL
1	D	743	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	224	HIS
1	A	225	GLN
1	A	277	ASN
1	A	333	GLN

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Mol	Chain	Res	Type
1	A	373	ASN
1	A	381	GLN
1	A	548	GLN
1	A	572	GLN
1	A	646	GLN
1	A	681	GLN
1	B	68	GLN
1	B	178	GLN
1	B	260	GLN
1	B	328	HIS
1	B	333	GLN
1	B	373	ASN
1	B	381	GLN
1	B	387	GLN
1	B	393	ASN
1	B	436	HIS
1	B	510	GLN
1	B	532	HIS
1	B	572	GLN
1	B	614	GLN
1	B	637	GLN
1	B	665	HIS
1	C	2	HIS
1	C	68	GLN
1	C	73	GLN
1	C	178	GLN
1	C	225	GLN
1	C	328	HIS
1	C	333	GLN
1	C	373	ASN
1	C	381	GLN
1	C	387	GLN
1	C	436	HIS
1	C	572	GLN
1	C	614	GLN
1	C	681	GLN
1	C	745	HIS
1	C	749	GLN
1	D	68	GLN
1	D	224	HIS
1	D	277	ASN
1	D	328	HIS

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Mol	Chain	Res	Type
1	D	333	GLN
1	D	373	ASN
1	D	377	ASN
1	D	381	GLN
1	D	548	GLN
1	D	637	GLN
1	D	745	HIS
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 oligosaccharides 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 [i](#)

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%)	-0.20	6 (0%) 82 69	21, 37, 67, 94	1 (0%)
1	B	726/756 (96%)	-0.14	13 (1%) 67 49	22, 37, 69, 95	1 (0%)
1	C	718/756 (94%)	-0.10	4 (0%) 85 74	20, 38, 69, 94	1 (0%)
1	D	720/756 (95%)	0.20	16 (2%) 62 44	22, 37, 68, 94	1 (0%)
All	All	2896/3024 (95%)	-0.06	39 (1%) 75 57	20, 38, 68, 95	4 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	ASP	3.7
1	D	185	THR	3.7
1	D	236	ALA	3.3
1	B	585	THR	3.0
1	B	524	VAL	3.0
1	A	102	SER	3.0
1	C	524	VAL	3.0
1	D	190	SER	2.8
1	D	524	VAL	2.8
1	A	435	GLU	2.8
1	B	128	MET	2.7
1	A	712	GLN	2.7
1	A	-1	GLY	2.6
1	D	105	PRO	2.6
1	D	209	ASP	2.5
1	D	150	LEU	2.5
1	D	146	ASP	2.5
1	D	189	GLU	2.5
1	B	393	ASN	2.4
1	B	234	ASP	2.4
1	B	187	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	235	LEU	2.3
1	D	184	PHE	2.3
1	D	128	MET	2.3
1	B	190	SER	2.3
1	C	151	SER	2.3
1	B	106	GLN	2.3
1	D	186	ARG	2.2
1	D	102	SER	2.2
1	B	395	LEU	2.2
1	A	604	SER	2.2
1	B	396	VAL	2.1
1	D	252	ASP	2.1
1	B	229	PRO	2.1
1	C	190	SER	2.1
1	D	153	SER	2.0
1	B	519	GLY	2.0
1	B	706	GLU	2.0
1	D	233	ASP	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 oligosaccharides 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
2	MN	D	5023	1/1	0.73	0.15	101,101,101,101	0
2	MN	B	5039	1/1	0.75	0.26	50,50,50,50	0
2	MN	A	5033	1/1	0.85	0.08	97,97,97,97	0
2	MN	A	5013	1/1	0.86	0.08	74,74,74,74	0
2	MN	A	5004	1/1	0.86	0.09	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MN	A	5003	1/1	0.87	0.07	79,79,79,79	0
2	MN	D	5035	1/1	0.87	0.08	116,116,116,116	0
2	MN	D	5038	1/1	0.87	0.06	88,88,88,88	0
2	MN	C	5018	1/1	0.88	0.05	115,115,115,115	0
2	MN	B	5010	1/1	0.88	0.14	99,99,99,99	0
2	MN	C	5017	1/1	0.89	0.05	86,86,86,86	0
2	MN	D	5024	1/1	0.90	0.07	109,109,109,109	0
2	MN	C	5016	1/1	0.90	0.09	101,101,101,101	0
2	MN	A	5027	1/1	0.90	0.11	52,52,52,52	0
2	MN	A	5034	1/1	0.91	0.16	85,85,85,85	0
2	MN	D	5031	1/1	0.91	0.08	83,83,83,83	0
2	MN	C	5025	1/1	0.91	0.07	109,109,109,109	0
2	MN	B	5009	1/1	0.91	0.07	80,80,80,80	0
2	MN	D	5022	1/1	0.92	0.06	72,72,72,72	0
2	MN	C	5019	1/1	0.92	0.09	94,94,94,94	0
2	MN	B	5037	1/1	0.93	0.18	78,78,78,78	0
2	MN	C	5030	1/1	0.93	0.17	80,80,80,80	0
2	MN	C	5032	1/1	0.93	0.12	95,95,95,95	0
2	MN	A	5005	1/1	0.94	0.04	51,51,51,51	0
2	MN	A	5026	1/1	0.94	0.05	64,64,64,64	0
2	MN	C	5036	1/1	0.95	0.05	116,116,116,116	0
2	MN	B	5007	1/1	0.96	0.05	40,40,40,40	0
2	MN	A	5006	1/1	0.96	0.03	36,36,36,36	0
2	MN	A	5029	1/1	0.96	0.16	67,67,67,67	0
2	MN	B	5012	1/1	0.96	0.08	51,51,51,51	0
2	MN	B	5028	1/1	0.96	0.04	63,63,63,63	0
2	MN	D	5021	1/1	0.96	0.04	36,36,36,36	0
2	MN	C	5014	1/1	0.97	0.04	50,50,50,50	0
2	MN	B	5011	1/1	0.97	0.03	51,51,51,51	0
2	MN	B	5008	1/1	0.98	0.04	27,27,27,27	0
2	MN	A	5001	1/1	0.98	0.05	34,34,34,34	0
2	MN	C	5015	1/1	0.99	0.03	40,40,40,40	0
2	MN	D	5020	1/1	0.99	0.03	41,41,41,41	0
2	MN	A	5002	1/1	0.99	0.03	21,21,21,21	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.