



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:00 AM UTC

PDB ID : 6JYT / pdb_00006jyt
Title : Delicate structural coordination of the Severe Acute Respiratory Syndrome coronavirus Nsp13 upon ATP hydrolysis
Authors : Yan, L.; Jia, Z.
Deposited on : 2019-04-28
Resolution : 2.80 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

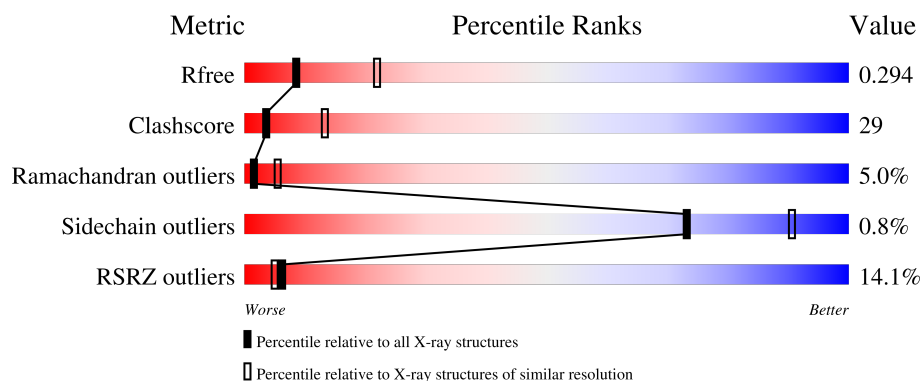
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	603	14% 53% 40% 5%
1	B	603	14% 54% 39% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9467 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 Helicase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	Se	0	0	0
			4655	2956	794	871	26	8			
1	B	597	Total	C	N	O	S	Se	0	0	0
			4657	2958	794	871	26	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASN	-	expression tag	UNP P0C6X7
A	0	SER	-	expression tag	UNP P0C6X7
B	-1	ASN	-	expression tag	UNP P0C6X7
B	0	SER	-	expression tag	UNP P0C6X7

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total	O	0	0
			69	69		
3	B	80	Total	O	0	0
			80	80		

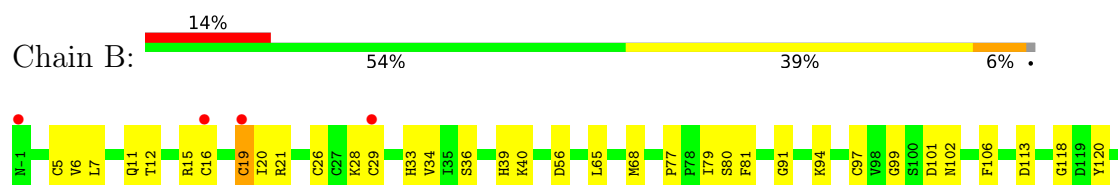
3 Residue-property plots

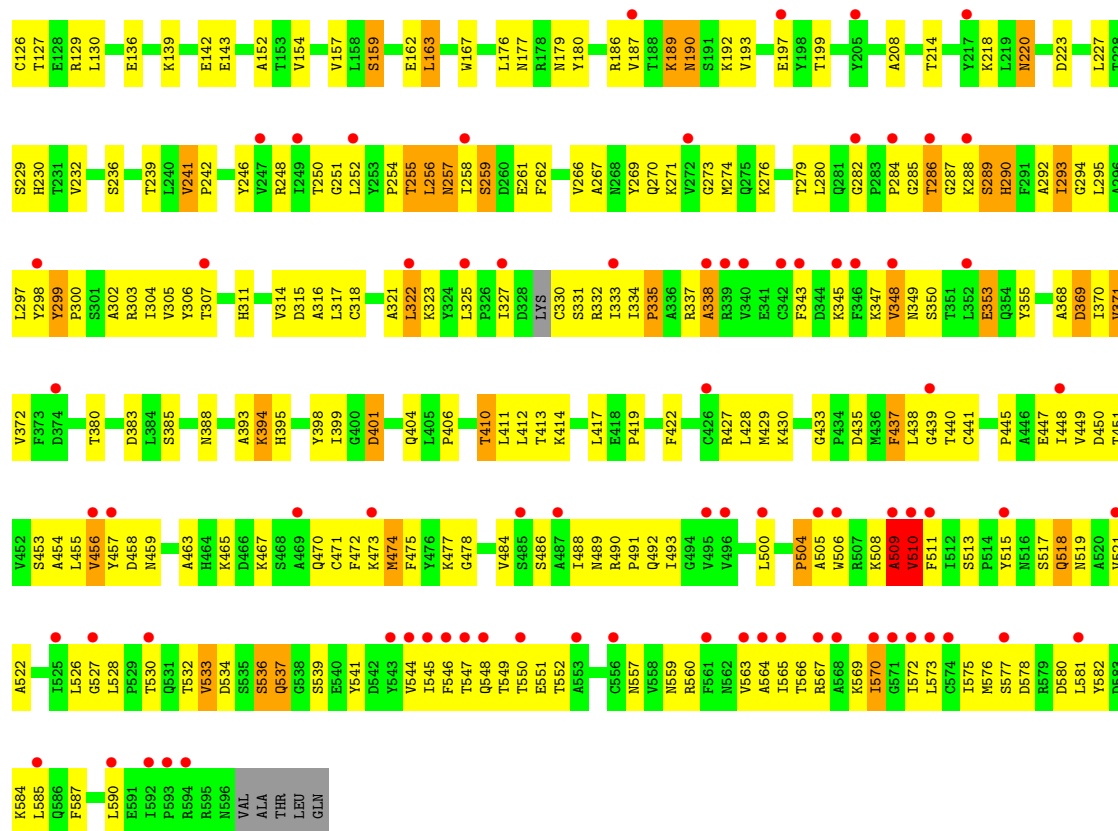
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Helicase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	191.99Å 189.15Å 57.33Å 90.00° 102.89° 90.00°	Depositor
Resolution (Å)	48.83 – 2.80 48.83 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.83-2.80) 99.4 (48.83-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.237 , 0.292 0.238 , 0.294	Depositor DCC
R_{free} test set	2533 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.909	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9467	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.52% 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

5.1 Standard geometry

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

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	0.81	0/4751	1.20	33/6450 (0.5%)
1	B	0.83	3/4753 (0.1%)	1.23	47/6451 (0.7%)
All	All	0.82	3/9504 (0.0%)	1.21	80/12901 (0.6%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	19	CYS	CA-CB	9.85	1.65	1.53
1	B	19	CYS	CB-SG	9.16	2.11	1.81
1	B	509	ALA	CA-C	5.04	1.59	1.52

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	451	THR	N-CA-C	-9.55	100.83	111.14
1	A	173	ARG	CA-C-N	9.32	126.37	119.66
1	A	173	ARG	C-N-CA	9.32	126.37	119.66
1	A	369	ASP	N-CA-C	-8.66	102.64	113.55
1	B	394	LYS	N-CA-C	-8.45	101.84	112.90
1	A	221	VAL	N-CA-C	-8.03	96.44	109.12
1	B	20	ILE	N-CA-C	7.72	119.42	110.62
1	B	369	ASP	N-CA-C	-7.57	104.01	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	CYS	CB-CA-C	7.27	121.72	110.67
1	B	299	TYR	CA-C-N	7.24	126.91	119.82
1	B	299	TYR	C-N-CA	7.24	126.91	119.82
1	A	591	GLU	N-CA-C	7.05	117.80	108.07
1	B	371	VAL	CA-C-N	-6.84	114.71	123.19
1	B	371	VAL	C-N-CA	-6.84	114.71	123.19
1	B	193	VAL	N-CA-C	6.82	118.12	108.17
1	B	241	VAL	CA-C-N	-6.81	112.44	120.13
1	B	241	VAL	C-N-CA	-6.81	112.44	120.13
1	B	322	LEU	N-CA-C	-6.66	104.30	112.88
1	B	257	ASN	N-CA-C	-6.62	106.15	114.56
1	B	510	VAL	CA-C-N	-6.59	111.27	122.33
1	B	510	VAL	C-N-CA	-6.59	111.27	122.33
1	B	282	GLY	CA-C-N	6.51	127.09	120.38
1	B	282	GLY	C-N-CA	6.51	127.09	120.38
1	B	20	ILE	CB-CA-C	-6.50	103.53	112.04
1	B	189	LYS	CA-C-N	6.40	133.22	121.70
1	B	189	LYS	C-N-CA	6.40	133.22	121.70
1	A	394	LYS	N-CA-C	-6.31	105.40	113.23
1	B	290	HIS	N-CA-C	-6.31	104.32	111.07
1	B	433	GLY	CA-C-N	6.29	125.91	119.56
1	B	433	GLY	C-N-CA	6.29	125.91	119.56
1	B	15	ARG	CA-C-N	-6.28	112.52	121.50
1	B	15	ARG	C-N-CA	-6.28	112.52	121.50
1	A	318	CYS	N-CA-C	-6.27	105.28	113.12
1	A	518	GLN	N-CA-C	-6.21	105.34	113.17
1	B	510	VAL	CB-CA-C	-6.21	101.85	110.91
1	A	513	SER	CA-C-N	6.16	127.54	119.84
1	A	513	SER	C-N-CA	6.16	127.54	119.84
1	A	45	VAL	N-CA-C	-6.12	104.00	112.50
1	A	159	SER	N-CA-C	6.12	116.32	108.24
1	A	0	SER	N-CA-C	-6.00	106.11	113.50
1	B	401	ASP	CA-C-N	5.98	126.76	120.12
1	B	401	ASP	C-N-CA	5.98	126.76	120.12
1	B	533	VAL	N-CA-C	5.93	116.67	110.62
1	A	325	LEU	CA-C-N	5.93	127.25	119.84
1	A	325	LEU	C-N-CA	5.93	127.25	119.84
1	A	503	ASN	CA-C-N	5.92	127.23	119.84
1	A	503	ASN	C-N-CA	5.92	127.23	119.84
1	B	220	ASN	CA-C-N	-5.92	115.37	122.35
1	B	220	ASN	C-N-CA	-5.92	115.37	122.35
1	B	437	PHE	N-CA-C	-5.91	103.14	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	GLN	N-CA-C	5.90	118.19	111.11
1	B	163	LEU	N-CA-C	5.90	118.04	109.07
1	A	374	ASP	CA-C-N	-5.81	113.84	123.37
1	A	374	ASP	C-N-CA	-5.81	113.84	123.37
1	A	590	LEU	CA-C-N	-5.80	113.65	122.23
1	A	590	LEU	C-N-CA	-5.80	113.65	122.23
1	A	396	TYR	CA-C-N	-5.76	115.67	123.10
1	A	396	TYR	C-N-CA	-5.76	115.67	123.10
1	A	8	CYS	N-CA-C	-5.74	106.06	114.39
1	B	293	ILE	N-CA-C	-5.63	105.62	111.58
1	B	39	HIS	CA-C-N	-5.61	113.75	122.67
1	B	39	HIS	C-N-CA	-5.61	113.75	122.67
1	B	101	ASP	CA-C-N	5.53	132.10	121.54
1	B	101	ASP	C-N-CA	5.53	132.10	121.54
1	B	159	SER	N-CA-C	5.38	115.23	108.45
1	A	241	VAL	CA-C-N	-5.36	114.07	120.13
1	A	241	VAL	C-N-CA	-5.36	114.07	120.13
1	A	564	ALA	N-CA-C	-5.36	106.68	113.43
1	B	518	GLN	N-CA-C	-5.28	106.52	113.17
1	A	551	GLU	CA-C-N	5.27	131.18	121.70
1	A	551	GLU	C-N-CA	5.27	131.18	121.70
1	B	510	VAL	N-CA-C	5.25	114.93	108.53
1	B	430	LYS	N-CA-C	-5.20	106.24	112.59
1	A	29	CYS	N-CA-C	-5.20	106.09	112.90
1	A	283	PRO	N-CA-C	5.20	117.04	110.70
1	B	353	GLU	N-CA-C	5.18	117.37	110.53
1	A	435	ASP	N-CA-C	-5.17	103.32	110.35
1	B	255	THR	N-CA-C	5.08	118.06	108.65
1	B	251	GLY	N-CA-C	-5.08	108.97	115.42
1	B	19	CYS	N-CA-C	-5.06	101.87	109.15

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4655	0	4620	266	0
1	B	4657	0	4624	281	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	69	0	0	18	0
3	B	80	0	0	25	1
All	All	9467	0	9244	546	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 29.

All (546) 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:B:19:CYS:CB	1:B:19:CYS:SG	2.11	1.37
1:B:21:ARG:NH1	1:B:136:GLU:HB3	1.43	1.34
1:B:21:ARG:HH11	1:B:136:GLU:CB	1.42	1.31
1:B:566:THR:OG1	1:B:567:ARG:NH2	1.72	1.22
1:B:509:ALA:C	1:B:528:LEU:HD23	1.70	1.17
1:B:21:ARG:NH1	1:B:136:GLU:OE1	1.80	1.15
1:A:334:ILE:HD11	1:A:343:PHE:O	1.47	1.13
1:B:447:GLU:OE1	1:B:470:GLN:NE2	1.81	1.11
1:B:427:ARG:NH1	3:B:801:HOH:O	1.81	1.11
1:B:510:VAL:HG22	1:B:511:PHE:N	1.65	1.06
1:B:510:VAL:CG2	1:B:511:PHE:N	2.18	1.06
1:A:214:THR:O	1:A:337:ARG:NH1	1.88	1.05
1:B:509:ALA:C	1:B:528:LEU:CD2	2.32	1.01
1:B:19:CYS:SG	1:B:33:HIS:NE2	2.30	1.01
1:B:563:VAL:HA	1:B:567:ARG:NH2	1.76	1.00
1:B:508:LYS:O	1:B:509:ALA:O	1.82	0.97
1:B:575:ILE:HD12	1:B:575:ILE:O	1.62	0.97
1:B:563:VAL:C	1:B:567:ARG:NH2	2.22	0.96
1:B:509:ALA:O	1:B:528:LEU:HD23	1.65	0.95
1:B:492:GLN:HG3	1:B:575:ILE:CD1	1.96	0.95
1:A:474:MSE:HE1	1:A:476:TYR:CG	2.03	0.94
1:B:285:GLY:H	1:B:288:LYS:HE3	1.31	0.93
1:A:351:THR:HG22	1:A:352:LEU:HG	1.50	0.93
1:B:21:ARG:NH1	1:B:136:GLU:CB	2.14	0.93
1:B:21:ARG:HH11	1:B:136:GLU:HB3	0.77	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LYS:HB3	1:B:190:ASN:HB3	1.52	0.92
1:A:303:ARG:NH1	1:A:367:THR:O	2.04	0.90
1:A:332:ARG:HE	1:A:343:PHE:HD2	1.15	0.90
1:B:455:LEU:HG	1:B:456:VAL:HG23	1.54	0.89
1:B:563:VAL:HA	1:B:567:ARG:HH22	1.37	0.88
1:A:332:ARG:NE	1:A:343:PHE:HB2	1.88	0.88
1:B:563:VAL:CA	1:B:567:ARG:NH2	2.37	0.88
1:A:168:GLU:CD	1:A:171:LYS:HE2	1.98	0.88
1:B:330:CYS:N	1:B:353:GLU:OE1	2.08	0.87
1:A:332:ARG:NH2	1:A:343:PHE:HB2	1.89	0.87
1:B:510:VAL:CG2	1:B:511:PHE:H	1.86	0.86
1:A:414:LYS:NZ	3:A:803:HOH:O	2.08	0.86
1:A:474:MSE:HE1	1:A:476:TYR:CD1	2.12	0.85
1:B:287:GLY:HA3	1:B:438:LEU:HD21	1.59	0.84
1:A:332:ARG:CZ	1:A:343:PHE:HB2	2.08	0.84
1:A:332:ARG:NE	1:A:343:PHE:HD2	1.75	0.84
1:B:489:ASN:H	1:B:518:GLN:HG3	1.41	0.84
1:B:330:CYS:N	3:B:808:HOH:O	2.11	0.83
1:A:471:CYS:HG	1:A:588:THR:HG1	1.25	0.83
1:B:21:ARG:NH1	1:B:136:GLU:CD	2.37	0.83
1:A:512:ILE:HD12	1:A:513:SER:H	1.41	0.83
1:A:21:ARG:HE	1:A:136:GLU:HG2	1.44	0.82
1:A:303:ARG:HH22	1:A:366:THR:HG21	1.45	0.82
1:B:437:PHE:HD2	1:B:438:LEU:H	1.27	0.81
1:B:189:LYS:N	1:B:190:ASN:O	2.11	0.81
1:B:492:GLN:OE1	1:B:575:ILE:HD13	1.81	0.81
1:A:303:ARG:HD3	1:A:303:ARG:C	2.06	0.81
1:B:510:VAL:HG23	1:B:511:PHE:H	1.45	0.81
1:A:332:ARG:HE	1:A:343:PHE:HB2	1.45	0.80
1:B:21:ARG:NH1	1:B:136:GLU:CG	2.45	0.79
1:B:288:LYS:O	1:B:290:HIS:N	2.16	0.79
1:B:492:GLN:HG3	1:B:575:ILE:HD11	1.62	0.78
1:B:129:ARG:NH2	3:B:809:HOH:O	2.15	0.78
1:B:255:THR:O	3:B:802:HOH:O	2.01	0.78
1:A:262:PHE:HE1	1:A:297:LEU:HD12	1.49	0.78
1:A:311:HIS:HD1	1:A:343:PHE:HE1	1.31	0.78
1:A:332:ARG:HH21	1:A:343:PHE:HB2	1.50	0.77
1:A:286:THR:O	1:A:288:LYS:N	2.18	0.77
1:A:303:ARG:HH12	1:A:366:THR:HG22	1.47	0.77
1:B:19:CYS:HG	1:B:33:HIS:HE2	0.84	0.77
1:B:159:SER:HB3	1:B:162:GLU:H	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:VAL:C	1:B:567:ARG:CZ	2.59	0.76
1:A:332:ARG:NE	1:A:343:PHE:CD2	2.53	0.76
1:B:398:TYR:OH	3:B:803:HOH:O	2.04	0.75
1:A:248:ARG:NH1	1:A:249:ILE:O	2.19	0.75
1:B:566:THR:HG1	1:B:567:ARG:HH22	1.33	0.75
1:A:512:ILE:HD12	1:A:513:SER:N	2.02	0.74
1:A:267:ALA:C	1:A:270:GLN:HG3	2.11	0.74
1:A:450:ASP:HA	1:A:453:SER:HB3	1.70	0.74
1:A:526:LEU:HD22	1:A:528:LEU:HD11	1.69	0.74
1:A:94:LYS:O	3:A:801:HOH:O	2.05	0.74
1:A:320:LYS:HA	1:A:323:LYS:HE2	1.70	0.73
1:B:287:GLY:CA	1:B:438:LEU:HD21	2.19	0.73
1:B:564:ALA:C	1:B:567:ARG:HE	1.96	0.72
1:A:181:VAL:O	3:A:802:HOH:O	2.08	0.72
1:B:21:ARG:HH12	1:B:136:GLU:CD	1.98	0.72
1:A:334:ILE:CD1	1:A:343:PHE:O	2.34	0.72
1:B:68:MSE:HG2	3:B:823:HOH:O	1.89	0.71
1:B:186:ARG:NH1	3:B:815:HOH:O	2.22	0.71
1:A:459:ASN:C	1:A:460:LYS:HD3	2.16	0.71
1:A:473:LYS:HB3	1:A:589:SER:HA	1.71	0.71
1:B:510:VAL:N	1:B:528:LEU:HD22	2.06	0.70
1:B:286:THR:H	1:B:288:LYS:HD2	1.56	0.70
1:A:376:ILE:HD11	1:A:429:MSE:HE2	1.74	0.70
1:B:564:ALA:CA	1:B:567:ARG:HE	2.05	0.70
1:A:266:VAL:HG22	1:A:298:TYR:HE1	1.55	0.70
1:B:474:MSE:SE	1:B:582:TYR:HB3	2.41	0.70
1:B:488:ILE:HA	1:B:518:GLN:HB2	1.73	0.70
1:A:147:LEU:O	3:A:804:HOH:O	2.09	0.69
1:B:305:VAL:HG22	1:B:371:VAL:HG22	1.73	0.69
1:A:188:THR:OG1	1:A:189:LYS:N	2.24	0.69
1:A:303:ARG:HH12	1:A:366:THR:CG2	2.05	0.69
1:A:320:LYS:NZ	3:A:812:HOH:O	2.23	0.69
1:B:471:CYS:HA	1:B:587:PHE:HB3	1.72	0.69
1:B:297:LEU:N	3:B:813:HOH:O	2.25	0.69
1:B:28:LYS:HG3	1:B:97:CYS:SG	2.33	0.68
1:B:548:GLN:HG3	1:B:576:MSE:HB2	1.75	0.68
1:A:162:GLU:O	1:A:163:LEU:HD23	1.92	0.68
1:B:36:SER:OG	3:B:805:HOH:O	2.10	0.68
1:B:179:ASN:N	3:B:811:HOH:O	2.18	0.68
1:B:449:VAL:HG11	1:B:463:ALA:HB2	1.75	0.68
1:B:262:PHE:HE2	1:B:297:LEU:HD12	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:SER:OG	1:A:519:ASN:OD1	2.11	0.67
1:B:250:THR:N	3:B:817:HOH:O	2.27	0.67
1:A:330:CYS:HB2	1:A:355:TYR:HB2	1.77	0.67
1:B:576:MSE:HG2	1:B:577:SER:N	2.09	0.67
1:B:242:PRO:O	3:B:807:HOH:O	2.11	0.67
1:B:564:ALA:N	1:B:567:ARG:HH21	1.93	0.67
1:A:40:LYS:HD2	1:A:59:ASP:OD1	1.96	0.66
1:A:446:ALA:HB3	1:A:467:LYS:HD2	1.76	0.66
1:B:152:ALA:HB2	1:B:167:TRP:CZ3	2.32	0.65
1:A:332:ARG:HE	1:A:343:PHE:CB	2.09	0.65
1:A:354:GLN:HG2	1:A:355:TYR:CE2	2.31	0.65
1:A:549:THR:O	1:A:577:SER:OG	2.07	0.65
1:A:142:GLU:HG2	1:A:411:LEU:HD12	1.78	0.65
1:B:255:THR:OG1	1:B:256:LEU:N	2.17	0.65
1:A:574:CYS:HB3	1:A:576:MSE:HE2	1.79	0.65
1:A:333:ILE:HG13	1:A:334:ILE:H	1.62	0.65
1:A:497:ARG:O	1:A:501:THR:OG1	2.15	0.65
1:A:333:ILE:O	1:A:334:ILE:HD13	1.98	0.64
1:B:289:SER:O	1:B:293:ILE:HG12	1.98	0.64
1:A:303:ARG:HD2	1:A:368:ALA:HA	1.80	0.64
1:A:12:THR:HB	1:A:26:CYS:HA	1.79	0.64
1:A:207:ASP:OD2	3:A:805:HOH:O	2.15	0.64
1:A:526:LEU:HD22	1:A:528:LEU:CD1	2.28	0.64
1:B:472:PHE:HD1	1:B:587:PHE:HB2	1.63	0.64
1:A:514:PRO:HD3	1:A:546:PHE:HE2	1.63	0.64
1:B:269:TYR:CD2	1:B:295:LEU:HD13	2.33	0.63
1:A:582:TYR:HA	1:A:585:LEU:HG	1.79	0.63
1:A:21:ARG:NE	1:A:136:GLU:HG2	2.13	0.63
1:A:280:LEU:HD11	1:A:438:LEU:HD23	1.80	0.63
1:A:292:ALA:O	1:A:306:TYR:OH	2.08	0.63
1:A:372:VAL:HG13	1:A:397:VAL:HG13	1.80	0.62
1:A:77:PRO:HG2	1:A:80:SER:HB3	1.81	0.62
1:A:473:LYS:NZ	1:A:578:ASP:OD2	2.26	0.62
1:B:472:PHE:CD1	1:B:587:PHE:HB2	2.34	0.62
1:B:332:ARG:HD2	1:B:347:LYS:O	2.00	0.62
1:B:472:PHE:HD2	1:B:474:MSE:HG3	1.65	0.62
1:B:284:PRO:HG2	1:B:566:THR:HG21	1.80	0.62
1:A:306:TYR:CD1	1:A:317:LEU:HD21	2.35	0.61
1:A:545:ILE:HG23	1:A:573:LEU:HG	1.81	0.61
1:B:322:LEU:HD22	1:B:327:ILE:HD12	1.82	0.61
1:A:159:SER:HB3	1:A:162:GLU:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ASP:HB3	1:A:570:ILE:HD12	1.82	0.61
1:B:509:ALA:C	1:B:528:LEU:HD22	2.21	0.61
1:B:547:THR:HG23	1:B:575:ILE:HD11	1.81	0.61
1:B:332:ARG:HH22	1:B:345:LYS:HB2	1.65	0.61
1:A:334:ILE:HD11	1:A:343:PHE:C	2.25	0.61
1:B:218:LYS:O	3:B:810:HOH:O	2.16	0.61
1:B:427:ARG:NE	3:B:814:HOH:O	2.21	0.61
1:A:553:ALA:HA	1:A:556:CYS:HB3	1.83	0.61
1:B:21:ARG:HH12	1:B:136:GLU:CG	2.13	0.61
1:B:447:GLU:CD	1:B:470:GLN:NE2	2.58	0.61
1:A:402:PRO:HG3	1:A:429:MSE:HE3	1.83	0.61
1:A:443:ARG:NH2	1:A:567:ARG:HA	2.16	0.60
1:B:302:ALA:O	1:B:304:ILE:HG13	2.01	0.60
1:B:286:THR:OG1	1:B:287:GLY:N	2.33	0.60
1:B:297:LEU:O	1:B:300:PRO:HG3	2.00	0.60
1:A:576:MSE:HE3	1:A:585:LEU:HD22	1.83	0.60
1:B:269:TYR:HD2	1:B:295:LEU:HD13	1.66	0.60
1:A:22:ARG:NH2	1:B:56:ASP:O	2.32	0.60
1:B:21:ARG:CZ	1:B:136:GLU:OE1	2.49	0.60
1:B:532:THR:O	1:B:536:SER:OG	2.18	0.60
1:B:177:ASN:HB3	3:B:811:HOH:O	2.01	0.59
1:A:287:GLY:N	3:A:817:HOH:O	2.35	0.59
1:B:304:ILE:HG12	1:B:370:ILE:HG23	1.84	0.59
1:B:143:GLU:HG3	1:B:230:HIS:O	2.01	0.59
1:A:214:THR:OG1	1:A:337:ARG:HD3	2.02	0.59
1:A:373:PHE:CE2	1:A:387:VAL:HG21	2.38	0.59
1:A:473:LYS:HG3	1:A:474:MSE:N	2.17	0.59
1:B:549:THR:OG1	1:B:550:THR:N	2.35	0.59
1:B:566:THR:OG1	1:B:567:ARG:CZ	2.48	0.59
1:B:266:VAL:O	1:B:270:GLN:HG3	2.03	0.59
1:B:445:PRO:HG3	1:B:570:ILE:HA	1.83	0.59
1:B:585:LEU:HB2	1:B:587:PHE:HE2	1.67	0.58
1:A:214:THR:C	1:A:337:ARG:NH1	2.60	0.58
1:A:473:LYS:HG3	1:A:474:MSE:H	1.67	0.58
1:A:497:ARG:HD2	1:A:525:ILE:HD11	1.85	0.58
1:A:454:ALA:O	1:A:456:VAL:N	2.32	0.58
1:A:60:VAL:HA	1:A:63:LEU:HD12	1.86	0.58
1:B:484:VAL:HG23	1:B:486:SER:H	1.67	0.58
1:A:303:ARG:HD3	1:A:304:ILE:N	2.18	0.58
1:A:471:CYS:HB2	1:A:587:PHE:HB3	1.84	0.58
1:A:242:PRO:O	3:A:807:HOH:O	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ARG:CD	1:A:343:PHE:HD2	2.17	0.57
1:B:564:ALA:N	1:B:567:ARG:NH2	2.52	0.57
1:A:526:LEU:HD22	1:A:528:LEU:CG	2.33	0.57
1:B:271:LYS:O	1:B:274:MSE:N	2.24	0.57
1:A:472:PHE:CE1	1:A:572:ILE:HG23	2.39	0.57
1:B:34:VAL:O	1:B:40:LYS:HE3	2.04	0.57
1:B:187:VAL:HG22	1:B:192:LYS:HD3	1.87	0.57
1:A:64:TYR:CD1	1:A:76:LYS:HD3	2.39	0.57
1:A:311:HIS:CD2	1:A:339:ARG:HG2	2.40	0.57
1:B:348:VAL:HG23	1:B:349:ASN:H	1.70	0.57
1:A:186:ARG:NH1	1:A:217:TYR:OH	2.37	0.57
1:B:334:ILE:HB	1:B:343:PHE:HE2	1.70	0.57
1:B:548:GLN:CG	1:B:576:MSE:HB2	2.34	0.57
1:A:155:ARG:NH2	3:A:820:HOH:O	2.37	0.57
1:B:575:ILE:O	1:B:575:ILE:CD1	2.46	0.57
1:B:563:VAL:O	1:B:567:ARG:CZ	2.52	0.57
1:B:77:PRO:HG2	1:B:80:SER:HB3	1.87	0.56
1:B:259:SER:HB2	1:B:261:GLU:OE1	2.05	0.56
1:B:477:LYS:HA	1:B:492:GLN:NE2	2.19	0.56
1:A:17:GLY:HA3	1:A:41:LEU:HD23	1.88	0.56
1:A:361:ASN:N	3:A:816:HOH:O	2.35	0.56
1:A:455:LEU:HD22	1:A:584:LYS:HE2	1.88	0.56
1:B:492:GLN:CG	1:B:575:ILE:CD1	2.77	0.56
1:B:490:ARG:HA	1:B:493:ILE:HG12	1.88	0.56
1:B:303:ARG:HG3	1:B:368:ALA:HA	1.88	0.56
1:A:311:HIS:ND1	1:A:343:PHE:HE1	2.02	0.56
1:A:419:PRO:HA	1:A:422:PHE:CE2	2.41	0.56
1:B:279:THR:HB	1:B:429:MSE:HE2	1.88	0.55
1:B:486:SER:HB3	1:B:515:TYR:HB3	1.87	0.55
1:A:154:VAL:HG23	1:A:223:ASP:O	2.06	0.55
1:B:177:ASN:HB3	1:B:180:TYR:HD2	1.71	0.55
1:A:473:LYS:HZ3	1:A:582:TYR:HB3	1.71	0.55
1:A:307:THR:HG21	1:A:363:LEU:HD11	1.88	0.55
1:B:315:ASP:O	1:B:318:CYS:N	2.31	0.55
1:A:472:PHE:CD1	1:A:573:LEU:HA	2.42	0.55
1:B:533:VAL:HG23	1:B:534:ASP:OD1	2.07	0.55
1:A:214:THR:HB	1:A:337:ARG:HH11	1.72	0.55
1:B:557:ASN:HB3	1:B:560:ARG:HB2	1.88	0.54
1:B:406:PRO:HB3	1:B:422:PHE:CZ	2.43	0.54
1:A:267:ALA:HA	1:A:270:GLN:HG3	1.90	0.54
1:A:393:ALA:C	1:A:394:LYS:HE2	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:PHE:HD2	1:B:438:LEU:N	2.02	0.54
1:B:545:ILE:HG23	1:B:573:LEU:HG	1.90	0.54
1:A:197:GLU:OE2	1:A:337:ARG:HG2	2.08	0.54
1:B:197:GLU:H	1:B:214:THR:HB	1.73	0.54
1:B:118:GLY:N	3:B:818:HOH:O	2.30	0.54
1:B:126:CYS:SG	1:B:130:LEU:HB3	2.47	0.54
1:B:254:PRO:HB3	1:B:298:TYR:CE1	2.43	0.54
1:B:489:ASN:CG	1:B:492:GLN:HB2	2.32	0.54
1:A:303:ARG:NH2	1:A:366:THR:HG21	2.19	0.53
1:A:474:MSE:CE	1:A:476:TYR:CD1	2.88	0.53
1:A:267:ALA:O	1:A:270:GLN:HG3	2.09	0.53
1:B:5:CYS:HB2	1:B:26:CYS:HB3	1.90	0.53
1:A:284:PRO:HB3	1:A:567:ARG:HH12	1.73	0.53
1:A:331:SER:HA	1:A:345:LYS:HG3	1.90	0.53
1:A:515:TYR:CE2	1:A:549:THR:HG21	2.44	0.53
1:B:518:GLN:HA	1:B:521:VAL:HG22	1.90	0.53
1:A:332:ARG:CD	1:A:343:PHE:CD2	2.92	0.53
1:A:354:GLN:HG2	1:A:355:TYR:CZ	2.43	0.53
1:B:241:VAL:HG22	1:B:242:PRO:HD2	1.89	0.53
1:B:509:ALA:CA	1:B:528:LEU:HD23	2.38	0.53
1:B:477:LYS:HD3	1:B:492:GLN:NE2	2.23	0.53
1:A:143:GLU:HG3	1:A:230:HIS:O	2.09	0.53
1:A:472:PHE:HE1	1:A:572:ILE:HG23	1.72	0.53
1:A:526:LEU:HD13	1:A:528:LEU:HD11	1.91	0.53
1:B:509:ALA:O	1:B:528:LEU:CD2	2.45	0.53
1:A:323:LYS:O	1:A:325:LEU:N	2.42	0.52
1:A:473:LYS:HE2	1:A:582:TYR:HD1	1.74	0.52
1:B:473:LYS:HD2	1:B:590:LEU:HB3	1.91	0.52
1:B:239:THR:O	1:B:388:ASN:ND2	2.42	0.52
1:A:267:ALA:CA	1:A:270:GLN:HG3	2.38	0.52
1:B:262:PHE:HE1	1:B:290:HIS:NE2	2.07	0.52
1:B:508:LYS:O	1:B:509:ALA:C	2.50	0.52
1:B:576:MSE:HG2	1:B:577:SER:H	1.74	0.52
1:A:132:LEU:HD21	1:A:237:ALA:O	2.09	0.52
1:A:286:THR:HG23	1:A:289:SER:H	1.75	0.52
1:A:332:ARG:NE	1:A:343:PHE:CB	2.66	0.52
1:A:578:ASP:OD1	1:A:581:LEU:N	2.42	0.52
1:B:582:TYR:HA	1:B:585:LEU:HG	1.91	0.52
1:B:254:PRO:HB3	1:B:298:TYR:HE1	1.75	0.52
1:A:445:PRO:O	1:A:449:VAL:HG23	2.10	0.51
1:B:286:THR:N	1:B:288:LYS:HD2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ILE:HG22	1:B:334:ILE:HG12	1.93	0.51
1:A:369:ASP:O	1:A:370:ILE:HD13	2.11	0.51
1:B:287:GLY:N	1:B:438:LEU:HD21	2.26	0.51
1:B:488:ILE:HD11	1:B:517:SER:HB2	1.93	0.51
1:B:68:MSE:N	3:B:823:HOH:O	2.33	0.51
1:B:477:LYS:HA	1:B:492:GLN:HE22	1.75	0.51
1:A:159:SER:O	1:A:218:LYS:NZ	2.44	0.50
1:B:471:CYS:SG	3:B:875:HOH:O	2.59	0.50
1:A:297:LEU:O	1:A:300:PRO:HG3	2.12	0.50
1:A:380:THR:O	1:A:383:ASP:N	2.41	0.50
1:B:292:ALA:O	1:B:306:TYR:OH	2.23	0.50
1:B:355:TYR:OH	3:B:806:HOH:O	2.10	0.50
1:B:515:TYR:CD2	1:B:549:THR:HG21	2.47	0.50
1:A:460:LYS:HD3	1:A:460:LYS:N	2.25	0.50
1:A:549:THR:HG23	1:A:551:GLU:H	1.77	0.50
1:B:564:ALA:HA	1:B:567:ARG:HE	1.76	0.50
1:A:72:CYS:O	1:A:76:LYS:HB2	2.12	0.50
1:B:286:THR:HB	1:B:441:CYS:HA	1.92	0.50
1:B:477:LYS:HD3	1:B:492:GLN:HE21	1.77	0.49
1:B:331:SER:O	1:B:331:SER:OG	2.28	0.49
1:A:214:THR:C	1:A:337:ARG:HH11	2.20	0.49
1:A:317:LEU:HD23	1:A:357:PHE:HE2	1.78	0.49
1:B:385:SER:OG	3:B:812:HOH:O	2.20	0.49
1:A:228:THR:OG1	3:A:809:HOH:O	2.20	0.49
1:A:90:PHE:CD1	1:A:94:LYS:HE3	2.48	0.49
1:A:250:THR:O	3:A:808:HOH:O	2.19	0.49
1:B:473:LYS:O	1:B:475:PHE:N	2.46	0.49
1:A:21:ARG:HE	1:A:136:GLU:CG	2.18	0.49
1:B:127:THR:HG22	1:B:129:ARG:H	1.78	0.49
1:A:473:LYS:HD2	1:A:585:LEU:HD11	1.94	0.49
1:B:437:PHE:CD2	1:B:438:LEU:N	2.78	0.49
1:A:308:ALA:HB2	1:A:374:ASP:HB3	1.94	0.49
1:B:580:ASP:O	1:B:584:LYS:HD2	2.12	0.49
1:B:262:PHE:CE2	1:B:297:LEU:HD12	2.44	0.49
1:A:303:ARG:C	1:A:303:ARG:CD	2.82	0.49
1:A:473:LYS:NZ	1:A:582:TYR:HB3	2.28	0.48
1:B:566:THR:H	1:B:567:ARG:NH2	2.11	0.48
1:A:271:LYS:O	1:A:274:MSE:N	2.47	0.48
1:A:303:ARG:NH1	1:A:366:THR:HG22	2.22	0.48
1:A:526:LEU:HD22	1:A:528:LEU:HG	1.95	0.48
1:A:333:ILE:C	1:A:334:ILE:HD13	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:PRO:O	1:B:449:VAL:HG23	2.12	0.48
1:B:447:GLU:OE1	1:B:470:GLN:CD	2.54	0.48
1:B:550:THR:C	1:B:552:THR:H	2.21	0.48
1:A:152:ALA:HB2	1:A:167:TRP:CZ3	2.47	0.48
1:A:194:GLN:HG3	1:A:195:ILE:N	2.28	0.48
1:A:406:PRO:HB3	1:A:422:PHE:CZ	2.48	0.48
1:B:250:THR:C	1:B:252:LEU:H	2.21	0.48
1:B:478:GLY:H	1:B:492:GLN:NE2	2.12	0.48
1:A:417:LEU:HD22	1:A:421:TYR:HB2	1.96	0.48
1:B:315:ASP:C	1:B:317:LEU:H	2.21	0.48
1:A:168:GLU:OE1	1:A:171:LYS:HE2	2.13	0.48
1:A:214:THR:CB	1:A:337:ARG:HH11	2.24	0.48
1:B:143:GLU:O	1:B:229:SER:HB2	2.14	0.48
1:A:286:THR:C	1:A:288:LYS:N	2.72	0.48
1:B:380:THR:O	1:B:383:ASP:N	2.43	0.48
1:B:492:GLN:HG3	1:B:575:ILE:HD13	1.87	0.48
1:A:214:THR:CB	1:A:337:ARG:HD3	2.44	0.48
1:B:280:LEU:HB3	1:B:399:ILE:HG23	1.96	0.47
1:A:353:GLU:HG3	1:A:354:GLN:N	2.29	0.47
1:A:361:ASN:HB2	3:A:816:HOH:O	2.13	0.47
1:B:315:ASP:C	1:B:317:LEU:N	2.71	0.47
1:A:73:LYS:HA	1:A:76:LYS:HE2	1.97	0.47
1:A:323:LYS:NZ	3:A:827:HOH:O	2.46	0.47
1:A:443:ARG:HH21	1:A:567:ARG:HA	1.79	0.47
1:B:581:LEU:HG	1:B:585:LEU:HD23	1.96	0.47
1:A:214:THR:HB	1:A:337:ARG:NH1	2.29	0.47
1:A:540:GLU:HB3	1:A:569:LYS:HE3	1.96	0.47
1:A:163:LEU:HG	1:A:211:TYR:CD1	2.49	0.47
1:A:520:ALA:C	1:A:522:ALA:H	2.22	0.47
1:B:266:VAL:HG13	1:B:298:TYR:CE2	2.50	0.47
1:B:545:ILE:HD12	1:B:573:LEU:HD21	1.96	0.47
1:A:317:LEU:HD23	1:A:357:PHE:CE2	2.50	0.47
1:A:376:ILE:HD11	1:A:429:MSE:CE	2.44	0.47
1:A:490:ARG:HA	1:A:493:ILE:HG12	1.96	0.47
1:A:544:VAL:HG13	1:A:572:ILE:HD13	1.97	0.47
1:A:532:THR:O	1:A:536:SER:OG	2.27	0.47
1:B:559:ASN:ND2	3:B:828:HOH:O	2.47	0.47
1:A:248:ARG:NH1	1:A:249:ILE:C	2.73	0.47
1:A:581:LEU:HG	1:A:585:LEU:HD23	1.97	0.47
1:B:334:ILE:CG2	1:B:337:ARG:H	2.28	0.47
1:A:262:PHE:CE1	1:A:297:LEU:HD12	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ILE:HG13	1:A:517:SER:HB2	1.97	0.46
1:A:521:VAL:HG12	1:A:524:LYS:HE2	1.97	0.46
1:A:31:TYR:C	1:A:31:TYR:CD2	2.93	0.46
1:A:409:ARG:O	1:A:410:THR:C	2.58	0.46
1:B:227:LEU:HD12	1:B:227:LEU:HA	1.53	0.46
1:B:294:GLY:C	3:B:813:HOH:O	2.57	0.46
1:A:378:MSE:HE3	1:A:378:MSE:HB3	1.79	0.46
1:A:446:ALA:HA	1:A:449:VAL:HB	1.97	0.46
1:B:246:TYR:HB2	1:B:274:MSE:HA	1.96	0.46
1:B:256:LEU:HB3	1:B:257:ASN:H	1.49	0.46
1:B:458:ASP:N	3:B:829:HOH:O	2.48	0.46
1:B:576:MSE:SE	1:B:578:ASP:HB2	2.65	0.46
1:B:585:LEU:HB2	1:B:587:PHE:CE2	2.49	0.46
1:B:163:LEU:O	1:B:208:ALA:HA	2.16	0.46
1:B:267:ALA:O	1:B:270:GLN:HB2	2.15	0.46
1:B:79:ILE:HD12	1:B:79:ILE:HA	1.82	0.46
1:B:428:LEU:HD23	1:B:428:LEU:HA	1.69	0.46
1:A:315:ASP:C	1:A:317:LEU:N	2.73	0.46
1:A:551:GLU:HA	1:A:552:THR:C	2.41	0.46
1:A:551:GLU:HA	1:A:552:THR:O	2.16	0.46
1:B:457:TYR:HB3	3:B:829:HOH:O	2.15	0.46
1:B:492:GLN:CD	1:B:575:ILE:HD13	2.39	0.46
1:A:393:ALA:HB3	1:A:396:TYR:CZ	2.50	0.46
1:A:466:ASP:O	1:A:468:SER:N	2.35	0.46
1:B:563:VAL:O	1:B:563:VAL:HG12	2.15	0.46
1:A:5:CYS:HB2	1:A:26:CYS:HB3	1.97	0.46
1:A:64:TYR:CG	1:A:76:LYS:HD3	2.51	0.46
1:B:113:ASP:OD1	1:B:113:ASP:C	2.58	0.46
1:B:139:LYS:HD3	1:B:232:VAL:HG13	1.98	0.46
1:B:477:LYS:NZ	1:B:576:MSE:HA	2.31	0.46
1:B:311:HIS:O	1:B:314:VAL:HG12	2.16	0.45
1:B:515:TYR:HD2	1:B:549:THR:HG21	1.81	0.45
1:B:142:GLU:HG2	1:B:411:LEU:HD12	1.98	0.45
1:A:321:ALA:O	1:A:325:LEU:HB2	2.17	0.45
1:B:544:VAL:HG13	1:B:572:ILE:HD13	1.98	0.45
1:A:215:THR:O	1:A:216:THR:HG22	2.15	0.45
1:A:439:GLY:HA2	1:A:440:THR:HB	1.98	0.45
1:A:473:LYS:NZ	1:A:585:LEU:HD21	2.32	0.45
1:A:503:ASN:OD1	1:A:504:PRO:HD2	2.17	0.45
1:B:334:ILE:HG13	1:B:338:ALA:HB2	1.97	0.45
1:B:513:SER:HA	1:B:546:PHE:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:TYR:HE2	1:A:549:THR:HG21	1.81	0.45
1:B:276:LYS:HD2	1:B:276:LYS:O	2.17	0.45
1:B:315:ASP:O	1:B:317:LEU:N	2.50	0.45
1:B:541:TYR:O	1:B:569:LYS:HG3	2.17	0.45
1:A:218:LYS:N	3:A:829:HOH:O	2.47	0.45
1:A:279:THR:O	1:A:435:ASP:HB2	2.17	0.45
1:B:448:ILE:HD13	1:B:565:ILE:HG22	1.99	0.45
1:B:484:VAL:HG23	1:B:486:SER:N	2.31	0.45
1:B:510:VAL:HG23	1:B:511:PHE:N	2.07	0.45
1:B:537:GLN:C	1:B:539:SER:H	2.25	0.45
1:A:206:GLY:C	1:A:208:ALA:H	2.23	0.45
1:A:15:ARG:HD2	1:A:24:PHE:CE1	2.52	0.45
1:A:122:LEU:HD12	1:A:122:LEU:HA	1.68	0.45
1:B:94:LYS:HE3	1:B:94:LYS:HB2	1.74	0.45
1:A:285:GLY:N	1:A:286:THR:HA	2.32	0.44
1:B:157:VAL:HA	1:B:163:LEU:HD12	1.99	0.44
1:B:325:LEU:HD22	1:B:355:TYR:CE2	2.52	0.44
1:B:261:GLU:OE1	1:B:261:GLU:N	2.32	0.44
1:B:457:TYR:C	1:B:459:ASN:H	2.24	0.44
1:A:478:GLY:H	1:A:492:GLN:NE2	2.15	0.44
1:A:514:PRO:HD3	1:A:546:PHE:CE2	2.48	0.44
1:A:541:TYR:O	1:A:569:LYS:N	2.51	0.44
1:B:293:ILE:C	1:B:295:LEU:N	2.76	0.44
1:B:453:SER:HB3	1:B:459:ASN:HA	1.99	0.44
1:A:315:ASP:O	1:A:317:LEU:N	2.51	0.44
1:A:315:ASP:O	1:A:318:CYS:N	2.30	0.44
1:B:490:ARG:N	1:B:491:PRO:HD2	2.33	0.44
1:B:154:VAL:HG23	1:B:223:ASP:O	2.18	0.44
1:A:506:TRP:HZ3	1:A:570:ILE:HD13	1.83	0.44
1:B:489:ASN:OD1	1:B:492:GLN:HB2	2.18	0.44
1:A:447:GLU:HG3	1:A:448:ILE:HG23	2.00	0.44
1:B:323:LYS:N	1:B:323:LYS:HD2	2.33	0.44
1:A:226:VAL:HG23	1:A:228:THR:HG23	1.99	0.43
1:B:440:THR:HG23	1:B:463:ALA:HA	2.00	0.43
1:B:511:PHE:HE2	1:B:519:ASN:HA	1.82	0.43
1:B:65:LEU:HD23	1:B:81:PHE:CZ	2.52	0.43
1:A:350:SER:HA	1:A:351:THR:HA	1.53	0.43
1:A:448:ILE:HG21	1:A:572:ILE:HG21	2.00	0.43
1:B:120:TYR:CE2	1:B:412:LEU:HB2	2.54	0.43
1:B:159:SER:HB3	1:B:162:GLU:N	2.27	0.43
1:B:332:ARG:HG3	1:B:347:LYS:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LYS:HE3	3:A:858:HOH:O	2.19	0.43
1:A:549:THR:OG1	1:A:550:THR:N	2.50	0.43
1:B:267:ALA:HA	1:B:270:GLN:OE1	2.18	0.43
1:A:176:LEU:HD23	1:A:176:LEU:HA	1.79	0.43
1:A:270:GLN:O	1:A:274:MSE:HG2	2.18	0.43
1:A:417:LEU:HD23	1:A:417:LEU:HA	1.77	0.43
1:B:394:LYS:HE2	1:B:394:LYS:N	2.34	0.43
1:B:401:ASP:OD2	1:B:404:GLN:HG3	2.19	0.43
1:A:215:THR:O	1:A:217:TYR:N	2.50	0.43
1:B:6:VAL:HG13	1:B:7:LEU:HG	1.99	0.43
1:B:510:VAL:CA	1:B:528:LEU:HD22	2.48	0.43
1:A:178:ARG:O	1:A:178:ARG:HG3	2.18	0.43
1:B:394:LYS:C	1:B:395:HIS:CG	2.97	0.42
1:B:412:LEU:HD12	1:B:414:LYS:H	1.83	0.42
1:B:578:ASP:OD1	1:B:581:LEU:N	2.33	0.42
1:A:120:TYR:CE2	1:A:412:LEU:HG	2.55	0.42
1:A:512:ILE:O	1:A:519:ASN:OD1	2.38	0.42
1:B:287:GLY:H	1:B:438:LEU:HD21	1.84	0.42
1:B:12:THR:HB	1:B:26:CYS:HA	2.01	0.42
1:B:186:ARG:NH1	1:B:220:ASN:OD1	2.53	0.42
1:B:248:ARG:HH21	1:B:250:THR:HA	1.84	0.42
1:B:413:THR:O	1:B:413:THR:OG1	2.36	0.42
1:B:417:LEU:HD23	1:B:417:LEU:HA	1.69	0.42
1:A:240:LEU:HA	1:A:240:LEU:HD23	1.64	0.42
1:A:262:PHE:HE2	1:A:290:HIS:NE2	2.17	0.42
1:A:567:ARG:HD2	1:A:567:ARG:N	2.34	0.42
1:B:29:CYS:SG	1:B:99:GLY:HA2	2.59	0.42
1:B:564:ALA:CA	1:B:567:ARG:NE	2.79	0.42
1:A:292:ALA:HB1	1:A:306:TYR:HE1	1.85	0.42
1:A:305:VAL:HG22	1:A:356:VAL:HB	2.01	0.42
1:A:503:ASN:HA	1:A:504:PRO:HD2	1.83	0.42
1:B:271:LYS:C	1:B:273:GLY:N	2.76	0.42
1:B:585:LEU:HD12	1:B:585:LEU:O	2.19	0.42
1:A:28:LYS:HG3	1:A:97:CYS:SG	2.60	0.42
1:A:215:THR:C	1:A:217:TYR:H	2.27	0.42
1:A:315:ASP:C	1:A:317:LEU:H	2.27	0.42
1:A:369:ASP:C	1:A:370:ILE:HD13	2.44	0.42
1:A:525:ILE:O	1:A:527:GLY:N	2.46	0.42
1:A:572:ILE:HD12	1:A:573:LEU:H	1.84	0.42
1:B:284:PRO:HG2	1:B:566:THR:CG2	2.49	0.42
1:B:298:TYR:C	1:B:300:PRO:HD3	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:THR:HG22	1:B:411:LEU:N	2.34	0.42
1:A:76:LYS:HB3	1:A:76:LYS:HE3	1.71	0.42
1:A:518:GLN:HA	1:A:521:VAL:HG22	2.01	0.42
1:A:552:THR:C	1:A:554:HIS:H	2.28	0.42
1:B:176:LEU:N	1:B:176:LEU:HD22	2.35	0.42
1:B:293:ILE:C	1:B:295:LEU:H	2.27	0.42
1:B:510:VAL:HG23	1:B:530:THR:HA	2.02	0.42
1:A:168:GLU:OE2	1:A:171:LYS:HE2	2.19	0.42
1:A:252:LEU:HD12	1:A:253:TYR:CE1	2.54	0.42
1:B:335:PRO:HG2	1:B:337:ARG:HH11	1.84	0.42
1:B:474:MSE:CE	1:B:585:LEU:HD21	2.50	0.42
1:B:118:GLY:CA	3:B:818:HOH:O	2.68	0.42
1:B:504:PRO:C	1:B:506:TRP:H	2.26	0.42
1:B:541:TYR:HD1	1:B:567:ARG:HB3	1.85	0.42
1:A:302:ALA:O	1:A:304:ILE:HG13	2.20	0.41
1:A:472:PHE:CG	1:A:573:LEU:HA	2.55	0.41
1:B:474:MSE:HE1	1:B:582:TYR:HB3	2.01	0.41
1:A:25:LEU:HD13	1:A:30:CYS:HA	2.02	0.41
1:A:235:LEU:HD23	1:A:235:LEU:HA	1.73	0.41
1:A:250:THR:N	3:A:808:HOH:O	2.53	0.41
1:A:405:LEU:HA	1:A:406:PRO:HD3	1.88	0.41
1:B:16:CYS:CB	1:B:19:CYS:SG	3.08	0.41
1:B:307:THR:HG22	1:B:372:VAL:O	2.20	0.41
1:B:419:PRO:HA	1:B:422:PHE:CE2	2.54	0.41
1:B:7:LEU:HD21	1:B:106:PHE:HB2	2.01	0.41
1:A:495:VAL:HG22	1:A:495:VAL:O	2.20	0.41
1:A:515:TYR:OH	1:A:549:THR:HG21	2.21	0.41
1:B:318:CYS:O	1:B:322:LEU:HG	2.21	0.41
1:B:541:TYR:CD1	1:B:567:ARG:HB3	2.55	0.41
1:A:14:LEU:HD21	1:A:90:PHE:O	2.20	0.41
1:A:65:LEU:HA	1:A:65:LEU:HD12	1.82	0.41
1:A:325:LEU:HA	1:A:326:PRO:HD3	1.81	0.41
1:A:476:TYR:HE1	1:A:595:ARG:HH12	1.66	0.41
1:A:484:VAL:HG23	1:A:486:SER:H	1.84	0.41
1:B:65:LEU:HA	1:B:65:LEU:HD12	1.69	0.41
1:B:330:CYS:SG	1:B:331:SER:N	2.91	0.41
1:B:393:ALA:C	1:B:394:LYS:HE2	2.45	0.41
1:B:450:ASP:HA	1:B:453:SER:OG	2.21	0.41
1:B:492:GLN:CG	1:B:575:ILE:HD13	2.49	0.41
1:A:378:MSE:O	1:A:407:ALA:HB2	2.20	0.41
1:A:419:PRO:HA	1:A:422:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:CYS:SG	1:A:588:THR:OG1	2.52	0.41
1:B:489:ASN:O	1:B:493:ILE:HG23	2.21	0.41
1:A:167:TRP:CG	1:A:173:ARG:HD2	2.56	0.41
1:A:456:VAL:HG23	1:A:456:VAL:O	2.21	0.41
1:B:335:PRO:HG2	1:B:337:ARG:NH1	2.36	0.41
1:A:152:ALA:HB1	1:A:165:LEU:HD22	2.02	0.41
1:A:332:ARG:HH21	1:A:343:PHE:CB	2.27	0.41
1:A:439:GLY:HA2	1:A:440:THR:O	2.20	0.41
1:B:252:LEU:HD23	1:B:299:TYR:CE1	2.56	0.41
1:B:449:VAL:HG12	1:B:450:ASP:OD2	2.21	0.41
1:A:269:TYR:HD1	1:A:298:TYR:CD1	2.38	0.41
1:A:286:THR:HG22	1:A:287:GLY:N	2.35	0.41
1:A:548:GLN:HB3	1:A:549:THR:H	1.53	0.41
1:B:578:ASP:OD2	1:B:582:TYR:N	2.54	0.41
1:B:261:GLU:HG2	1:B:262:PHE:CD1	2.56	0.41
1:B:269:TYR:HB3	1:B:299:TYR:HE2	1.86	0.41
1:B:564:ALA:HA	1:B:567:ARG:NE	2.36	0.41
1:A:178:ARG:HH12	1:A:340:VAL:HG23	1.85	0.40
1:B:91:GLY:O	1:B:94:LYS:HG2	2.21	0.40
1:B:302:ALA:HA	1:B:369:ASP:OD2	2.21	0.40
1:A:180:TYR:HA	3:A:843:HOH:O	2.21	0.40
1:A:227:LEU:HD12	1:A:227:LEU:HA	1.72	0.40
1:A:546:PHE:O	1:A:575:ILE:HG13	2.22	0.40
1:B:522:ALA:O	1:B:526:LEU:HA	2.21	0.40
1:A:214:THR:HB	1:A:337:ARG:HD3	2.04	0.40
1:B:445:PRO:HA	1:B:465:LYS:HE3	2.03	0.40
1:A:506:TRP:HB3	1:A:543:TYR:CE2	2.56	0.40
1:A:578:ASP:CG	1:A:581:LEU:HB3	2.46	0.40
1:B:190:ASN:OD1	1:B:190:ASN:C	2.64	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:B:874:HOH:O	3:B:878:HOH:O[1_556]	2.01	0.19

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	593/603 (98%)	472 (80%)	91 (15%)	30 (5%)	1	5
1	B	593/603 (98%)	472 (80%)	92 (16%)	29 (5%)	1	6
All	All	1186/1206 (98%)	944 (80%)	183 (15%)	59 (5%)	1	5

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	THR
1	A	216	THR
1	A	287	GLY
1	A	323	LYS
1	A	324	TYR
1	A	353	GLU
1	A	410	THR
1	A	454	ALA
1	A	504	PRO
1	A	513	SER
1	B	102	ASN
1	B	258	ILE
1	B	259	SER
1	B	410	THR
1	B	439	GLY
1	B	474	MSE
1	B	509	ALA
1	B	536	SER
1	A	204	ASP
1	A	348	VAL
1	A	436	MSE
1	A	455	LEU
1	A	458	ASP
1	A	467	LYS
1	A	521	VAL

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Mol	Chain	Res	Type
1	A	552	THR
1	A	580	ASP
1	B	190	ASN
1	B	256	LEU
1	B	500	LEU
1	B	504	PRO
1	B	537	GLN
1	A	321	ALA
1	A	440	THR
1	A	551	GLU
1	B	338	ALA
1	B	348	VAL
1	B	350	SER
1	B	467	LYS
1	B	505	ALA
1	B	551	GLU
1	A	335	PRO
1	A	459	ASN
1	B	289	SER
1	B	316	ALA
1	B	321	ALA
1	B	335	PRO
1	B	454	ALA
1	A	316	ALA
1	A	350	SER
1	A	553	ALA
1	B	286	THR
1	B	570	ILE
1	A	236	SER
1	B	236	SER
1	B	456	VAL
1	A	340	VAL
1	A	527	GLY
1	B	527	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	518/517 (100%)	514 (99%)	4 (1%)	73	90
1	B	518/517 (100%)	514 (99%)	4 (1%)	73	90
All	All	1036/1034 (100%)	1028 (99%)	8 (1%)	73	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	CYS
1	A	286	THR
1	A	416	THR
1	A	443	ARG
1	B	11	GLN
1	B	199	THR
1	B	435	ASP
1	B	510	VAL

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

Mol	Chain	Res	Type
1	A	51	ASN
1	A	116	ASN
1	A	492	GLN
1	A	548	GLN
1	A	562	ASN
1	B	86	ASN
1	B	177	ASN
1	B	464	HIS
1	B	554	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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

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	589/603 (97%)	0.88	84 (14%) 6 5	32, 73, 173, 206	0
1	B	589/603 (97%)	0.84	82 (13%) 6 5	33, 71, 175, 208	0
All	All	1178/1206 (97%)	0.86	166 (14%) 6 5	32, 72, 174, 208	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	PRO	4.8
1	B	545	ILE	4.6
1	A	457	TYR	4.6
1	A	342	CYS	4.6
1	A	334	ILE	4.4
1	A	455	LEU	4.2
1	A	339	ARG	4.1
1	A	338	ALA	4.1
1	A	346	PHE	4.1
1	A	561	PHE	4.1
1	B	564	ALA	4.1
1	A	343	PHE	4.1
1	B	574	CYS	4.0
1	A	344	ASP	3.9
1	B	561	PHE	3.9
1	A	333	ILE	3.8
1	B	340	VAL	3.8
1	B	16	CYS	3.6
1	A	484	VAL	3.6
1	B	345	LYS	3.5
1	A	475	PHE	3.5
1	A	340	VAL	3.5
1	B	509	ALA	3.5
1	B	546	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	258	ILE	3.4
1	B	525	ILE	3.4
1	A	303	ARG	3.4
1	A	521	VAL	3.3
1	B	346	PHE	3.3
1	B	550	THR	3.3
1	B	592	ILE	3.2
1	A	510	VAL	3.2
1	B	272	VAL	3.2
1	A	286	THR	3.2
1	A	487	ALA	3.2
1	B	548	GLN	3.1
1	B	543	TYR	3.1
1	A	336	ALA	3.1
1	A	500	LEU	3.1
1	B	521	VAL	3.0
1	A	156	GLU	3.0
1	B	343	PHE	3.0
1	B	448	ILE	3.0
1	B	590	LEU	3.0
1	B	288	LYS	3.0
1	B	573	LEU	3.0
1	B	19	CYS	3.0
1	B	456	VAL	3.0
1	A	348	VAL	2.9
1	B	252	LEU	2.9
1	B	348	VAL	2.9
1	B	333	ILE	2.9
1	B	593	PRO	2.9
1	B	339	ARG	2.9
1	A	252	LEU	2.9
1	B	327	ILE	2.9
1	B	510	VAL	2.8
1	B	544	VAL	2.8
1	A	493	ILE	2.8
1	A	288	LYS	2.8
1	A	337	ARG	2.7
1	A	249	ILE	2.7
1	A	67	GLY	2.7
1	A	479	VAL	2.7
1	A	505	ALA	2.7
1	A	375	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	579	ARG	2.6
1	B	284	PRO	2.6
1	B	338	ALA	2.6
1	A	205	TYR	2.6
1	A	543	TYR	2.6
1	B	556	CYS	2.6
1	B	469	ALA	2.6
1	A	593	PRO	2.6
1	A	345	LYS	2.6
1	B	322	LEU	2.6
1	A	592	ILE	2.6
1	B	572	ILE	2.6
1	A	464	HIS	2.6
1	A	295	LEU	2.6
1	A	565	ILE	2.6
1	B	307	THR	2.6
1	A	463	ALA	2.6
1	B	568	ALA	2.6
1	B	565	ILE	2.5
1	A	590	LEU	2.5
1	A	525	ILE	2.5
1	B	530	THR	2.5
1	A	574	CYS	2.5
1	A	456	VAL	2.5
1	B	567	ARG	2.5
1	B	-1	ASN	2.5
1	A	585	LEU	2.5
1	B	570	ILE	2.5
1	B	547	THR	2.5
1	A	297	LEU	2.4
1	B	585	LEU	2.4
1	B	577	SER	2.4
1	A	444	CYS	2.4
1	A	570	ILE	2.4
1	B	511	PHE	2.4
1	A	258	ILE	2.4
1	B	505	ALA	2.4
1	A	481	THR	2.4
1	A	438	LEU	2.4
1	B	571	GLY	2.4
1	A	517	SER	2.4
1	A	568	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	322	LEU	2.3
1	A	526	LEU	2.3
1	B	553	ALA	2.3
1	A	581	LEU	2.3
1	B	581	LEU	2.3
1	B	506	TRP	2.3
1	A	188	THR	2.3
1	B	457	TYR	2.3
1	B	282	GLY	2.3
1	B	249	ILE	2.3
1	A	327	ILE	2.3
1	B	286	THR	2.3
1	B	496	VAL	2.3
1	B	563	VAL	2.3
1	A	478	GLY	2.3
1	A	191	SER	2.2
1	B	495	VAL	2.2
1	A	254	PRO	2.2
1	B	205	TYR	2.2
1	A	572	ILE	2.2
1	A	491	PRO	2.2
1	B	247	VAL	2.2
1	B	426	CYS	2.2
1	B	485	SER	2.2
1	A	325	LEU	2.2
1	A	506	TRP	2.2
1	B	298	TYR	2.2
1	A	577	SER	2.2
1	A	347	LYS	2.1
1	A	285	GLY	2.1
1	A	351	THR	2.1
1	B	473	LYS	2.1
1	B	527	GLY	2.1
1	B	352	LEU	2.1
1	A	269	TYR	2.1
1	B	515	TYR	2.1
1	A	441	CYS	2.1
1	B	342	CYS	2.1
1	A	399	ILE	2.1
1	B	187	VAL	2.1
1	A	546	PHE	2.1
1	B	325	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	500	LEU	2.1
1	B	217	TYR	2.1
1	B	594	ARG	2.1
1	B	29	CYS	2.1
1	A	452	VAL	2.1
1	B	439	GLY	2.1
1	A	448	ILE	2.1
1	A	520	ALA	2.1
1	B	197	GLU	2.1
1	A	29	CYS	2.1
1	B	487	ALA	2.1
1	A	426	CYS	2.0
1	A	374	ASP	2.0
1	A	571	GLY	2.0
1	A	547	THR	2.0
1	B	374	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	ZN	B	703	1/1	0.88	0.31	337,337,337,337	0
2	ZN	A	701	1/1	0.98	0.06	54,54,54,54	0
2	ZN	B	702	1/1	0.99	0.08	109,109,109,109	0
2	ZN	B	701	1/1	0.99	0.04	50,50,50,50	0
2	ZN	A	703	1/1	1.00	0.02	30,30,30,30	0
2	ZN	A	702	1/1	1.00	0.04	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.