



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:16 PM UTC

PDB ID : 1OHF / pdb_00001ohf
Title : The refined structure of Nudaurelia capensis omega virus
Authors : Helgstrand, C.; Munshi, S.; Johnson, J.E.; Liljas, L.
Deposited on : 2003-05-26
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
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

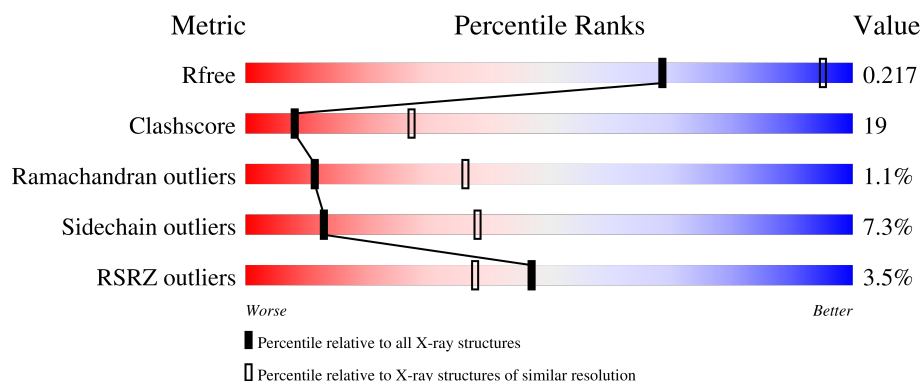
1 Overall quality at a glance

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	570	2% 53% 31% 6% 11%
1	B	570	4% 56% 30% 6% 8%
1	C	570	2% 64% 25% 8%
1	D	570	2% 62% 26% 5% 7%
2	E	74	3% 24% 15% 61%

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Mol	Chain	Length	Quality of chain
2	F	74	15%12%73%
2	G	74	7%46%32%8%12%
2	H	74	16%49%19%11%20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17851 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 p70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			3925	2496	651	766	12			
1	B	527	Total	C	N	O	S	0	0	0
			4044	2565	672	795	12			
1	C	525	Total	C	N	O	S	0	0	0
			4034	2558	671	793	12			
1	D	528	Total	C	N	O	S	0	0	0
			4052	2571	673	796	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	ARG	HIS	variant	UNP Q4TVS9
A	204	THR	ALA	variant	UNP Q4TVS9
B	37	ARG	HIS	variant	UNP Q4TVS9
B	204	THR	ALA	variant	UNP Q4TVS9
C	37	ARG	HIS	variant	UNP Q4TVS9
C	204	THR	ALA	variant	UNP Q4TVS9
D	37	ARG	HIS	variant	UNP Q4TVS9
D	204	THR	ALA	variant	UNP Q4TVS9

- Molecule 2 is a protein called p70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	29	Total	C	N	O	S	0	0	0
			209	136	32	40	1			
2	F	20	Total	C	N	O	S	0	0	0
			143	94	22	26	1			
2	G	65	Total	C	N	O	S	0	0	0
			485	303	99	81	2			
2	H	59	Total	C	N	O	S	0	0	0
			439	275	88	74	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	576	LEU	SER	variant	UNP Q4TVS9
F	576	LEU	SER	variant	UNP Q4TVS9
G	576	LEU	SER	variant	UNP Q4TVS9
H	576	LEU	SER	variant	UNP Q4TVS9

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

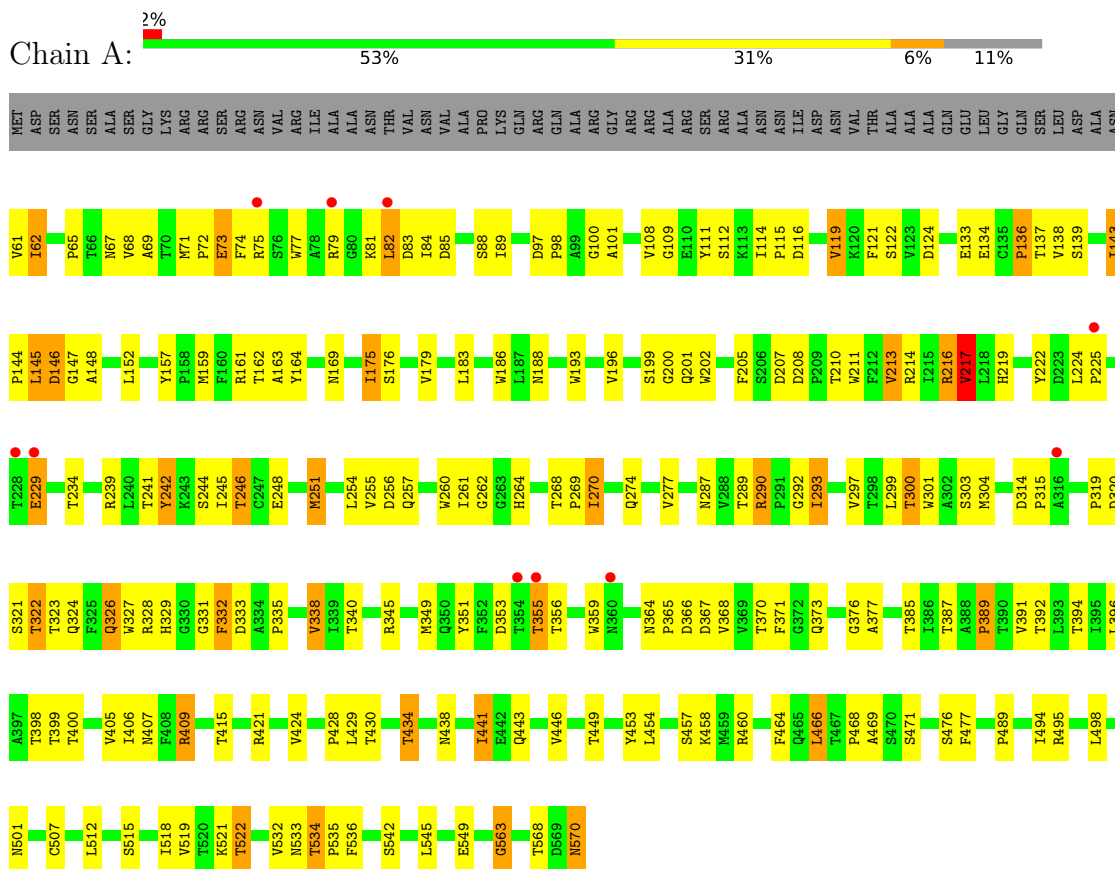
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	97	Total O 97 97	0	0
4	B	127	Total O 127 127	0	0
4	C	148	Total O 148 148	0	0
4	D	144	Total O 144 144	0	0

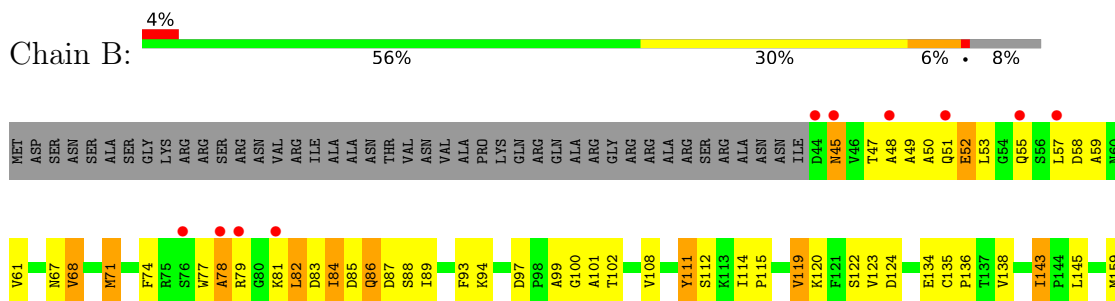
3 Residue-property plots [i](#)

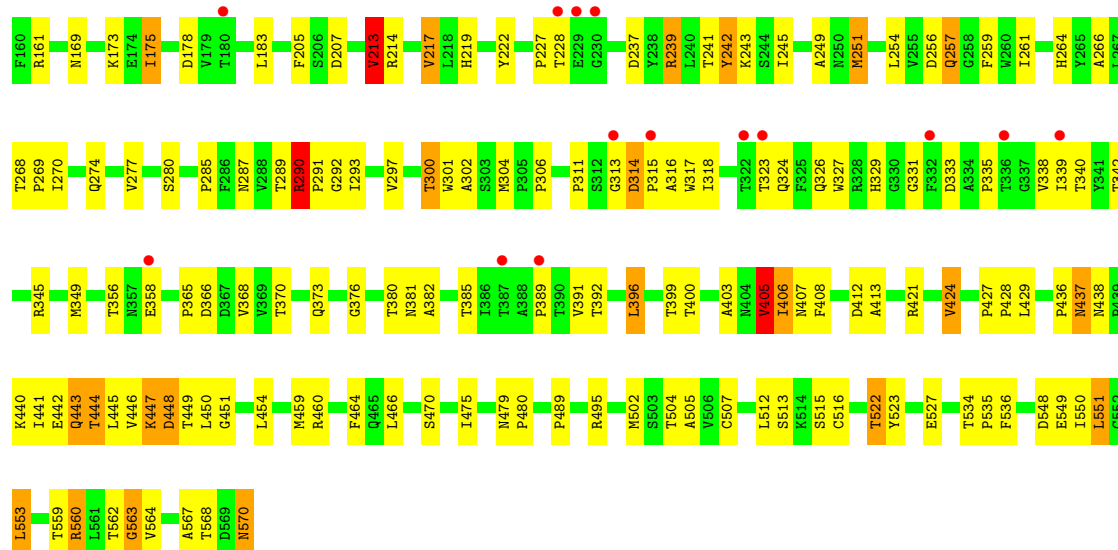
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: p70

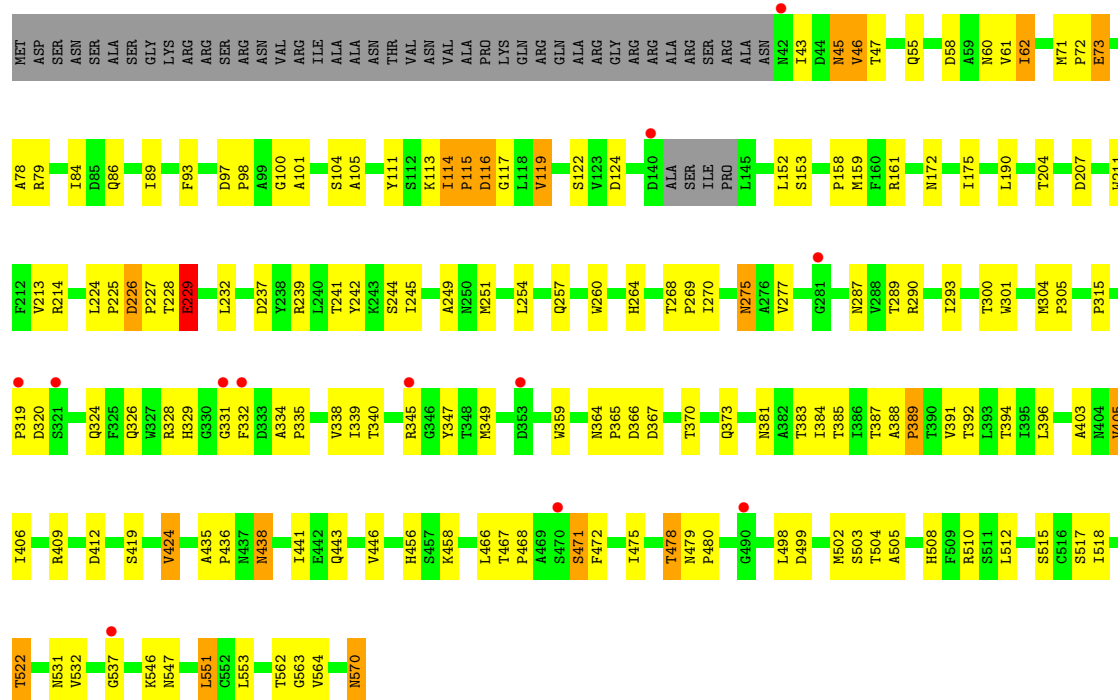


• Molecule 1: p70

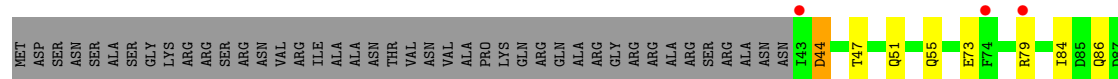


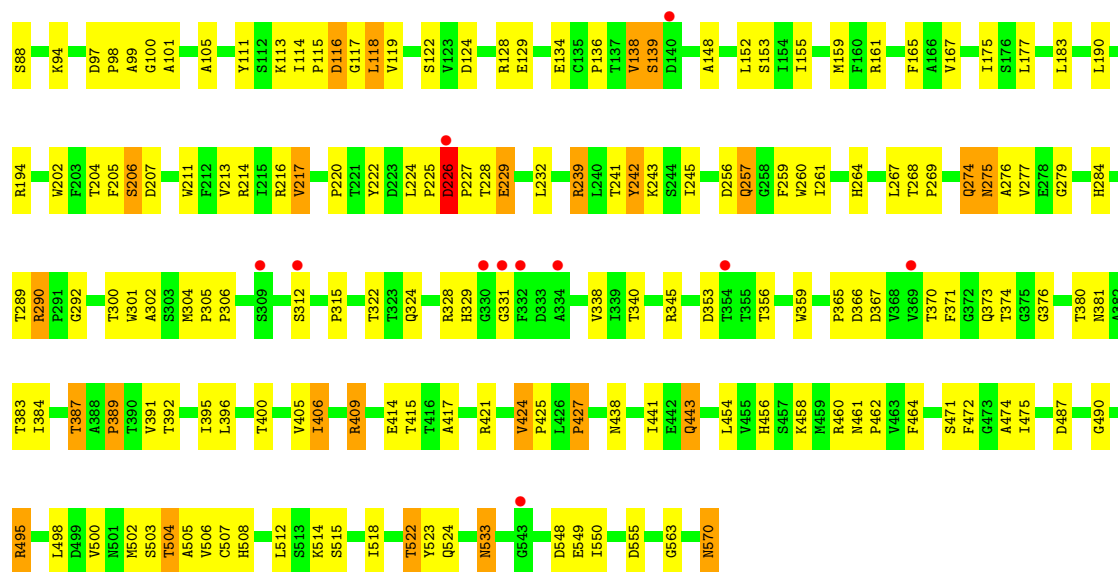


• Molecule 1: p70

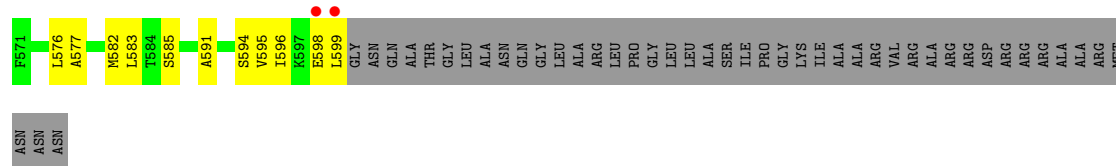


• Molecule 1: p70

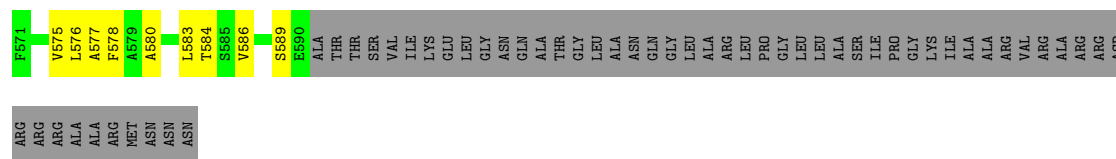




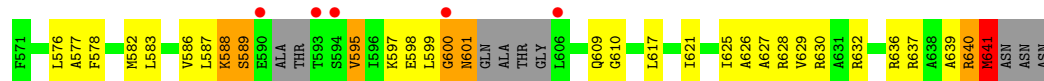
- Molecule 2: p70



- Molecule 2: p70



- Molecule 2: p70



- Molecule 2: p70





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	413.55Å 410.22Å 419.67Å 59.13° 58.90° 64.04°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	50.9 (20.00-2.80) 50.8 (20.00-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.07 (at 2.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.221 0.214 , 0.217	Depositor DCC
R_{free} test set	24978 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 97.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.045 for h-l,h,h-k 0.045 for k,k-l,-h+k 0.046 for -k,-h,-l 0.046 for -h+l,-k+l,l 0.046 for k-l,h-l,-l 0.046 for -h,-h+l,-h+k 0.046 for -k+l,-k,h-k	Xtriage
F_o, F_c correlation	0.24	EDS
Total number of atoms	17851	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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: MG

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	0/4034	1.00	23/5532 (0.4%)
1	B	0.50	0/4153	1.02	24/5695 (0.4%)
1	C	0.47	0/4141	0.98	21/5676 (0.4%)
1	D	0.46	0/4161	1.01	18/5706 (0.3%)
2	E	0.64	0/210	0.96	1/284 (0.4%)
2	F	0.59	0/144	0.96	1/194 (0.5%)
2	G	0.72	1/486 (0.2%)	0.95	1/648 (0.2%)
2	H	0.85	0/441	1.13	4/590 (0.7%)
All	All	0.50	1/17770 (0.0%)	1.00	93/24325 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	641	MET	SD-CE	6.68	1.96	1.79

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	614	LEU	CA-C-N	9.78	132.07	119.84
2	H	614	LEU	C-N-CA	9.78	132.07	119.84
1	B	143	ILE	CA-C-N	9.68	129.31	119.24
1	B	143	ILE	C-N-CA	9.68	129.31	119.24
1	A	207	ASP	N-CA-C	-9.20	101.25	111.28
1	D	274	GLN	N-CA-C	-8.53	102.89	113.38
1	A	145	LEU	N-CA-C	-8.47	100.57	111.92
1	C	207	ASP	N-CA-C	-8.01	102.53	111.82
1	A	405	VAL	N-CA-C	7.78	120.05	108.46
1	D	290	ARG	CA-C-N	7.70	127.25	119.24
1	D	290	ARG	C-N-CA	7.70	127.25	119.24
1	B	207	ASP	N-CA-C	-7.59	102.98	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	290	ARG	CA-C-N	7.53	128.21	119.47
1	C	290	ARG	C-N-CA	7.53	128.21	119.47
1	B	290	ARG	CA-C-N	7.47	127.01	119.24
1	B	290	ARG	C-N-CA	7.47	127.01	119.24
1	D	207	ASP	N-CA-C	-7.35	103.41	112.38
1	B	405	VAL	N-CA-C	7.03	120.20	108.81
1	C	116	ASP	N-CA-C	7.00	118.70	111.14
1	B	349	MET	N-CA-C	6.95	120.76	110.48
1	D	256	ASP	N-CA-C	6.89	122.42	111.81
1	D	117	GLY	N-CA-C	-6.84	102.08	114.46
1	A	322	THR	N-CA-C	-6.80	99.49	109.63
2	E	577	ALA	N-CA-C	-6.71	103.89	111.07
1	A	349	MET	N-CA-C	6.64	120.31	110.48
1	D	405	VAL	N-CA-C	6.56	119.43	108.81
1	D	406	ILE	N-CA-C	-6.54	98.96	108.11
1	B	119	VAL	N-CA-C	6.46	117.90	108.53
1	C	471	SER	N-CA-C	6.46	120.99	113.18
1	B	45	ASN	N-CA-C	-6.39	104.97	112.89
1	D	206	SER	N-CA-C	6.31	119.82	109.85
1	D	279	GLY	N-CA-C	6.23	118.45	111.85
1	A	290	ARG	CA-C-N	6.20	126.39	119.32
1	A	290	ARG	C-N-CA	6.20	126.39	119.32
1	B	71	MET	CA-C-N	6.16	127.54	119.84
1	B	71	MET	C-N-CA	6.16	127.54	119.84
1	B	87	ASP	N-CA-C	-6.12	104.16	111.69
1	C	405	VAL	N-CA-C	6.08	118.47	108.99
1	D	427	PRO	N-CA-C	-6.02	103.36	110.70
1	B	111	TYR	N-CA-C	6.00	120.30	113.15
1	A	406	ILE	N-CA-C	-6.00	99.71	108.11
1	D	275	ASN	N-CA-C	5.89	119.27	109.96
1	C	502	MET	N-CA-C	5.79	118.23	110.35
1	B	213	VAL	CB-CA-C	-5.78	103.27	111.19
1	D	276	ALA	N-CA-C	-5.72	98.61	110.80
1	C	515	SER	N-CA-C	-5.71	106.31	113.28
1	B	219	HIS	N-CA-C	5.67	121.26	113.77
2	H	615	PRO	N-CA-C	5.65	124.10	112.47
1	A	270	ILE	N-CA-C	-5.63	100.29	108.17
1	A	111	TYR	N-CA-C	5.63	119.68	113.21
2	F	577	ALA	N-CA-C	-5.62	105.05	111.07
1	C	111	TYR	N-CA-C	5.62	119.61	112.87
1	C	438	ASN	CA-C-N	5.61	125.22	119.56
1	C	438	ASN	C-N-CA	5.61	125.22	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	254	LEU	N-CA-C	5.61	117.47	111.36
1	D	119	VAL	N-CA-C	5.61	117.98	109.12
1	B	502	MET	N-CA-C	5.57	117.73	110.43
1	B	443	GLN	N-CA-C	5.55	117.55	108.55
1	A	332	PHE	N-CA-C	-5.54	105.78	112.54
1	A	119	VAL	N-CA-C	5.50	116.91	108.71
1	C	332	PHE	N-CA-C	-5.50	105.37	111.36
1	D	111	TYR	N-CA-C	5.50	119.60	113.01
1	B	447	LYS	N-CA-C	-5.46	105.41	111.36
1	D	515	SER	N-CA-C	-5.38	106.56	113.23
1	C	119	VAL	N-CA-C	5.37	116.72	108.71
1	C	229	GLU	N-CA-C	-5.37	105.59	111.82
1	A	534	THR	CA-C-N	5.30	124.91	119.56
1	A	534	THR	C-N-CA	5.30	124.91	119.56
1	B	567	ALA	N-CA-C	-5.30	105.62	111.71
1	D	563	GLY	N-CA-C	-5.29	108.02	115.32
1	B	427	PRO	N-CA-C	-5.28	104.25	110.70
1	C	60	ASN	N-CA-C	5.28	119.03	112.59
1	A	202	TRP	N-CA-C	-5.28	100.70	109.46
1	A	471	SER	N-CA-C	5.25	119.69	113.28
1	B	57	LEU	N-CA-C	5.24	120.53	113.72
1	B	436	PRO	N-CA-C	5.21	120.37	113.86
1	C	115	PRO	CA-C-N	5.17	127.48	120.44
1	C	115	PRO	C-N-CA	5.17	127.48	120.44
1	B	437	ASN	N-CA-C	5.15	119.52	112.88
2	H	596	ILE	CB-CA-C	-5.15	105.11	111.70
1	A	147	GLY	N-CA-C	-5.10	101.08	113.18
1	A	143	ILE	CA-C-N	5.09	126.21	119.84
1	A	143	ILE	C-N-CA	5.09	126.21	119.84
1	C	117	GLY	N-CA-C	-5.09	106.11	114.76
1	D	502	MET	N-CA-C	5.08	117.23	110.53
1	B	406	ILE	N-CA-C	-5.07	101.02	108.11
1	A	217	VAL	N-CA-CB	-5.06	106.08	112.60
1	C	114	ILE	CA-C-N	5.05	126.15	119.84
1	C	114	ILE	C-N-CA	5.05	126.15	119.84
1	A	219	HIS	N-CA-C	5.05	119.81	113.25
1	A	303	SER	N-CA-C	5.03	118.71	112.47
2	G	577	ALA	N-CA-C	-5.03	105.68	111.07
1	A	563	GLY	N-CA-C	-5.00	108.42	115.32

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	3925	0	3764	185	0
1	B	4044	0	3872	176	0
1	C	4034	0	3860	152	0
1	D	4052	0	3883	134	0
2	E	209	0	223	14	0
2	F	143	0	149	14	0
2	G	485	0	529	44	0
2	H	439	0	480	31	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	97	0	0	3	0
4	B	127	0	0	5	0
4	C	148	0	0	1	0
4	D	144	0	0	4	0
All	All	17851	0	16760	663	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (663) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:PRO:HB2	1:A:434:THR:HG22	1.34	1.08
1:A:175:ILE:HD11	1:A:429:LEU:HB3	1.37	1.06
1:B:342:THR:HG22	1:B:368:VAL:HG22	1.35	1.04
1:B:269:PRO:HB3	1:B:424:VAL:HG13	1.39	0.99
1:A:329:HIS:CE1	1:A:373:GLN:HE22	1.79	0.98
2:E:596:ILE:HG21	1:B:47:THR:HG22	1.46	0.98
1:A:570:ASN:C	1:A:570:ASN:HD22	1.72	0.97
1:D:269:PRO:HB3	1:D:424:VAL:HG13	1.47	0.96
1:C:570:ASN:HD22	1:C:570:ASN:C	1.72	0.96
1:C:385:THR:HG22	1:C:394:THR:HG22	1.48	0.94
1:A:329:HIS:HE1	1:A:373:GLN:HE22	0.97	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:MET:HE3	1:D:475:ILE:HD12	1.49	0.93
1:D:570:ASN:C	1:D:570:ASN:HD22	1.74	0.93
2:E:596:ILE:HG21	1:B:47:THR:CG2	1.98	0.93
1:A:157:TYR:HB2	1:A:159:MET:HE2	1.51	0.91
1:D:257:GLN:H	1:D:257:GLN:HE21	1.16	0.91
1:B:570:ASN:C	1:B:570:ASN:HD22	1.75	0.91
1:B:440:LYS:HD2	1:B:562:THR:HG22	1.52	0.90
1:C:101:ALA:N	2:G:576:LEU:HD11	1.88	0.89
1:A:152:LEU:HD23	1:A:518:ILE:HD12	1.55	0.89
1:A:385:THR:HG22	1:A:394:THR:HG22	1.53	0.89
1:B:78:ALA:HB3	1:B:81:LYS:HD2	1.53	0.88
1:B:228:THR:HG22	1:B:323:THR:HG21	1.55	0.87
1:D:292:GLY:HA2	1:D:400:THR:HG22	1.56	0.87
1:A:84:ILE:HG23	1:A:89:ILE:HD11	1.55	0.86
1:B:560:ARG:HG3	1:C:72:PRO:HD2	1.54	0.86
1:B:169:ASN:ND2	1:B:173:LYS:H	1.74	0.86
1:D:329:HIS:HE1	1:D:373:GLN:HE22	1.22	0.85
1:C:159:MET:HE3	1:C:475:ILE:HD12	1.56	0.84
1:B:314:ASP:HA	1:B:315:PRO:C	1.99	0.84
1:D:257:GLN:H	1:D:257:GLN:NE2	1.76	0.83
2:H:593:THR:HG22	2:H:594:SER:H	1.42	0.83
1:B:84:ILE:HD12	1:B:84:ILE:H	1.42	0.83
1:A:175:ILE:HD11	1:A:429:LEU:CB	2.10	0.81
1:B:444:THR:HG21	1:B:448:ASP:OD2	1.81	0.80
2:H:587:LEU:HD23	2:H:596:ILE:HD13	1.61	0.80
1:B:159:MET:HE3	1:B:475:ILE:HD12	1.63	0.80
1:A:101:ALA:HA	2:E:576:LEU:HD22	1.64	0.79
2:G:600:GLY:O	2:G:601:ASN:HB2	1.82	0.78
1:A:570:ASN:C	1:A:570:ASN:ND2	2.37	0.78
1:D:99:ALA:HB1	1:D:570:ASN:HD21	1.48	0.78
1:B:570:ASN:C	1:B:570:ASN:ND2	2.40	0.77
1:D:257:GLN:HE21	1:D:257:GLN:N	1.80	0.77
1:B:169:ASN:HD22	1:B:173:LYS:H	1.30	0.77
1:C:97:ASP:HB3	2:G:576:LEU:HD21	1.65	0.77
1:D:101:ALA:N	2:H:576:LEU:HD11	2.01	0.76
1:D:533:ASN:N	1:D:533:ASN:HD22	1.83	0.76
2:G:639:ALA:C	2:G:641:MET:H	1.95	0.75
1:C:62:ILE:HD12	1:D:128:ARG:HD2	1.68	0.74
1:A:254:LEU:HG	1:A:255:VAL:HG13	1.69	0.74
1:B:300:THR:HB	1:B:326:GLN:HG3	1.68	0.74
1:B:268:THR:OG1	1:B:460:ARG:HD2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:570:ASN:C	1:D:570:ASN:ND2	2.46	0.73
1:B:292:GLY:HA2	1:B:400:THR:HG22	1.70	0.73
1:D:97:ASP:HB3	2:H:576:LEU:CD2	2.19	0.72
1:D:100:GLY:C	2:H:576:LEU:HD11	2.14	0.72
1:C:347:TYR:HB3	1:C:349:MET:HE3	1.71	0.72
1:A:73:GLU:HG2	1:A:545:LEU:HD13	1.72	0.72
1:A:329:HIS:HE1	1:A:373:GLN:NE2	1.81	0.72
1:B:85:ASP:O	1:B:86:GLN:HB2	1.90	0.71
1:A:329:HIS:CE1	1:A:373:GLN:NE2	2.57	0.71
1:B:340:THR:HG22	1:B:370:THR:HG22	1.71	0.71
1:B:329:HIS:HE1	1:B:373:GLN:OE1	1.73	0.71
1:A:97:ASP:CG	2:E:576:LEU:HD11	2.16	0.71
1:A:430:THR:O	1:A:434:THR:HG23	1.91	0.71
1:C:570:ASN:O	1:C:570:ASN:ND2	2.23	0.71
1:D:329:HIS:CE1	1:D:373:GLN:HE22	2.07	0.71
1:D:97:ASP:HB3	2:H:576:LEU:HD21	1.71	0.71
1:D:381:ASN:HB3	1:D:396:LEU:HD11	1.73	0.71
2:H:590:GLU:HG3	2:H:591:ALA:H	1.55	0.71
1:A:293:ILE:N	1:A:293:ILE:HD12	2.06	0.70
1:C:381:ASN:HB3	1:C:396:LEU:HD11	1.72	0.70
1:A:217:VAL:HG21	1:A:222:TYR:CD1	2.26	0.70
1:A:260:TRP:O	1:A:443:GLN:HG2	1.90	0.70
1:C:116:ASP:OD1	1:C:239:ARG:NH2	2.25	0.70
1:A:146:ASP:HB3	1:A:148:ALA:H	1.56	0.70
1:C:319:PRO:HG2	1:D:322:THR:HG23	1.73	0.70
2:H:581:ASN:ND2	2:H:601:ASN:HD22	1.90	0.70
1:C:152:LEU:HD23	1:C:518:ILE:HD12	1.74	0.70
1:B:274:GLN:HG3	1:B:421:ARG:NH1	2.07	0.69
1:A:84:ILE:CG2	1:A:89:ILE:HD11	2.21	0.69
1:B:85:ASP:HB3	1:B:88:SER:HB2	1.73	0.69
1:A:287:ASN:HD21	1:A:289:THR:HG22	1.56	0.69
1:D:101:ALA:HA	2:H:576:LEU:HD11	1.75	0.69
1:C:320:ASP:HB3	1:C:326:GLN:HG2	1.73	0.69
1:C:116:ASP:CG	1:C:239:ARG:HH22	2.00	0.69
1:D:570:ASN:ND2	1:D:570:ASN:O	2.26	0.68
1:A:199:SER:O	1:A:201:GLN:N	2.25	0.68
1:C:100:GLY:C	2:G:576:LEU:HD11	2.19	0.68
2:H:592:THR:HG22	2:H:596:ILE:HD11	1.75	0.68
1:A:322:THR:HG22	1:A:323:THR:H	1.59	0.68
1:A:73:GLU:HG2	1:A:545:LEU:CD1	2.24	0.68
1:D:101:ALA:CA	2:H:576:LEU:HD11	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:VAL:O	1:D:139:SER:HB3	1.95	0.67
1:A:329:HIS:HD2	1:A:331:GLY:H	1.43	0.67
1:B:315:PRO:HG2	1:B:333:ASP:O	1.94	0.67
1:C:97:ASP:HB3	2:G:576:LEU:CD2	2.23	0.67
1:D:44:ASP:OD2	1:D:47:THR:HG23	1.95	0.66
1:C:62:ILE:CD1	1:D:128:ARG:HD2	2.25	0.66
1:D:217:VAL:HG21	1:D:222:TYR:CD1	2.31	0.66
1:A:133:GLU:OE2	1:A:216:ARG:HD2	1.94	0.66
1:B:270:ILE:CD1	1:C:471:SER:HA	2.25	0.66
1:D:88:SER:HB3	1:D:550:ILE:HG13	1.77	0.66
1:C:385:THR:HG22	1:C:394:THR:CG2	2.25	0.66
2:G:597:LYS:HG2	2:G:636:ARG:HH12	1.61	0.66
1:A:340:THR:HG22	1:A:370:THR:HG22	1.78	0.65
1:D:113:LYS:HE3	1:D:124:ASP:OD1	1.97	0.65
1:C:229:GLU:H	1:C:229:GLU:CD	2.02	0.65
1:C:260:TRP:O	1:C:443:GLN:HG2	1.96	0.65
1:A:385:THR:HG22	1:A:394:THR:CG2	2.24	0.65
1:B:51:GLN:O	1:B:55:GLN:HG3	1.97	0.65
1:D:268:THR:OG1	1:D:460:ARG:HD2	1.96	0.65
1:B:245:ILE:HG12	1:B:522:THR:HB	1.79	0.65
1:B:560:ARG:NH2	1:C:58:ASP:OD2	2.28	0.65
2:F:586:VAL:O	2:F:589:SER:HB3	1.96	0.65
1:B:101:ALA:HA	2:F:576:LEU:CD2	2.27	0.65
1:A:62:ILE:HD12	1:A:62:ILE:N	2.12	0.64
1:A:199:SER:C	1:A:201:GLN:H	2.05	0.64
1:C:71:MET:HB3	1:C:73:GLU:OE2	1.97	0.64
1:A:319:PRO:HG3	1:A:327:TRP:CH2	2.32	0.64
1:D:214:ARG:HD3	1:D:216:ARG:NE	2.13	0.64
2:H:640:ARG:HG2	2:H:640:ARG:O	1.97	0.64
1:B:58:ASP:H	1:B:67:ASN:HD21	1.45	0.64
1:B:342:THR:CG2	1:B:368:VAL:HG22	2.22	0.64
1:A:251:MET:HE2	1:A:256:ASP:CA	2.27	0.64
1:A:161:ARG:HG2	1:A:222:TYR:HA	1.80	0.63
1:B:340:THR:HG22	1:B:370:THR:CG2	2.27	0.63
1:B:86:GLN:NE2	1:B:108:VAL:HG21	2.13	0.63
1:C:438:ASN:HB3	1:C:441:ILE:HG23	1.79	0.63
1:C:315:PRO:CG	1:C:331:GLY:HA3	2.28	0.63
1:A:101:ALA:HA	2:E:576:LEU:CD2	2.29	0.63
1:C:245:ILE:HG12	1:C:522:THR:HB	1.79	0.63
1:B:489:PRO:HB3	1:C:277:VAL:HG11	1.80	0.62
1:D:353:ASP:OD2	1:D:356:THR:HG23	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ASN:HB3	1:B:441:ILE:HG12	1.82	0.62
1:A:229:GLU:OE2	1:A:321:SER:HB2	1.98	0.62
1:B:97:ASP:CG	2:F:576:LEU:HD11	2.25	0.62
1:C:275:ASN:HD22	1:C:275:ASN:H	1.47	0.62
1:A:364:ASN:HB3	1:A:365:PRO:HD2	1.81	0.62
1:D:301:TRP:CD2	1:D:304:MET:HG3	2.34	0.62
1:B:293:ILE:HA	1:B:399:THR:HG22	1.82	0.62
1:A:428:PRO:CB	1:A:434:THR:HG22	2.22	0.61
1:A:67:ASN:HD21	1:A:69:ALA:CB	2.12	0.61
1:A:67:ASN:HD21	1:A:69:ALA:HB3	1.65	0.61
1:A:269:PRO:CG	1:A:498:LEU:HD23	2.30	0.61
1:B:454:LEU:HD11	1:B:507:CYS:HB2	1.80	0.61
1:C:249:ALA:CB	1:C:251:MET:HE2	2.30	0.61
2:H:588:LYS:C	2:H:590:GLU:H	2.06	0.61
1:C:101:ALA:CA	2:G:576:LEU:HD11	2.30	0.61
1:C:113:LYS:HE2	1:C:122:SER:OG	2.01	0.61
1:D:245:ILE:HG12	1:D:522:THR:HB	1.81	0.61
1:A:269:PRO:HG3	1:A:498:LEU:HD23	1.82	0.61
2:G:586:VAL:HG12	2:G:587:LEU:HD23	1.82	0.61
1:D:101:ALA:HA	2:H:576:LEU:CD1	2.31	0.61
1:B:88:SER:HB3	1:B:550:ILE:CD1	2.31	0.61
1:B:280:SER:HB3	1:B:413:ALA:HA	1.83	0.61
1:C:98:PRO:CG	1:C:244:SER:HB3	2.31	0.60
1:C:338:VAL:CG1	1:C:370:THR:HB	2.31	0.60
1:A:533:ASN:HD22	1:C:480:PRO:HG3	1.66	0.60
1:A:239:ARG:HB3	1:A:466:LEU:HD12	1.82	0.60
1:A:345:ARG:HA	1:A:365:PRO:HB3	1.84	0.60
1:B:449:THR:O	1:B:451:GLY:N	2.29	0.60
2:G:610:GLY:HA3	2:G:621:ILE:O	2.01	0.60
1:A:245:ILE:HG12	1:A:522:THR:HB	1.84	0.59
1:C:225:PRO:C	1:C:227:PRO:HD3	2.27	0.59
2:E:582:MET:HE1	1:B:71:MET:SD	2.42	0.59
1:B:85:ASP:O	1:B:86:GLN:CB	2.50	0.59
1:B:161:ARG:O	1:B:217:VAL:HG22	2.02	0.59
1:A:320:ASP:O	1:A:321:SER:HB3	2.00	0.59
1:D:241:THR:O	1:D:242:TYR:HB3	2.02	0.59
1:A:315:PRO:HG2	1:A:333:ASP:O	2.03	0.59
1:C:359:TRP:CZ3	1:C:409:ARG:HG3	2.37	0.59
1:D:228:THR:HG1	1:D:472:PHE:HE2	1.51	0.59
1:B:381:ASN:HB3	1:B:396:LEU:HD21	1.83	0.59
1:B:88:SER:HB3	1:B:550:ILE:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:THR:O	1:B:564:VAL:N	2.35	0.59
1:A:300:THR:HB	1:A:326:GLN:HG2	1.84	0.59
1:D:456:HIS:HD2	1:D:503:SER:O	1.86	0.59
1:A:67:ASN:ND2	1:A:69:ALA:CB	2.66	0.58
1:A:329:HIS:CD2	1:A:331:GLY:H	2.19	0.58
1:D:161:ARG:HG2	1:D:222:TYR:HA	1.83	0.58
1:D:315:PRO:CG	1:D:331:GLY:HA3	2.33	0.58
1:B:489:PRO:HB3	1:C:277:VAL:CG1	2.32	0.58
1:C:438:ASN:HB3	1:C:441:ILE:CG2	2.33	0.58
1:D:99:ALA:CB	1:D:570:ASN:HD21	2.17	0.58
1:D:504:THR:HG23	4:D:2071:HOH:O	2.03	0.58
1:A:68:VAL:HG22	2:G:582:MET:HE1	1.85	0.58
1:B:251:MET:HG3	1:B:256:ASP:HA	1.85	0.58
1:A:65:PRO:HG2	2:G:578:PHE:CE1	2.39	0.58
1:C:329:HIS:HE1	1:C:373:GLN:OE1	1.87	0.58
2:G:597:LYS:HG2	2:G:636:ARG:NH1	2.19	0.58
1:B:99:ALA:HB1	1:B:570:ASN:HD21	1.67	0.57
1:A:161:ARG:HD3	4:A:2033:HOH:O	2.04	0.57
1:C:161:ARG:NH2	1:C:226:ASP:OD1	2.32	0.57
1:D:97:ASP:OD1	1:D:100:GLY:N	2.36	0.57
1:D:329:HIS:HD2	1:D:331:GLY:H	1.53	0.57
1:A:145:LEU:HD22	1:A:254:LEU:HD23	1.87	0.57
1:D:167:VAL:HG22	1:D:213:VAL:HG12	1.86	0.57
1:A:340:THR:HG22	1:A:370:THR:CG2	2.34	0.57
1:B:67:ASN:HB2	4:B:2004:HOH:O	2.03	0.57
1:A:251:MET:HE2	1:A:256:ASP:HA	1.87	0.57
1:D:116:ASP:OD2	1:D:239:ARG:NH2	2.38	0.57
1:A:108:VAL:HG12	1:A:109:GLY:N	2.19	0.56
1:D:226:ASP:N	1:D:227:PRO:HD3	2.19	0.56
1:A:292:GLY:HA2	1:A:400:THR:HG22	1.86	0.56
1:B:78:ALA:HB3	1:B:81:LYS:CD	2.31	0.56
1:C:114:ILE:C	1:C:116:ASP:H	2.13	0.56
1:C:405:VAL:HG22	1:C:406:ILE:N	2.19	0.56
1:D:113:LYS:HE2	1:D:122:SER:OG	2.05	0.56
1:C:249:ALA:HB1	1:C:251:MET:HE2	1.87	0.56
1:D:454:LEU:HD11	1:D:507:CYS:HB2	1.87	0.56
1:A:119:VAL:HG21	1:A:122:SER:HB3	1.88	0.56
1:A:188:ASN:CG	1:A:476:SER:HB2	2.30	0.56
1:A:205:PHE:CE2	1:A:213:VAL:HG13	2.41	0.56
1:B:264:HIS:CD2	1:B:505:ALA:HB2	2.41	0.56
1:B:313:GLY:O	1:B:314:ASP:HB3	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ALA:O	2:G:637:ARG:NH2	2.34	0.55
1:A:365:PRO:O	1:A:366:ASP:HB2	2.05	0.55
1:C:98:PRO:HG3	1:C:244:SER:HB3	1.88	0.55
1:C:239:ARG:HD2	1:C:466:LEU:CD2	2.36	0.55
1:C:365:PRO:O	1:C:366:ASP:HB2	2.06	0.55
2:H:592:THR:CG2	2:H:596:ILE:HD11	2.36	0.55
1:B:205:PHE:CD2	1:B:213:VAL:CG2	2.90	0.55
1:D:228:THR:OG1	1:D:472:PHE:HE2	1.90	0.55
1:A:320:ASP:CG	1:A:328:ARG:HD2	2.31	0.55
1:A:290:ARG:HD3	1:A:398:THR:O	2.05	0.55
1:B:115:PRO:O	1:B:551:LEU:HD21	2.07	0.55
1:B:329:HIS:CE1	1:B:373:GLN:OE1	2.58	0.55
1:C:62:ILE:CD1	1:D:128:ARG:HH11	2.20	0.55
1:C:275:ASN:HD22	1:C:275:ASN:N	2.04	0.55
1:A:246:THR:HG23	1:A:521:LYS:O	2.07	0.54
2:H:639:ALA:C	2:H:641:MET:H	2.16	0.54
1:D:338:VAL:CG1	1:D:370:THR:HB	2.38	0.54
1:D:533:ASN:HD22	1:D:533:ASN:H	1.52	0.54
1:B:213:VAL:HG12	1:B:214:ARG:H	1.72	0.54
1:A:67:ASN:ND2	1:A:69:ALA:HB2	2.23	0.54
1:D:243:LYS:HD2	1:D:524:GLN:OE1	2.08	0.54
1:A:268:THR:OG1	1:A:460:ARG:HD2	2.07	0.54
1:B:101:ALA:HA	2:F:576:LEU:HD22	1.88	0.54
1:B:285:PRO:HD2	1:B:302:ALA:HB3	1.89	0.54
1:C:161:ARG:HG3	1:C:161:ARG:HH11	1.73	0.54
1:D:373:GLN:HB2	1:D:384:ILE:CD1	2.38	0.54
1:D:373:GLN:HB2	1:D:384:ILE:HD13	1.89	0.54
1:D:421:ARG:NH1	1:D:487:ASP:HB3	2.22	0.54
1:A:82:LEU:HD13	1:A:549:GLU:CB	2.38	0.54
1:A:287:ASN:ND2	1:A:289:THR:CG2	2.71	0.54
1:B:559:THR:HG23	1:C:119:VAL:O	2.08	0.54
1:D:290:ARG:O	1:D:400:THR:HA	2.07	0.54
1:A:246:THR:HG21	1:A:570:ASN:OD1	2.08	0.54
1:C:456:HIS:HD2	1:C:503:SER:O	1.90	0.54
1:D:225:PRO:C	1:D:227:PRO:HD3	2.33	0.54
1:D:373:GLN:HG2	1:D:374:THR:N	2.22	0.54
1:D:284:HIS:HE1	1:D:414:GLU:OE1	1.91	0.53
1:B:560:ARG:NH1	1:C:71:MET:HE2	2.23	0.53
1:A:359:TRP:CZ3	1:A:409:ARG:HB3	2.43	0.53
1:B:287:ASN:HD21	1:B:403:ALA:HA	1.73	0.53
1:B:560:ARG:HD2	1:C:73:GLU:OE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:THR:C	1:B:564:VAL:H	2.15	0.53
1:B:269:PRO:CB	1:B:424:VAL:HG13	2.27	0.53
1:D:461:ASN:HD22	1:D:462:PRO:CD	2.21	0.53
1:B:97:ASP:HB3	2:F:576:LEU:HG	1.91	0.53
1:D:267:LEU:HD22	1:D:425:PRO:HG2	1.90	0.53
1:D:274:GLN:HB2	1:D:421:ARG:HB2	1.90	0.53
1:B:329:HIS:HD2	1:B:331:GLY:H	1.57	0.53
1:C:287:ASN:HD21	1:C:403:ALA:HA	1.73	0.53
1:A:300:THR:HB	1:A:326:GLN:CG	2.39	0.53
1:C:301:TRP:CD2	1:C:304:MET:HG3	2.43	0.53
1:B:143:ILE:HD12	1:B:515:SER:HB3	1.90	0.53
1:C:570:ASN:C	1:C:570:ASN:ND2	2.46	0.53
2:G:640:ARG:O	2:G:640:ARG:HG2	2.08	0.53
1:C:43:ILE:HD12	2:H:635:ARG:HD3	1.90	0.53
1:A:287:ASN:HD21	1:A:289:THR:CG2	2.22	0.53
1:C:471:SER:O	1:C:472:PHE:HB2	2.09	0.53
1:D:365:PRO:O	1:D:366:ASP:HB2	2.09	0.53
1:B:101:ALA:HA	2:F:576:LEU:HD21	1.89	0.52
1:B:119:VAL:HG21	1:B:122:SER:HB3	1.90	0.52
1:A:340:THR:HA	1:A:370:THR:HG22	1.92	0.52
1:A:438:ASN:HB3	1:A:441:ILE:HG12	1.92	0.52
2:E:591:ALA:O	2:E:594:SER:HB3	2.10	0.52
1:D:548:ASP:O	1:D:549:GLU:C	2.51	0.52
1:C:329:HIS:HD2	1:C:331:GLY:H	1.58	0.52
1:C:97:ASP:OD2	2:G:576:LEU:HG	2.10	0.52
1:A:251:MET:HE1	1:A:446:VAL:CG1	2.39	0.52
1:B:94:LYS:HE3	1:B:111:TYR:CE1	2.45	0.52
1:B:315:PRO:HB2	1:B:335:PRO:HG3	1.91	0.52
1:D:500:VAL:HG12	4:D:2123:HOH:O	2.09	0.52
1:C:55:GLN:HE22	1:C:71:MET:HE1	1.75	0.52
1:C:269:PRO:CG	1:C:498:LEU:HD23	2.39	0.52
1:D:152:LEU:HD23	1:D:518:ILE:HD12	1.92	0.52
2:F:578:PHE:CE1	1:C:73:GLU:HG2	2.45	0.52
1:C:153:SER:OG	1:C:508:HIS:HD2	1.93	0.52
1:C:226:ASP:N	1:C:227:PRO:HD3	2.24	0.52
1:A:74:PHE:CD2	2:G:586:VAL:HG21	2.45	0.52
1:B:112:SER:HB2	1:B:124:ASP:OD1	2.10	0.52
1:D:461:ASN:HD22	1:D:462:PRO:HD2	1.74	0.52
1:A:161:ARG:O	1:A:217:VAL:HG22	2.10	0.51
1:A:239:ARG:O	1:A:239:ARG:HG2	2.09	0.51
1:A:290:ARG:HH21	1:A:376:GLY:HA2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:GLN:OE1	1:B:495:ARG:NH2	2.43	0.51
1:A:468:PRO:CB	1:C:270:ILE:HD11	2.40	0.51
1:A:301:TRP:CD2	1:A:304:MET:HG3	2.44	0.51
1:B:339:ILE:O	1:B:370:THR:HA	2.11	0.51
1:C:435:ALA:HB3	1:C:436:PRO:HD3	1.92	0.51
1:D:148:ALA:HB1	1:D:514:LYS:HD2	1.93	0.51
1:A:251:MET:HE2	1:A:256:ASP:C	2.35	0.51
1:A:290:ARG:NH1	1:A:399:THR:HG22	2.25	0.51
1:D:161:ARG:O	1:D:217:VAL:HG22	2.09	0.51
1:A:533:ASN:HD22	1:C:480:PRO:CG	2.23	0.51
1:B:84:ILE:H	1:B:84:ILE:CD1	2.17	0.51
1:C:62:ILE:HD12	1:D:128:ARG:HH11	1.75	0.51
1:C:275:ASN:HD21	1:C:419:SER:H	1.59	0.51
1:D:533:ASN:N	1:D:533:ASN:ND2	2.55	0.51
1:C:45:ASN:O	1:C:46:VAL:C	2.54	0.51
1:C:101:ALA:HA	2:G:576:LEU:HD11	1.92	0.51
1:C:329:HIS:CD2	1:C:331:GLY:H	2.29	0.51
1:B:217:VAL:HG21	1:B:222:TYR:CD1	2.46	0.51
1:B:560:ARG:HG3	1:C:71:MET:HA	1.92	0.51
1:C:228:THR:OG1	1:C:472:PHE:HE2	1.94	0.51
1:A:144:PRO:O	1:A:145:LEU:HB2	2.10	0.51
1:C:315:PRO:HG2	1:C:331:GLY:HA3	1.93	0.51
1:D:99:ALA:CB	1:D:570:ASN:ND2	2.74	0.51
1:D:261:ILE:HG12	1:D:443:GLN:HB2	1.92	0.51
1:D:458:LYS:HD3	1:D:464:PHE:CZ	2.46	0.51
1:D:500:VAL:HG22	1:D:500:VAL:O	2.10	0.51
1:B:178:ASP:HB3	4:B:2047:HOH:O	2.11	0.50
1:B:301:TRP:CD2	1:B:304:MET:HG3	2.45	0.50
1:A:193:TRP:CE3	1:A:494:ILE:HG23	2.46	0.50
1:A:224:LEU:HD13	1:A:234:THR:HG22	1.92	0.50
1:D:84:ILE:HD12	2:H:587:LEU:HD21	1.93	0.50
1:A:364:ASN:O	1:A:367:ASP:HB2	2.12	0.50
1:B:449:THR:C	1:B:451:GLY:H	2.17	0.50
1:A:251:MET:HE1	1:A:446:VAL:HG12	1.92	0.50
1:B:376:GLY:HA2	1:B:380:THR:O	2.11	0.50
1:C:251:MET:HE1	1:C:446:VAL:HG12	1.92	0.50
2:F:580:ALA:O	2:F:584:THR:HG23	2.11	0.50
1:C:338:VAL:HG11	1:C:370:THR:HB	1.93	0.50
1:A:79:ARG:HD3	1:A:81:LYS:HD2	1.94	0.50
1:A:161:ARG:NH2	1:A:469:ALA:O	2.42	0.50
1:B:49:ALA:HA	1:B:52:GLU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:HA	1:B:549:GLU:HG3	1.93	0.50
1:B:257:GLN:OE1	1:B:513:SER:HB2	2.12	0.50
1:D:205:PHE:CE2	1:D:213:VAL:HG13	2.47	0.50
1:A:454:LEU:HD11	1:A:507:CYS:HB2	1.92	0.50
1:C:237:ASP:HB3	1:C:466:LEU:HB3	1.94	0.50
1:A:368:VAL:O	1:A:389:PRO:HD3	2.12	0.50
1:B:97:ASP:OD2	2:F:575:VAL:HB	2.10	0.50
1:B:217:VAL:HG11	1:B:222:TYR:CD2	2.47	0.50
1:A:175:ILE:HG23	1:A:211:TRP:CH2	2.47	0.50
1:D:94:LYS:O	1:D:98:PRO:HG3	2.12	0.49
1:C:101:ALA:HA	2:G:576:LEU:CD1	2.43	0.49
2:H:639:ALA:O	2:H:641:MET:N	2.46	0.49
1:B:145:LEU:HD22	1:B:254:LEU:HD23	1.94	0.49
1:B:391:VAL:HG12	1:B:392:THR:N	2.28	0.49
1:C:269:PRO:HG3	1:C:498:LEU:HD23	1.93	0.49
2:H:581:ASN:HD21	2:H:601:ASN:HD22	1.57	0.49
1:B:97:ASP:OD1	1:B:100:GLY:N	2.43	0.49
1:C:115:PRO:O	1:C:546:LYS:HA	2.12	0.49
1:A:98:PRO:HG2	1:A:244:SER:HB3	1.95	0.49
1:C:172:ASN:O	1:C:510:ARG:NH2	2.46	0.49
1:A:164:TYR:CE1	1:A:216:ARG:HG3	2.47	0.49
1:A:536:PHE:CD2	1:A:536:PHE:N	2.79	0.49
1:B:358:GLU:HB3	1:C:345:ARG:NH2	2.28	0.49
2:H:593:THR:O	2:H:596:ILE:HG13	2.13	0.49
1:A:143:ILE:HD12	1:A:515:SER:HB3	1.93	0.49
1:A:277:VAL:O	1:A:415:THR:HA	2.13	0.49
1:A:512:LEU:HD11	1:A:518:ILE:HD11	1.95	0.49
1:D:427:PRO:CG	1:D:506:VAL:HG11	2.43	0.49
1:A:533:ASN:ND2	1:C:480:PRO:HG3	2.27	0.49
4:A:2038:HOH:O	1:C:478:THR:HG22	2.12	0.49
1:A:97:ASP:OD1	1:A:100:GLY:N	2.45	0.49
1:A:489:PRO:HB3	1:B:277:VAL:HG12	1.95	0.49
1:B:264:HIS:HE1	1:B:563:GLY:O	1.96	0.49
1:B:280:SER:HB3	1:B:413:ALA:CA	2.43	0.49
1:A:315:PRO:HG3	1:A:331:GLY:HA3	1.95	0.49
1:C:159:MET:HE3	1:C:475:ILE:CD1	2.36	0.48
1:A:82:LEU:HD12	1:A:83:ASP:N	2.28	0.48
1:C:161:ARG:HG3	1:C:161:ARG:NH1	2.29	0.48
1:D:153:SER:OG	1:D:508:HIS:HD2	1.97	0.48
1:A:251:MET:HG3	1:A:256:ASP:HA	1.94	0.48
1:B:241:THR:O	1:B:242:TYR:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:GLN:HG3	1:B:421:ARG:HH12	1.76	0.48
1:C:264:HIS:HE1	1:C:563:GLY:O	1.96	0.48
1:D:229:GLU:CD	1:D:229:GLU:H	2.20	0.48
1:B:270:ILE:HD13	1:C:471:SER:HA	1.94	0.48
1:D:183:LEU:HD13	1:D:213:VAL:HG11	1.94	0.48
1:D:205:PHE:CD2	1:D:213:VAL:HG13	2.48	0.48
1:A:138:VAL:HG12	1:A:139:SER:N	2.28	0.48
2:G:583:LEU:HD11	2:G:587:LEU:HD12	1.95	0.48
1:C:227:PRO:HB3	1:C:229:GLU:OE1	2.14	0.48
1:A:293:ILE:N	1:A:293:ILE:CD1	2.75	0.48
1:A:121:PHE:HA	1:A:542:SER:HA	1.95	0.48
1:B:205:PHE:CD2	1:B:213:VAL:HG23	2.49	0.48
1:A:391:VAL:HG12	1:A:392:THR:N	2.28	0.48
1:C:264:HIS:CD2	1:C:505:ALA:HB2	2.49	0.48
1:D:322:THR:HG22	1:D:322:THR:O	2.14	0.48
1:A:353:ASP:OD2	1:A:356:THR:HG23	2.13	0.47
1:B:300:THR:HB	1:B:326:GLN:HE21	1.79	0.47
1:B:382:ALA:O	1:B:396:LEU:HD23	2.14	0.47
1:C:269:PRO:HB3	1:C:424:VAL:HG22	1.96	0.47
1:A:82:LEU:HD12	1:A:82:LEU:C	2.38	0.47
1:B:266:ALA:HB2	1:B:459:MET:HE2	1.95	0.47
1:B:290:ARG:O	1:B:400:THR:HA	2.15	0.47
1:A:108:VAL:CG1	1:A:109:GLY:N	2.77	0.47
1:C:98:PRO:HG2	1:C:244:SER:HB3	1.96	0.47
2:H:593:THR:HG22	2:H:594:SER:N	2.21	0.47
1:A:61:VAL:O	1:A:61:VAL:HG12	2.14	0.47
1:A:387:THR:HG22	1:A:392:THR:OG1	2.15	0.47
1:B:536:PHE:CD2	1:B:536:PHE:N	2.80	0.47
1:A:201:GLN:HE21	1:A:400:THR:HG21	1.80	0.47
1:D:376:GLY:HA2	1:D:380:THR:O	2.14	0.47
1:D:495:ARG:CG	1:D:495:ARG:HH11	2.27	0.47
1:A:264:HIS:HE1	1:A:563:GLY:O	1.97	0.47
1:A:533:ASN:ND2	1:C:480:PRO:CG	2.78	0.47
1:B:68:VAL:HG13	1:B:74:PHE:HB2	1.96	0.47
1:B:83:ASP:O	1:B:85:ASP:N	2.47	0.47
1:B:315:PRO:O	1:B:335:PRO:HB3	2.15	0.47
1:C:105:ALA:HB2	2:G:630:ARG:HG2	1.96	0.47
1:C:224:LEU:HD22	1:C:232:LEU:HD21	1.97	0.47
2:H:640:ARG:O	2:H:640:ARG:CG	2.62	0.47
1:B:428:PRO:HB3	1:C:532:VAL:HG12	1.97	0.47
1:A:241:THR:O	1:A:242:TYR:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:THR:O	1:A:323:THR:HB	2.14	0.47
1:A:338:VAL:HG22	1:A:371:PHE:O	2.15	0.47
1:B:365:PRO:O	1:B:366:ASP:HB2	2.15	0.47
1:C:113:LYS:HE3	1:C:124:ASP:OD1	2.13	0.47
1:A:68:VAL:CG1	1:A:68:VAL:O	2.62	0.47
1:B:78:ALA:CB	1:B:81:LYS:HD2	2.36	0.47
1:B:213:VAL:HG12	1:B:214:ARG:N	2.30	0.47
1:A:62:ILE:N	1:A:62:ILE:CD1	2.79	0.46
1:B:45:ASN:O	1:B:48:ALA:HB3	2.15	0.46
1:B:97:ASP:CG	2:F:576:LEU:CD1	2.88	0.46
1:B:315:PRO:CG	1:B:331:GLY:HA3	2.46	0.46
1:D:116:ASP:HB3	1:D:118:LEU:HB2	1.98	0.46
1:A:315:PRO:HB2	1:A:335:PRO:HG3	1.97	0.46
1:A:489:PRO:HB3	1:B:277:VAL:CG1	2.45	0.46
1:B:84:ILE:CG2	1:B:89:ILE:HD11	2.45	0.46
1:B:93:PHE:HB3	2:F:576:LEU:HD23	1.96	0.46
1:C:373:GLN:HG3	1:C:384:ILE:HD13	1.97	0.46
1:B:269:PRO:HB3	1:B:424:VAL:CG1	2.28	0.46
1:B:306:PRO:HD3	1:B:324:GLN:HA	1.96	0.46
1:B:338:VAL:HG11	1:B:370:THR:HB	1.97	0.46
4:D:2142:HOH:O	2:H:624:LYS:HE2	2.15	0.46
1:A:169:ASN:HA	1:A:210:THR:O	2.15	0.46
1:A:175:ILE:CD1	1:A:429:LEU:HD13	2.46	0.46
1:B:101:ALA:CA	2:F:576:LEU:HD21	2.45	0.46
1:C:204:THR:HG23	1:C:211:TRP:O	2.15	0.46
2:E:595:VAL:O	2:E:598:GLU:HB2	2.14	0.46
1:D:315:PRO:HG3	1:D:331:GLY:HA3	1.97	0.46
1:D:340:THR:HA	1:D:370:THR:HG22	1.97	0.46
1:A:287:ASN:ND2	1:A:289:THR:HG22	2.28	0.46
1:D:105:ALA:HB2	2:H:630:ARG:HG2	1.97	0.46
1:D:338:VAL:HG11	1:D:370:THR:HB	1.98	0.46
1:D:458:LYS:NZ	1:D:555:ASP:OD1	2.49	0.46
1:C:239:ARG:O	1:C:239:ARG:HG2	2.16	0.46
1:C:441:ILE:HD12	1:C:441:ILE:C	2.41	0.46
1:A:82:LEU:HD13	1:A:549:GLU:CG	2.46	0.46
1:B:293:ILE:HA	1:B:399:THR:CG2	2.45	0.46
1:C:405:VAL:CG2	1:C:406:ILE:N	2.79	0.45
1:D:461:ASN:ND2	1:D:462:PRO:HD2	2.30	0.45
1:D:495:ARG:NH1	4:D:2121:HOH:O	2.48	0.45
1:B:317:TRP:O	1:B:318:ILE:HD13	2.16	0.45
1:D:51:GLN:HA	1:D:73:GLU:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:ILE:HG12	1:D:406:ILE:HG13	1.98	0.45
1:D:138:VAL:O	1:D:139:SER:CB	2.62	0.45
1:B:86:GLN:HE21	1:B:108:VAL:HG21	1.81	0.45
2:G:626:ALA:HB3	2:G:629:VAL:HG23	1.98	0.45
1:A:239:ARG:HD2	1:A:466:LEU:HD11	1.98	0.45
1:A:290:ARG:HD3	1:A:398:THR:C	2.41	0.45
1:B:314:ASP:HA	1:B:316:ALA:N	2.31	0.45
1:B:405:VAL:CG2	1:B:406:ILE:N	2.79	0.45
1:D:260:TRP:HA	1:D:508:HIS:O	2.16	0.45
1:C:340:THR:HA	1:C:370:THR:HG22	1.99	0.45
1:D:226:ASP:N	1:D:227:PRO:CD	2.79	0.45
2:H:573:ALA:HB1	2:H:576:LEU:HD12	1.99	0.45
1:D:224:LEU:CD2	1:D:232:LEU:HD21	2.46	0.45
1:D:274:GLN:HG2	1:D:490:GLY:O	2.16	0.45
1:D:275:ASN:ND2	1:D:417:ALA:O	2.49	0.45
1:B:338:VAL:CG1	1:B:370:THR:HB	2.47	0.45
2:G:595:VAL:HG12	2:G:599:LEU:CD1	2.47	0.45
2:G:595:VAL:HG22	2:G:640:ARG:NH2	2.31	0.45
1:D:387:THR:HG22	1:D:392:THR:OG1	2.16	0.45
1:C:98:PRO:HG2	1:C:244:SER:CB	2.46	0.45
2:G:588:LYS:O	2:G:588:LYS:HG3	2.17	0.45
2:G:639:ALA:C	2:G:641:MET:N	2.66	0.45
1:D:391:VAL:HG12	1:D:392:THR:N	2.32	0.45
1:B:175:ILE:CD1	1:B:429:LEU:HB3	2.46	0.45
4:B:2091:HOH:O	1:C:61:VAL:HB	2.16	0.45
1:C:175:ILE:HA	1:C:211:TRP:CZ2	2.51	0.45
1:C:320:ASP:HB2	1:C:328:ARG:HG2	1.98	0.45
2:G:639:ALA:O	2:G:641:MET:N	2.43	0.45
1:D:284:HIS:HD2	1:D:302:ALA:O	1.99	0.45
2:H:590:GLU:HG3	2:H:591:ALA:N	2.28	0.44
1:C:84:ILE:HG12	2:G:587:LEU:HD13	1.97	0.44
1:C:89:ILE:HG21	2:G:599:LEU:HD12	1.99	0.44
1:C:190:LEU:HD23	1:C:190:LEU:HA	1.83	0.44
1:C:213:VAL:HG22	1:C:214:ARG:N	2.32	0.44
1:C:293:ILE:HD12	1:C:293:ILE:N	2.32	0.44
1:D:194:ARG:HG2	1:D:222:TYR:OH	2.17	0.44
1:D:269:PRO:CB	1:D:424:VAL:HG13	2.31	0.44
1:A:214:ARG:HD3	1:A:216:ARG:CZ	2.48	0.44
1:D:183:LEU:CD1	1:D:213:VAL:HG11	2.47	0.44
1:D:190:LEU:HD12	1:D:190:LEU:HA	1.85	0.44
1:D:277:VAL:O	1:D:415:THR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LEU:CD2	1:C:232:LEU:HD21	2.47	0.44
2:H:590:GLU:O	2:H:591:ALA:HB2	2.17	0.44
1:A:534:THR:HA	1:A:535:PRO:HD3	1.76	0.44
1:B:407:ASN:HD22	1:B:408:PHE:H	1.66	0.44
1:B:428:PRO:HD3	1:C:531:ASN:OD1	2.16	0.44
1:C:153:SER:CB	1:C:508:HIS:HD2	2.31	0.44
1:D:305:PRO:HA	1:D:306:PRO:HD3	1.87	0.44
1:B:243:LYS:HA	1:B:523:TYR:O	2.18	0.44
1:C:100:GLY:C	2:G:576:LEU:CD1	2.87	0.44
1:C:158:PRO:HB2	1:C:499:ASP:HB3	2.00	0.44
1:A:176:SER:OG	1:A:179:VAL:HG23	2.17	0.44
1:A:458:LYS:HE2	1:A:458:LYS:HB3	1.80	0.44
1:B:249:ALA:CB	1:B:446:VAL:CG1	2.96	0.44
1:C:269:PRO:HG3	1:C:498:LEU:CD2	2.48	0.44
1:A:224:LEU:HA	1:A:225:PRO:HD3	1.92	0.43
1:D:471:SER:O	1:D:472:PHE:HB2	2.18	0.43
1:A:428:PRO:HB2	1:A:434:THR:CG2	2.24	0.43
2:E:596:ILE:HD13	1:B:47:THR:HA	1.99	0.43
1:D:345:ARG:HA	1:D:365:PRO:HB3	2.00	0.43
1:A:116:ASP:OD2	1:A:239:ARG:NH2	2.51	0.43
1:A:248:GLU:HB2	1:A:519:VAL:HB	2.00	0.43
1:A:290:ARG:HD3	1:A:399:THR:HA	2.00	0.43
1:A:82:LEU:HA	1:B:79:ARG:HH12	1.83	0.43
1:A:217:VAL:HG11	1:A:222:TYR:CD2	2.53	0.43
1:A:315:PRO:CG	1:A:331:GLY:HA3	2.48	0.43
1:A:332:PHE:O	1:A:377:ALA:HA	2.19	0.43
1:D:114:ILE:HA	1:D:115:PRO:HD3	1.79	0.43
1:B:356:THR:O	1:B:358:GLU:HG2	2.18	0.43
1:A:85:ASP:HB3	1:A:88:SER:HB2	2.00	0.43
1:A:112:SER:HB2	1:A:124:ASP:OD1	2.18	0.43
1:A:421:ARG:HG3	1:A:476:SER:OG	2.18	0.43
1:C:345:ARG:HA	1:C:365:PRO:HB3	1.99	0.43
1:D:306:PRO:HG3	1:D:324:GLN:N	2.34	0.43
1:A:97:ASP:CG	2:E:576:LEU:CD1	2.90	0.43
1:A:322:THR:O	1:A:324:GLN:N	2.50	0.43
2:F:578:PHE:HE1	1:C:73:GLU:HG2	1.83	0.43
1:C:239:ARG:HD2	1:C:466:LEU:HD23	2.00	0.43
1:A:205:PHE:HD2	1:A:213:VAL:HG22	1.84	0.43
1:A:449:THR:O	1:A:568:THR:HG23	2.19	0.43
4:B:2107:HOH:O	1:C:229:GLU:HG3	2.18	0.43
1:C:268:THR:HA	1:C:269:PRO:HD3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:MET:HE3	1:B:475:ILE:CD1	2.42	0.43
1:B:447:LYS:HG3	4:B:2066:HOH:O	2.19	0.43
1:B:479:ASN:CG	1:B:480:PRO:HD2	2.43	0.43
1:C:114:ILE:C	1:C:116:ASP:N	2.77	0.43
1:C:458:LYS:HB3	1:C:458:LYS:HE2	1.83	0.43
2:G:588:LYS:O	2:G:589:SER:CB	2.66	0.43
1:D:175:ILE:HA	1:D:211:TRP:CZ2	2.54	0.43
1:D:264:HIS:CD2	1:D:505:ALA:HB2	2.54	0.43
1:A:458:LYS:HD3	1:A:464:PHE:CE1	2.54	0.43
1:B:327:TRP:CG	1:B:339:ILE:HD13	2.54	0.43
1:B:289:THR:O	1:B:291:PRO:HD3	2.19	0.42
1:C:547:ASN:O	1:C:551:LEU:HD22	2.19	0.42
1:D:214:ARG:HD3	1:D:216:ARG:CD	2.48	0.42
1:B:114:ILE:HD13	1:B:464:PHE:CG	2.54	0.42
1:A:269:PRO:HG2	1:A:498:LEU:HD23	1.99	0.42
1:B:259:PHE:HD1	1:B:445:LEU:HD23	1.84	0.42
2:G:632:ARG:NH1	2:G:632:ARG:CB	2.82	0.42
1:D:129:GLU:O	1:D:522:THR:HG23	2.19	0.42
2:H:571:PHE:O	2:H:574:ALA:HB2	2.18	0.42
1:B:88:SER:HB3	1:B:550:ILE:HD11	2.00	0.42
1:B:237:ASP:HB3	1:B:466:LEU:HB3	2.02	0.42
1:B:437:ASN:OD1	1:C:537:GLY:HA3	2.19	0.42
1:D:225:PRO:C	1:D:227:PRO:CD	2.93	0.42
1:D:359:TRP:CZ3	1:D:409:ARG:HB3	2.54	0.42
1:A:114:ILE:HA	1:A:115:PRO:HD3	1.82	0.42
1:A:385:THR:CG2	1:A:394:THR:HG22	2.35	0.42
1:B:115:PRO:HG2	1:B:550:ILE:HD11	2.01	0.42
1:B:534:THR:HA	1:B:535:PRO:HD3	1.77	0.42
1:D:338:VAL:HG13	1:D:371:PHE:O	2.18	0.42
1:B:77:TRP:CD1	1:B:77:TRP:C	2.98	0.42
2:G:595:VAL:HA	2:G:640:ARG:NH2	2.34	0.42
1:A:186:TRP:HH2	1:A:196:VAL:HG11	1.84	0.42
1:A:351:TYR:HE1	1:A:353:ASP:HB2	1.84	0.42
1:A:398:THR:HG22	1:A:399:THR:N	2.35	0.42
1:B:227:PRO:HG2	1:B:470:SER:CB	2.50	0.42
1:C:43:ILE:HG23	1:C:47:THR:HB	2.01	0.42
1:C:249:ALA:HB3	1:C:251:MET:HE2	2.01	0.42
1:A:65:PRO:HG2	2:G:578:PHE:HE1	1.82	0.42
1:A:262:GLY:O	1:A:441:ILE:HD13	2.20	0.42
2:E:596:ILE:CG2	1:B:47:THR:HG22	2.34	0.42
1:B:58:ASP:O	1:B:59:ALA:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:PRO:HD3	1:B:338:VAL:O	2.18	0.42
1:C:478:THR:CG2	1:C:479:ASN:N	2.81	0.42
1:A:77:TRP:CD1	1:A:77:TRP:C	2.97	0.42
1:B:251:MET:HB3	1:B:516:CYS:SG	2.59	0.42
1:B:460:ARG:HA	1:C:466:LEU:HD12	2.02	0.42
1:C:467:THR:HG22	1:C:468:PRO:HD2	2.00	0.42
1:D:183:LEU:HB2	1:D:205:PHE:CE1	2.55	0.42
1:A:75:ARG:O	1:A:79:ARG:HB2	2.20	0.42
1:B:239:ARG:NH1	1:B:527:GLU:OE2	2.48	0.42
1:C:334:ALA:HA	1:C:335:PRO:HD3	1.96	0.42
1:A:74:PHE:CE1	2:G:582:MET:HE2	2.55	0.41
1:A:270:ILE:N	1:A:270:ILE:HD12	2.35	0.41
1:B:97:ASP:OD2	2:F:576:LEU:HD12	2.20	0.41
2:G:598:GLU:CD	2:G:640:ARG:NH2	2.78	0.41
1:D:438:ASN:HB3	1:D:441:ILE:HG23	2.00	0.41
2:H:588:LYS:C	2:H:590:GLU:N	2.76	0.41
1:A:84:ILE:O	1:A:84:ILE:HG22	2.20	0.41
2:E:596:ILE:HD13	1:B:47:THR:HG22	2.02	0.41
1:C:78:ALA:O	1:C:79:ARG:HB2	2.21	0.41
2:G:628:ARG:NH1	2:G:628:ARG:HB2	2.34	0.41
4:A:2038:HOH:O	1:C:478:THR:CG2	2.68	0.41
2:E:596:ILE:HG21	1:B:47:THR:HG23	1.91	0.41
1:B:49:ALA:O	1:B:53:LEU:HB2	2.19	0.41
1:C:387:THR:HG22	1:C:392:THR:HG23	2.02	0.41
2:G:617:LEU:HD22	2:G:617:LEU:N	2.35	0.41
1:D:259:PHE:CZ	1:D:443:GLN:HG2	2.54	0.41
1:D:474:ALA:HB2	1:D:495:ARG:HE	1.85	0.41
1:A:68:VAL:CG2	2:G:582:MET:HE1	2.48	0.41
1:A:97:ASP:HB3	2:E:576:LEU:HG	2.03	0.41
1:A:453:TYR:CG	1:A:570:ASN:HB2	2.56	0.41
2:G:627:ALA:HB1	1:D:55:GLN:HB2	2.01	0.41
1:A:532:VAL:HG12	1:A:533:ASN:N	2.36	0.41
1:B:315:PRO:HG3	1:B:331:GLY:HA3	2.02	0.41
1:D:204:THR:HG22	1:D:206:SER:H	1.86	0.41
1:A:274:GLN:OE1	1:A:495:ARG:NH2	2.53	0.41
1:A:351:TYR:CE1	1:A:353:ASP:HB2	2.55	0.41
1:B:99:ALA:HB1	1:B:570:ASN:ND2	2.35	0.41
1:B:270:ILE:HD11	1:C:471:SER:HA	2.01	0.41
1:C:381:ASN:CB	1:C:396:LEU:HD11	2.48	0.41
1:A:261:ILE:HG13	1:A:443:GLN:HB2	2.02	0.41
1:A:274:GLN:HB2	1:A:421:ARG:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:PHE:CD1	1:A:477:PHE:N	2.89	0.41
1:B:99:ALA:CB	1:B:570:ASN:ND2	2.84	0.41
1:B:553:LEU:HD23	1:B:553:LEU:HA	1.78	0.41
1:C:562:THR:HG23	4:C:2127:HOH:O	2.20	0.41
2:G:598:GLU:C	2:G:600:GLY:H	2.29	0.41
1:D:367:ASP:HB2	1:D:389:PRO:HG2	2.02	0.41
1:C:241:THR:O	1:C:242:TYR:HB3	2.21	0.41
2:G:632:ARG:HH11	2:G:632:ARG:HB3	1.85	0.41
1:D:136:PRO:HG3	1:D:202:TRP:CD1	2.55	0.41
1:A:67:ASN:ND2	1:A:69:ALA:HB3	2.32	0.41
1:C:364:ASN:O	1:C:367:ASP:HB2	2.21	0.41
1:B:261:ILE:HG12	1:B:443:GLN:HB3	2.02	0.41
1:C:104:SER:HA	2:G:625:ILE:HD13	2.03	0.41
1:C:456:HIS:CD2	1:C:503:SER:O	2.72	0.41
1:D:155:ILE:HB	1:D:165:PHE:HB2	2.03	0.41
1:B:228:THR:CG2	1:B:323:THR:HG21	2.39	0.40
1:B:345:ARG:HA	1:B:365:PRO:HB3	2.03	0.40
1:C:93:PHE:HD2	2:G:576:LEU:HD22	1.86	0.40
1:C:339:ILE:O	1:C:370:THR:HA	2.22	0.40
1:C:383:THR:HG22	1:C:385:THR:HG23	2.02	0.40
1:D:79:ARG:HH12	2:H:590:GLU:HB2	1.87	0.40
1:A:71:MET:HA	1:A:72:PRO:HD2	1.91	0.40
1:A:457:SER:OG	1:B:120:LYS:HE2	2.21	0.40
1:B:329:HIS:CD2	1:B:331:GLY:H	2.37	0.40
1:B:438:ASN:HB3	1:B:441:ILE:CG1	2.49	0.40
1:A:82:LEU:HD13	1:A:549:GLU:HG3	2.04	0.40
1:A:208:ASP:HB3	1:A:211:TRP:HD1	1.86	0.40
1:A:355:THR:HG22	1:A:356:THR:HG23	2.03	0.40
1:B:85:ASP:HB3	1:B:88:SER:CB	2.46	0.40
1:B:135:CYS:HB3	1:B:138:VAL:HG23	2.03	0.40
1:B:441:ILE:CG2	1:B:442:GLU:N	2.85	0.40
1:D:243:LYS:HA	1:D:523:TYR:O	2.21	0.40
1:A:163:ALA:O	1:A:164:TYR:HB3	2.21	0.40
1:B:61:VAL:O	1:B:61:VAL:HG12	2.21	0.40
1:C:388:ALA:O	1:C:389:PRO:C	2.63	0.40
1:B:47:THR:O	1:B:50:ALA:HB3	2.22	0.40
1:C:304:MET:O	1:C:305:PRO:C	2.63	0.40

There are no symmetry-related clashes.

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	508/570 (89%)	471 (93%)	34 (7%)	3 (1%)	21	51
1	B	525/570 (92%)	482 (92%)	36 (7%)	7 (1%)	9	31
1	C	521/570 (91%)	499 (96%)	19 (4%)	3 (1%)	21	51
1	D	526/570 (92%)	496 (94%)	27 (5%)	3 (1%)	21	51
2	E	27/74 (36%)	24 (89%)	3 (11%)	0	100	100
2	F	18/74 (24%)	18 (100%)	0	0	100	100
2	G	59/74 (80%)	53 (90%)	3 (5%)	3 (5%)	1	5
2	H	55/74 (74%)	44 (80%)	6 (11%)	5 (9%)	0	1
All	All	2239/2576 (87%)	2087 (93%)	128 (6%)	24 (1%)	11	36

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	589	SER
1	D	139	SER
2	H	615	PRO
2	H	640	ARG
1	A	200	GLY
1	B	86	GLN
1	B	450	LEU
2	G	640	ARG
1	D	242	TYR
1	B	78	ALA
1	B	563	GLY
2	H	590	GLU
2	H	591	ALA
1	B	448	ASP
1	C	45	ASN
2	H	594	SER
1	B	242	TYR

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Mol	Chain	Res	Type
1	A	136	PRO
1	A	242	TYR
1	B	84	ILE
1	C	46	VAL
1	C	226	ASP
1	D	226	ASP
2	G	600	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	428/474 (90%)	392 (92%)	36 (8%)	10	32
1	B	440/474 (93%)	406 (92%)	34 (8%)	12	36
1	C	439/474 (93%)	417 (95%)	22 (5%)	22	54
1	D	441/474 (93%)	411 (93%)	30 (7%)	14	42
2	E	22/53 (42%)	19 (86%)	3 (14%)	3	13
2	F	14/53 (26%)	13 (93%)	1 (7%)	13	39
2	G	47/53 (89%)	42 (89%)	5 (11%)	6	22
2	H	43/53 (81%)	38 (88%)	5 (12%)	5	18
All	All	1874/2108 (89%)	1738 (93%)	136 (7%)	13	38

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	A	73	GLU
1	A	82	LEU
1	A	134	GLU
1	A	136	PRO
1	A	137	THR
1	A	146	ASP
1	A	162	THR

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Mol	Chain	Res	Type
1	A	175	ILE
1	A	183	LEU
1	A	213	VAL
1	A	216	ARG
1	A	217	VAL
1	A	229	GLU
1	A	246	THR
1	A	251	MET
1	A	257	GLN
1	A	293	ILE
1	A	297	VAL
1	A	299	LEU
1	A	300	THR
1	A	314	ASP
1	A	326	GLN
1	A	338	VAL
1	A	355	THR
1	A	389	PRO
1	A	396	LEU
1	A	407	ASN
1	A	409	ARG
1	A	424	VAL
1	A	434	THR
1	A	441	ILE
1	A	466	LEU
1	A	501	ASN
1	A	522	THR
1	A	570	ASN
2	E	583	LEU
2	E	585	SER
2	E	599	LEU
1	B	52	GLU
1	B	68	VAL
1	B	82	LEU
1	B	102	THR
1	B	123	VAL
1	B	134	GLU
1	B	136	PRO
1	B	175	ILE
1	B	183	LEU
1	B	213	VAL
1	B	217	VAL

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Mol	Chain	Res	Type
1	B	239	ARG
1	B	251	MET
1	B	257	GLN
1	B	290	ARG
1	B	297	VAL
1	B	300	THR
1	B	314	ASP
1	B	385	THR
1	B	389	PRO
1	B	396	LEU
1	B	405	VAL
1	B	412	ASP
1	B	424	VAL
1	B	444	THR
1	B	504	THR
1	B	512	LEU
1	B	522	THR
1	B	548	ASP
1	B	551	LEU
1	B	553	LEU
1	B	560	ARG
1	B	568	THR
1	B	570	ASN
2	F	583	LEU
1	C	62	ILE
1	C	73	GLU
1	C	86	GLN
1	C	229	GLU
1	C	257	GLN
1	C	275	ASN
1	C	289	THR
1	C	300	THR
1	C	324	GLN
1	C	389	PRO
1	C	391	VAL
1	C	412	ASP
1	C	424	VAL
1	C	478	THR
1	C	504	THR
1	C	512	LEU
1	C	517	SER
1	C	522	THR

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Mol	Chain	Res	Type
1	C	551	LEU
1	C	553	LEU
1	C	564	VAL
1	C	570	ASN
2	G	588	LYS
2	G	595	VAL
2	G	601	ASN
2	G	609	GLN
2	G	641	MET
1	D	44	ASP
1	D	86	GLN
1	D	116	ASP
1	D	118	LEU
1	D	134	GLU
1	D	138	VAL
1	D	177	LEU
1	D	217	VAL
1	D	220	PRO
1	D	226	ASP
1	D	229	GLU
1	D	239	ARG
1	D	257	GLN
1	D	289	THR
1	D	300	THR
1	D	312	SER
1	D	328	ARG
1	D	383	THR
1	D	387	THR
1	D	389	PRO
1	D	409	ARG
1	D	424	VAL
1	D	443	GLN
1	D	495	ARG
1	D	498	LEU
1	D	504	THR
1	D	512	LEU
1	D	522	THR
1	D	533	ASN
1	D	570	ASN
2	H	592	THR
2	H	593	THR
2	H	598	GLU

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Mol	Chain	Res	Type
2	H	615	PRO
2	H	641	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	149	GLN
1	A	201	GLN
1	A	219	HIS
1	A	264	HIS
1	A	287	ASN
1	A	326	GLN
1	A	329	HIS
1	A	357	ASN
1	A	373	GLN
1	A	407	ASN
1	A	443	GLN
1	A	533	ASN
1	A	570	ASN
1	B	45	ASN
1	B	55	GLN
1	B	67	ASN
1	B	86	GLN
1	B	169	ASN
1	B	201	GLN
1	B	264	HIS
1	B	287	ASN
1	B	326	GLN
1	B	329	HIS
1	B	357	ASN
1	B	381	ASN
1	B	407	ASN
1	B	420	ASN
1	B	443	GLN
1	B	479	ASN
1	B	533	ASN
1	C	86	GLN
1	C	264	HIS
1	C	275	ASN
1	C	284	HIS
1	C	287	ASN

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Mol	Chain	Res	Type
1	C	329	HIS
1	C	443	GLN
1	C	456	HIS
1	C	508	HIS
2	G	581	ASN
2	G	601	ASN
1	D	149	GLN
1	D	181	ASN
1	D	257	GLN
1	D	264	HIS
1	D	284	HIS
1	D	329	HIS
1	D	364	ASN
1	D	373	GLN
1	D	443	GLN
1	D	456	HIS
1	D	461	ASN
1	D	508	HIS
1	D	531	ASN
1	D	533	ASN
1	D	570	ASN
2	H	581	ASN
2	H	601	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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	510/570 (89%)	0.18	10 (1%) 65 56	19, 35, 68, 107	0
1	B	527/570 (92%)	0.35	24 (4%) 37 29	20, 34, 77, 143	0
1	C	525/570 (92%)	0.14	12 (2%) 61 51	20, 33, 61, 122	0
1	D	528/570 (92%)	0.17	14 (2%) 56 46	19, 32, 62, 105	0
2	E	29/74 (39%)	0.43	2 (6%) 23 16	24, 36, 97, 129	0
2	F	20/74 (27%)	0.13	0 100 100	24, 31, 66, 86	0
2	G	65/74 (87%)	0.37	5 (7%) 19 14	24, 38, 104, 112	0
2	H	59/74 (79%)	0.82	12 (20%) 3 2	24, 38, 127, 162	0
All	All	2263/2576 (87%)	0.23	79 (3%) 47 38	19, 34, 74, 162	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	79	ARG	9.1
1	B	44	ASP	7.3
1	C	42	ASN	5.0
1	B	78	ALA	4.9
2	H	598	GLU	4.8
2	H	601	ASN	4.5
2	G	600	GLY	4.4
2	H	600	GLY	4.3
1	D	43	ILE	4.2
2	H	594	SER	4.1
1	B	229	GLU	4.0
2	H	599	LEU	3.9
1	D	543	GLY	3.8
1	B	45	ASN	3.7
1	B	55	GLN	3.7
2	G	590	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	387	THR	3.4
1	D	140	ASP	3.3
1	D	334	ALA	3.2
1	A	228	THR	3.2
1	D	312	SER	3.2
1	B	322	THR	3.1
1	C	140	ASP	3.0
1	D	330	GLY	3.0
1	A	225	PRO	3.0
1	B	358	GLU	3.0
2	G	594	SER	3.0
1	C	470	SER	3.0
1	D	331	GLY	2.9
1	A	75	ARG	2.9
1	B	389	PRO	2.9
2	H	591	ALA	2.9
2	G	593	THR	2.9
1	B	315	PRO	2.8
2	H	614	LEU	2.8
2	H	597	LYS	2.8
1	C	331	GLY	2.8
2	E	599	LEU	2.7
1	D	79	ARG	2.7
2	H	641	MET	2.7
2	E	598	GLU	2.7
1	B	51	GLN	2.7
1	A	354	THR	2.7
1	B	48	ALA	2.6
1	C	332	PHE	2.6
2	H	592	THR	2.6
1	D	309	SER	2.5
1	C	345	ARG	2.5
1	A	360	ASN	2.5
1	B	76	SER	2.4
1	A	229	GLU	2.4
1	D	369	VAL	2.4
1	C	321	SER	2.4
1	B	180	THR	2.4
1	B	228	THR	2.4
1	D	226	ASP	2.4
1	A	79	ARG	2.3
1	C	281	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	336	THR	2.3
1	C	319	PRO	2.2
1	C	490	GLY	2.2
1	D	74	PHE	2.2
1	B	323	THR	2.2
1	A	316	ALA	2.2
1	C	353	ASP	2.2
1	B	81	LYS	2.2
1	B	230	GLY	2.2
1	B	313	GLY	2.2
1	A	355	THR	2.1
1	B	57	LEU	2.1
2	H	615	PRO	2.1
1	C	537	GLY	2.1
1	B	332	PHE	2.1
1	D	354	THR	2.1
1	D	332	PHE	2.1
1	B	339	ILE	2.1
1	A	82	LEU	2.0
2	G	606	LEU	2.0
2	H	595	VAL	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($\text{\AA}^2$)	Q<0.9
3	MG	A	1645	1/1	0.92	0.11	43,43,43,43	0
3	MG	C	1645	1/1	0.96	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	1645	1/1	0.97	0.07	24,24,24,24	0
3	MG	D	1645	1/1	0.98	0.04	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.