



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:46 AM UTC

PDB ID : 1HR7 / pdb_00001hr7
Title : Yeast Mitochondrial Processing Peptidase beta-E73Q Mutant
Authors : Taylor, A.B.; Smith, B.S.; Kitada, S.; Kojima, K.; Miyaura, H.; Otwinowski, Z.; Ito, A.; Deisenhofer, J.
Deposited on : 2000-12-21
Resolution : 2.55 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

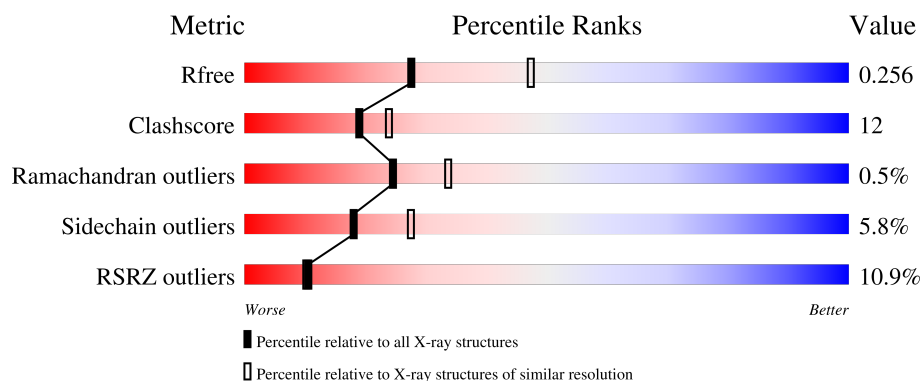
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	475	8% 72% 21% • •
1	C	475	5% 71% 19% • 7%
1	E	475	7% 70% 21% • 6%
1	G	475	8% 70% 21% • 5%
2	B	443	9% 72% 23% • •

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Mol	Chain	Length	Quality of chain
2	D	443	8% 70% 25% 5%
2	F	443	12% 72% 24% • •
2	H	443	29% 70% 26% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27725 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 MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3531	2233	599	680	19			
1	C	444	Total	C	N	O	S	0	0	0
			3447	2183	582	663	19			
1	E	448	Total	C	N	O	S	0	0	0
			3478	2201	590	668	19			
1	G	450	Total	C	N	O	S	0	0	0
			3485	2206	592	668	19			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	GLY	GLU	SEE REMARK 999	UNP P11914
A	217	GLY	GLU	SEE REMARK 999	UNP P11914
A	483	HIS	-	expression tag	UNP P11914
A	484	HIS	-	expression tag	UNP P11914
A	485	HIS	-	expression tag	UNP P11914
A	486	HIS	-	expression tag	UNP P11914
A	487	HIS	-	expression tag	UNP P11914
A	488	HIS	-	expression tag	UNP P11914
C	177	GLY	GLU	SEE REMARK 999	UNP P11914
C	217	GLY	GLU	SEE REMARK 999	UNP P11914
C	483	HIS	-	expression tag	UNP P11914
C	484	HIS	-	expression tag	UNP P11914
C	485	HIS	-	expression tag	UNP P11914
C	486	HIS	-	expression tag	UNP P11914
C	487	HIS	-	expression tag	UNP P11914
C	488	HIS	-	expression tag	UNP P11914
E	177	GLY	GLU	SEE REMARK 999	UNP P11914
E	217	GLY	GLU	SEE REMARK 999	UNP P11914
E	483	HIS	-	expression tag	UNP P11914
E	484	HIS	-	expression tag	UNP P11914

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Chain	Residue	Modelled	Actual	Comment	Reference
E	485	HIS	-	expression tag	UNP P11914
E	486	HIS	-	expression tag	UNP P11914
E	487	HIS	-	expression tag	UNP P11914
E	488	HIS	-	expression tag	UNP P11914
G	177	GLY	GLU	SEE REMARK 999	UNP P11914
G	217	GLY	GLU	SEE REMARK 999	UNP P11914
G	483	HIS	-	expression tag	UNP P11914
G	484	HIS	-	expression tag	UNP P11914
G	485	HIS	-	expression tag	UNP P11914
G	486	HIS	-	expression tag	UNP P11914
G	487	HIS	-	expression tag	UNP P11914
G	488	HIS	-	expression tag	UNP P11914

- Molecule 2 is a protein called MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	439	Total	C	N	O	S	0	0	0
			3414	2148	591	668	7			
2	D	441	Total	C	N	O	S	0	0	0
			3431	2159	594	671	7			
2	F	440	Total	C	N	O	S	0	0	0
			3422	2154	592	669	7			
2	H	440	Total	C	N	O	S	0	0	0
			3422	2154	592	669	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	ALA	-	cloning artifact	UNP P10507
B	73	GLN	GLU	engineered mutation	UNP P10507
B	84	PRO	SER	SEE REMARK 999	UNP P10507
B	350	ARG	GLN	SEE REMARK 999	UNP P10507
D	20	ALA	-	cloning artifact	UNP P10507
D	73	GLN	GLU	engineered mutation	UNP P10507
D	84	PRO	SER	SEE REMARK 999	UNP P10507
D	350	ARG	GLN	SEE REMARK 999	UNP P10507
F	20	ALA	-	cloning artifact	UNP P10507
F	73	GLN	GLU	engineered mutation	UNP P10507
F	84	PRO	SER	SEE REMARK 999	UNP P10507
F	350	ARG	GLN	SEE REMARK 999	UNP P10507
H	20	ALA	-	cloning artifact	UNP P10507

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Chain	Residue	Modelled	Actual	Comment	Reference
H	73	GLN	GLU	engineered mutation	UNP P10507
H	84	PRO	SER	SEE REMARK 999	UNP P10507
H	350	ARG	GLN	SEE REMARK 999	UNP P10507

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0

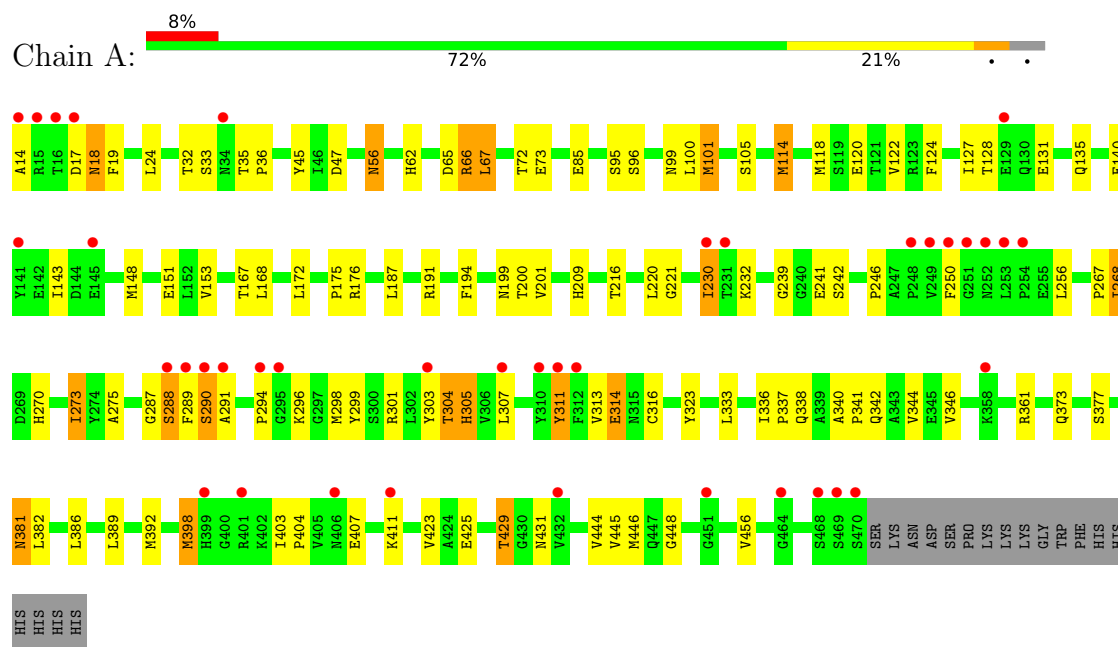
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	20	Total O 20 20	0	0
4	B	27	Total O 27 27	0	0
4	C	13	Total O 13 13	0	0
4	D	10	Total O 10 10	0	0
4	E	9	Total O 9 9	0	0
4	F	4	Total O 4 4	0	0
4	G	7	Total O 7 7	0	0
4	H	1	Total O 1 1	0	0

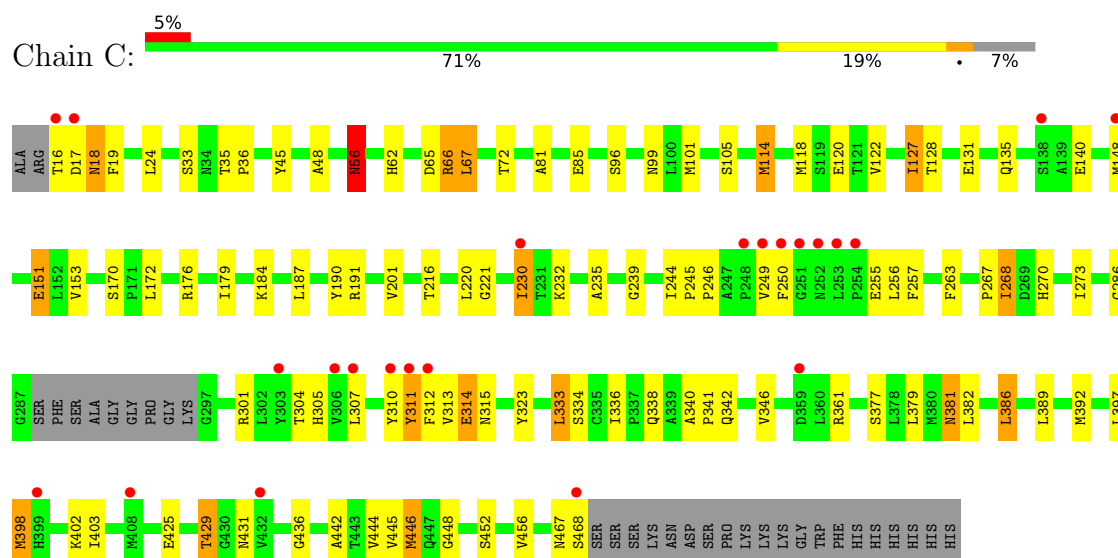
3 Residue-property plots [i](#)

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: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT



• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT



Chain E:

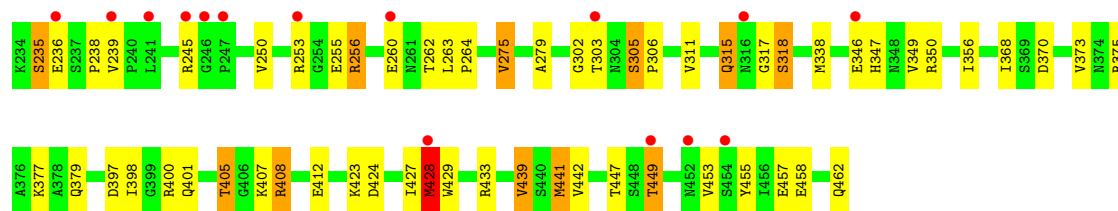
70% 21% 6% 7%

[illegible]

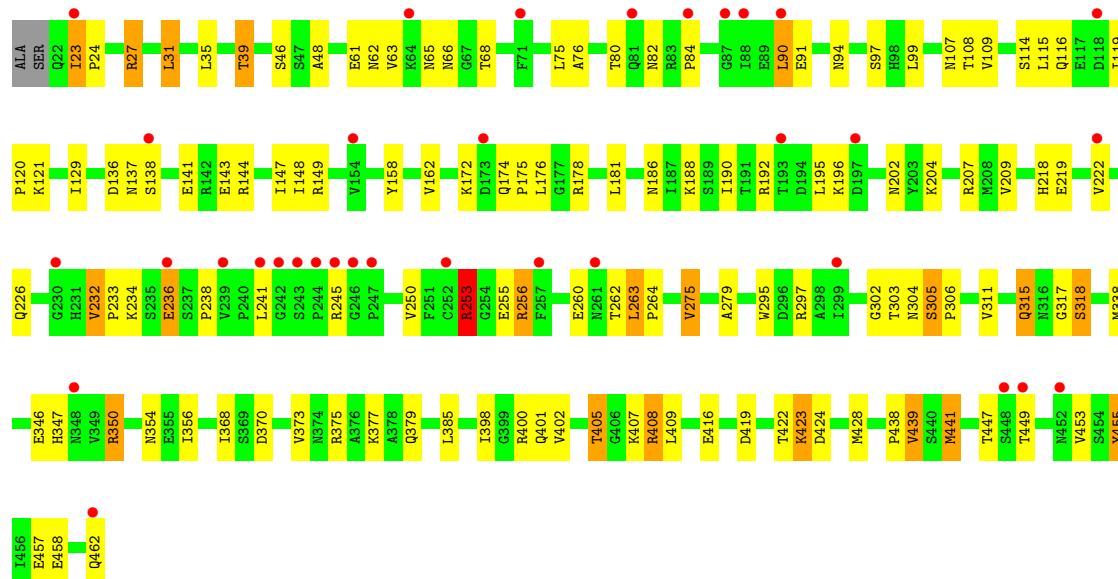
Chain B:

9% 72% 23%

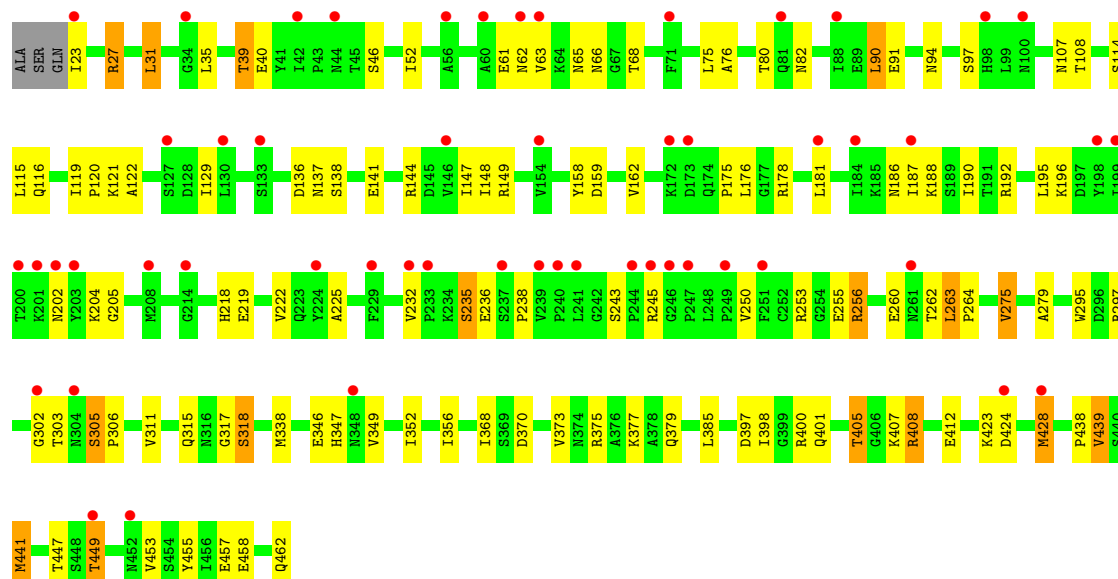
ALA SER GLN ILE P24 R27 T28 S29 K30 L31 T34 L35 T36 I37 A38 T39 E40 A48 A56 A60 E61 N62 V63 A64 N65 N66 G67 T68 L75 A76 Q86 R87 I88 E89 L90 E91 T92 E93 N94 S97 A98 L99 M107 T108 S114 L115 Q116 E117



• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

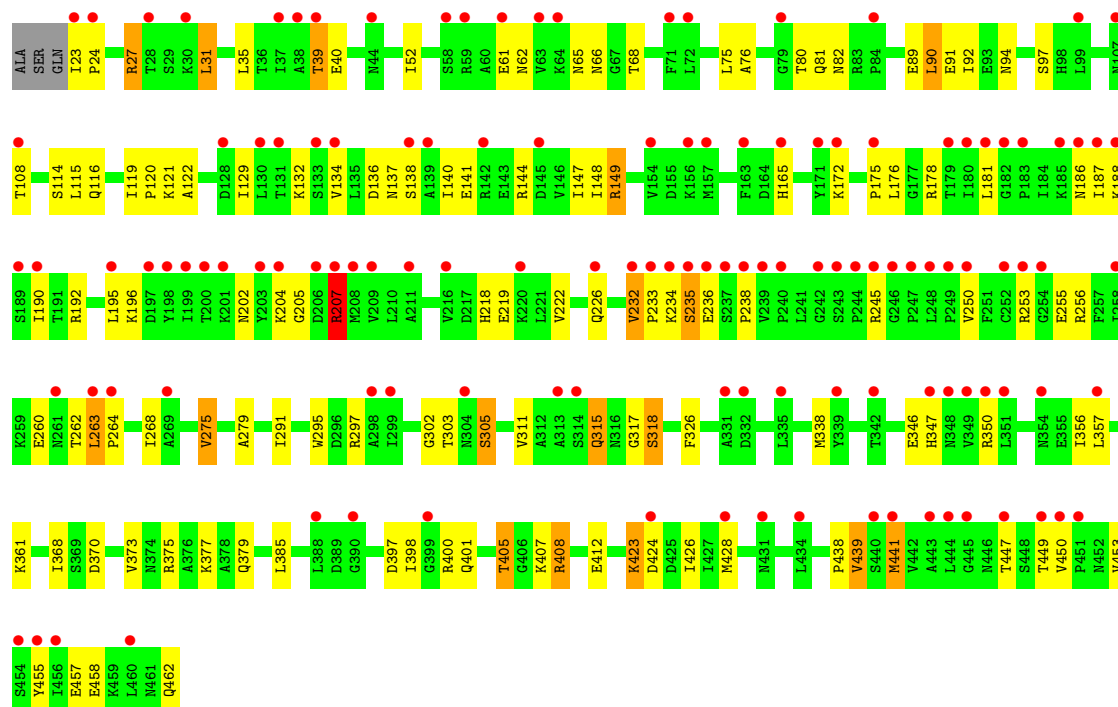


• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT



• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.20Å 178.62Å 201.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.53 – 2.55 47.53 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.53-2.55) 98.7 (47.53-2.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.256 0.242 , 0.256	Depositor DCC
R_{free} test set	2025 reflections (1.29%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27725	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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	0.79	3/3604 (0.1%)	1.04	12/4877 (0.2%)
1	C	0.78	4/3517 (0.1%)	1.07	20/4760 (0.4%)
1	E	0.74	2/3548 (0.1%)	1.08	21/4800 (0.4%)
1	G	0.71	0/3556	1.05	12/4811 (0.2%)
2	B	0.77	2/3478 (0.1%)	1.08	15/4720 (0.3%)
2	D	0.74	1/3495 (0.0%)	1.14	32/4744 (0.7%)
2	F	0.63	0/3486	1.05	20/4732 (0.4%)
2	H	0.62	0/3486	1.09	22/4732 (0.5%)
All	All	0.73	12/28170 (0.0%)	1.07	154/38176 (0.4%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	114	MET	SD-CE	-7.33	1.61	1.79
1	A	114	MET	SD-CE	-7.30	1.61	1.79
2	B	428	MET	SD-CE	6.91	1.96	1.79
2	B	441	MET	SD-CE	5.85	1.94	1.79
1	E	114	MET	SD-CE	-5.72	1.65	1.79
1	A	148	MET	SD-CE	5.72	1.93	1.79
1	C	245	PRO	CA-C	5.67	1.54	1.51
1	E	312	PHE	CA-C	5.39	1.59	1.52
1	C	398	MET	SD-CE	5.26	1.92	1.79
1	A	101	MET	SD-CE	-5.24	1.66	1.79
1	C	148	MET	SD-CE	5.22	1.92	1.79
2	D	109	VAL	CA-CB	5.14	1.61	1.54

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	253	ARG	NE-CZ-NH2	10.59	128.73	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	350	ARG	NE-CZ-NH2	10.21	128.39	119.20
2	D	350	ARG	CG-CD-NE	-10.08	89.83	112.00
2	H	207	ARG	NE-CZ-NH2	9.98	128.19	119.20
2	H	207	ARG	NE-CZ-NH1	-9.45	112.05	121.50
2	D	253	ARG	NE-CZ-NH1	-9.35	112.15	121.50
1	C	18	ASN	N-CA-C	-9.34	101.19	112.58
1	E	422	ARG	NE-CZ-NH2	8.98	127.28	119.20
1	E	422	ARG	NE-CZ-NH1	-8.73	112.77	121.50
2	D	350	ARG	NE-CZ-NH1	-8.72	112.78	121.50
2	H	149	ARG	NE-CZ-NH2	-8.26	111.76	119.20
2	D	305	SER	CA-C-N	7.87	127.80	119.85
2	D	305	SER	C-N-CA	7.87	127.80	119.85
2	H	450	VAL	N-CA-C	7.70	115.25	108.63
2	B	305	SER	CA-C-N	7.54	127.47	119.85
2	B	305	SER	C-N-CA	7.54	127.47	119.85
1	A	239	GLY	N-CA-C	-7.47	101.75	112.81
2	H	149	ARG	CD-NE-CZ	7.38	134.73	124.40
1	C	244	ILE	CA-C-N	7.28	124.98	119.66
1	C	244	ILE	C-N-CA	7.28	124.98	119.66
2	D	253	ARG	CD-NE-CZ	7.24	134.54	124.40
2	F	232	VAL	CA-C-N	7.14	127.54	119.83
2	F	232	VAL	C-N-CA	7.14	127.54	119.83
2	D	236	GLU	CB-CA-C	-7.06	99.75	110.90
2	F	305	SER	CA-C-N	7.03	126.95	119.85
2	F	305	SER	C-N-CA	7.03	126.95	119.85
1	A	18	ASN	N-CA-C	-7.03	102.50	111.92
2	H	149	ARG	NE-CZ-NH1	7.02	128.52	121.50
2	F	235	SER	N-CA-C	-7.00	101.29	110.53
2	H	235	SER	N-CA-C	-6.88	101.94	110.41
2	H	232	VAL	CA-C-N	6.87	127.25	119.83
2	H	232	VAL	C-N-CA	6.87	127.25	119.83
1	E	153	VAL	N-CA-C	6.84	116.98	110.42
2	H	305	SER	CA-C-N	6.74	126.66	119.85
2	H	305	SER	C-N-CA	6.74	126.66	119.85
2	D	241	LEU	N-CA-C	6.65	120.27	111.75
1	E	422	ARG	CD-NE-CZ	6.59	133.62	124.40
1	C	446	MET	N-CA-C	6.55	119.03	109.07
1	E	172	LEU	N-CA-C	-6.52	104.36	112.90
1	G	172	LEU	N-CA-C	-6.50	104.38	112.90
2	B	108	THR	N-CA-C	-6.46	98.37	108.90
2	H	207	ARG	CD-NE-CZ	6.45	133.43	124.40
1	A	105	SER	N-CA-C	-6.44	98.48	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	170	SER	N-CA-C	-6.39	101.72	109.83
2	H	315	GLN	N-CA-C	6.38	118.95	110.53
2	B	107	ASN	N-CA-C	6.35	118.60	109.14
2	D	347	HIS	N-CA-C	6.32	119.77	109.59
1	A	304	THR	N-CA-C	6.32	117.83	111.07
2	F	108	THR	N-CA-C	-6.28	98.66	108.90
1	E	239	GLY	N-CA-C	-6.19	102.70	112.61
2	F	347	HIS	N-CA-C	6.17	119.52	109.59
1	G	194	PHE	N-CA-C	6.10	121.38	113.88
2	H	347	HIS	N-CA-C	6.08	119.38	109.59
2	D	23	ILE	CA-C-N	6.05	126.37	119.83
2	D	23	ILE	C-N-CA	6.05	126.37	119.83
1	G	105	SER	N-CA-C	-6.04	99.16	109.24
2	H	108	THR	N-CA-C	-6.03	98.57	108.76
2	D	108	THR	N-CA-C	-6.03	99.08	108.90
2	H	202	ASN	N-CA-C	6.03	120.76	113.41
1	C	398	MET	N-CA-C	6.01	118.73	111.40
2	F	263	LEU	CA-C-N	6.00	125.55	119.19
2	F	263	LEU	C-N-CA	6.00	125.55	119.19
1	E	56	ASN	N-CA-C	5.99	118.77	111.82
1	C	179	ILE	CB-CA-C	-5.96	108.04	114.35
1	E	266	LEU	CA-C-N	5.92	125.83	119.85
1	E	266	LEU	C-N-CA	5.92	125.83	119.85
1	A	221	GLY	N-CA-C	5.92	119.80	112.64
1	C	257	PHE	N-CA-C	-5.92	100.97	110.14
2	D	232	VAL	N-CA-C	5.88	113.69	108.63
1	A	232	LYS	N-CA-C	5.87	118.33	107.99
2	B	302	GLY	N-CA-C	-5.86	107.15	115.30
2	D	423	LYS	N-CA-C	-5.85	104.90	111.28
1	C	56	ASN	N-CA-C	5.83	118.58	111.82
2	D	107	ASN	N-CA-C	5.83	118.05	109.24
2	B	235	SER	N-CA-C	-5.79	102.88	110.53
1	C	239	GLY	N-CA-C	-5.79	103.34	112.61
2	D	263	LEU	CA-C-N	5.79	125.16	118.85
2	D	263	LEU	C-N-CA	5.79	125.16	118.85
1	A	194	PHE	N-CA-C	5.78	120.99	113.88
2	B	232	VAL	CA-C-N	5.75	126.03	119.83
2	B	232	VAL	C-N-CA	5.75	126.03	119.83
1	A	56	ASN	N-CA-C	5.71	118.45	111.82
1	C	221	GLY	N-CA-C	5.70	119.78	112.83
1	G	153	VAL	N-CA-C	5.69	116.42	110.62
2	F	232	VAL	N-CA-C	5.66	113.50	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	208	MET	N-CA-C	5.64	117.97	109.23
2	H	263	LEU	CA-C-N	5.64	124.99	118.85
2	H	263	LEU	C-N-CA	5.64	124.99	118.85
1	G	446	MET	N-CA-C	5.63	117.63	109.07
2	F	302	GLY	N-CA-C	-5.62	107.48	115.30
2	H	385	LEU	N-CA-C	5.62	120.63	113.55
2	F	115	LEU	N-CA-C	-5.61	102.72	110.35
1	G	257	PHE	N-CA-C	-5.61	101.45	110.14
2	D	63	VAL	N-CA-C	5.59	116.32	110.62
2	F	23	ILE	CA-C-N	5.59	126.83	119.84
2	F	23	ILE	C-N-CA	5.59	126.83	119.84
1	E	301	ARG	N-CA-C	5.57	117.80	111.11
1	G	56	ASN	N-CA-C	5.57	118.28	111.82
2	B	315	GLN	N-CA-C	5.55	118.04	110.55
2	B	114	SER	N-CA-C	5.54	116.69	108.60
2	D	234	LYS	N-CA-C	-5.54	103.07	110.55
1	E	287	GLY	N-CA-C	-5.54	102.63	112.54
1	G	239	GLY	N-CA-C	-5.53	103.77	112.61
2	D	385	LEU	N-CA-C	5.51	120.50	113.55
2	B	202	ASN	N-CA-C	5.49	120.11	113.41
1	E	257	PHE	N-CA-C	-5.49	101.63	110.14
1	G	221	GLY	N-CA-C	5.49	119.53	112.83
2	H	423	LYS	N-CA-C	-5.49	105.30	111.28
2	D	350	ARG	CD-NE-CZ	5.48	132.08	124.40
1	A	398	MET	N-CA-C	5.48	118.08	111.40
1	E	105	SER	N-CA-C	-5.45	100.53	109.40
2	F	385	LEU	N-CA-C	5.44	120.41	113.55
1	G	304	THR	N-CA-C	5.43	116.88	111.07
2	F	63	VAL	N-CA-C	5.42	116.05	110.36
2	H	302	GLY	N-CA-C	-5.40	107.79	115.30
1	E	15	ARG	N-CA-C	5.40	121.03	110.56
1	A	153	VAL	N-CA-C	5.39	115.60	110.53
2	D	115	LEU	N-CA-C	-5.38	103.03	110.35
1	E	232	LYS	N-CA-C	5.38	117.76	107.75
2	F	202	ASN	N-CA-C	5.38	119.97	113.41
1	A	301	ARG	N-CA-C	5.37	117.83	111.33
1	E	398	MET	N-CA-C	5.35	117.93	111.40
1	G	108	ASN	N-CA-C	5.34	117.80	111.33
1	E	194	PHE	N-CA-C	5.33	120.80	113.97
2	B	347	HIS	N-CA-C	5.27	118.08	109.59
1	A	172	LEU	N-CA-C	-5.27	105.59	112.23
2	F	107	ASN	N-CA-C	5.25	116.96	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	455	TYR	N-CA-C	-5.24	105.48	111.14
2	D	315	GLN	N-CA-C	5.24	117.62	110.55
1	C	232	LYS	N-CA-C	5.22	117.46	107.75
1	C	304	THR	N-CA-C	5.21	116.64	111.07
1	C	170	SER	N-CA-C	-5.20	103.23	109.83
1	C	172	LEU	N-CA-C	-5.19	105.69	112.23
1	C	452	SER	N-CA-C	5.17	119.06	112.34
2	D	409	LEU	N-CA-C	-5.17	102.21	109.96
1	E	24	LEU	N-CA-C	-5.17	103.10	110.59
2	B	115	LEU	N-CA-C	-5.15	103.24	110.50
1	C	245	PRO	CA-C-N	5.15	125.08	119.78
1	C	245	PRO	C-N-CA	5.15	125.08	119.78
1	E	101	MET	N-CA-C	5.14	117.61	109.50
2	H	115	LEU	N-CA-C	-5.11	103.40	110.35
1	C	301	ARG	N-CA-C	5.11	117.24	111.11
1	G	301	ARG	N-CA-C	5.11	117.24	111.11
1	E	179	ILE	CB-CA-C	-5.10	108.94	114.35
2	D	232	VAL	CA-C-N	5.10	125.33	119.83
2	D	232	VAL	C-N-CA	5.10	125.33	119.83
2	B	232	VAL	N-CA-C	5.08	113.93	108.95
2	D	84	PRO	N-CA-C	-5.07	104.13	111.22
2	F	243	SER	CA-C-N	5.06	126.17	119.84
2	F	243	SER	C-N-CA	5.06	126.17	119.84
2	D	302	GLY	N-CA-C	-5.06	108.30	115.43
1	C	153	VAL	N-CA-C	5.02	115.25	110.53
1	C	105	SER	N-CA-C	-5.01	101.23	109.40
2	D	202	ASN	N-CA-C	5.01	119.52	113.41

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	3531	0	3488	82	0
1	C	3447	0	3406	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3478	0	3442	80	0
1	G	3485	0	3448	85	0
2	B	3414	0	3414	86	0
2	D	3431	0	3432	82	0
2	F	3422	0	3424	83	0
2	H	3422	0	3424	94	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	A	20	0	0	0	0
4	B	27	0	0	0	0
4	C	13	0	0	0	0
4	D	10	0	0	0	0
4	E	9	0	0	0	0
4	F	4	0	0	0	0
4	G	7	0	0	0	0
4	H	1	0	0	0	0
All	All	27725	0	27478	648	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 12.

All (648) 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:33:SER:HB3	1:A:392:MET:HE1	1.16	1.13
1:C:33:SER:HB3	1:C:392:MET:HE1	1.12	1.08
1:E:33:SER:HB3	1:E:392:MET:HE1	1.10	1.07
1:G:33:SER:HB3	1:G:392:MET:HE1	1.07	1.04
1:A:230:ILE:HD12	1:A:230:ILE:H	1.29	0.98
1:G:24:LEU:HD11	1:G:216:THR:HG22	1.43	0.97
1:G:311:TYR:HD2	1:G:311:TYR:N	1.60	0.96
1:C:230:ILE:HD12	1:C:230:ILE:H	1.29	0.95
1:C:24:LEU:HD11	1:C:216:THR:HG22	1.48	0.94
2:D:256:ARG:HG3	2:D:256:ARG:HH11	1.31	0.94
1:E:33:SER:CB	1:E:392:MET:HE1	1.96	0.93
1:G:230:ILE:H	1:G:230:ILE:HD12	1.30	0.93
1:A:24:LEU:HD11	1:A:216:THR:HG22	1.50	0.93
1:G:33:SER:CB	1:G:392:MET:HE1	1.98	0.92
1:C:33:SER:CB	1:C:392:MET:HE1	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:ILE:HD12	1:E:230:ILE:H	1.31	0.92
2:F:256:ARG:HG3	2:F:256:ARG:HH11	1.34	0.91
1:G:311:TYR:N	1:G:311:TYR:CD2	2.35	0.90
2:B:256:ARG:HG3	2:B:256:ARG:HH11	1.32	0.90
1:A:33:SER:CB	1:A:392:MET:HE1	2.03	0.89
1:E:268:ILE:HD11	1:E:398:MET:SD	2.14	0.86
1:C:99:ASN:HD22	1:C:101:MET:HE3	1.42	0.85
1:A:99:ASN:HD22	1:A:101:MET:HE3	1.42	0.85
1:G:99:ASN:HD22	1:G:101:MET:HE3	1.41	0.85
2:H:256:ARG:HH11	2:H:256:ARG:HG3	1.39	0.84
1:E:24:LEU:HD11	1:E:216:THR:HG22	1.59	0.84
1:C:246:PRO:HG3	1:C:448:GLY:HA2	1.59	0.83
2:H:62:ASN:H	2:H:65:ASN:HB3	1.43	0.83
1:G:311:TYR:HD2	1:G:311:TYR:H	0.84	0.83
2:B:62:ASN:H	2:B:65:ASN:HB3	1.43	0.82
1:E:99:ASN:HD22	1:E:101:MET:HE3	1.44	0.82
2:F:62:ASN:H	2:F:65:ASN:HB3	1.45	0.81
1:A:14:ALA:HB3	1:A:404:PRO:HB3	1.60	0.81
1:A:268:ILE:HD11	1:A:398:MET:SD	2.20	0.81
1:C:429:THR:CG2	1:C:431:ASN:HD22	1.94	0.81
1:C:230:ILE:HD12	1:C:230:ILE:N	1.95	0.80
1:C:268:ILE:HD11	1:C:398:MET:SD	2.22	0.80
1:A:429:THR:CG2	1:A:431:ASN:HD22	1.96	0.79
1:G:268:ILE:HD11	1:G:398:MET:SD	2.23	0.78
2:D:338:MET:HG2	2:D:356:ILE:HD13	1.66	0.77
2:D:62:ASN:H	2:D:65:ASN:HB3	1.49	0.77
1:A:230:ILE:HD12	1:A:230:ILE:N	1.98	0.77
1:G:33:SER:HB3	1:G:392:MET:CE	2.03	0.77
1:G:425:GLU:O	1:G:429:THR:HB	1.85	0.77
1:E:230:ILE:HD12	1:E:230:ILE:N	2.00	0.77
1:A:425:GLU:O	1:A:429:THR:HB	1.85	0.76
1:E:296:LYS:HE2	1:E:298:MET:HE2	1.66	0.76
1:E:429:THR:CG2	1:E:431:ASN:HD22	1.99	0.76
2:H:275:VAL:HG22	2:H:279:ALA:CB	2.15	0.76
2:H:338:MET:HG2	2:H:356:ILE:HD13	1.68	0.76
1:G:230:ILE:HD12	1:G:230:ILE:N	1.99	0.76
2:H:144:ARG:O	2:H:148:ILE:HG12	1.86	0.75
1:G:429:THR:CG2	1:G:431:ASN:HD22	2.00	0.75
2:B:338:MET:HG2	2:B:356:ILE:HD13	1.69	0.75
1:C:230:ILE:H	1:C:230:ILE:CD1	1.99	0.75
2:F:31:LEU:HD22	2:F:35:LEU:HD23	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:429:THR:HG21	1:G:431:ASN:HD22	1.52	0.74
1:C:425:GLU:O	1:C:429:THR:HB	1.86	0.74
1:E:246:PRO:HG3	1:E:448:GLY:HA2	1.69	0.74
1:G:19:PHE:CD1	1:G:392:MET:HE2	2.23	0.73
1:C:429:THR:HG21	1:C:431:ASN:HD22	1.52	0.73
1:C:96:SER:HB3	1:C:99:ASN:OD1	1.89	0.73
2:B:40:GLU:OE1	2:B:408:ARG:NH2	2.20	0.73
1:G:96:SER:HB3	1:G:99:ASN:OD1	1.88	0.73
2:H:186:ASN:O	2:H:190:ILE:HG12	1.88	0.73
1:E:425:GLU:O	1:E:429:THR:HB	1.89	0.73
2:B:458:GLU:O	2:B:462:GLN:HB2	1.88	0.73
2:F:245:ARG:HE	2:F:245:ARG:HA	1.54	0.73
2:F:303:THR:HG22	2:F:305:SER:H	1.54	0.73
1:A:230:ILE:H	1:A:230:ILE:CD1	2.00	0.72
2:B:186:ASN:O	2:B:190:ILE:HG12	1.88	0.72
2:F:338:MET:HG2	2:F:356:ILE:HD13	1.72	0.72
2:H:458:GLU:O	2:H:462:GLN:HB2	1.90	0.72
2:F:458:GLU:O	2:F:462:GLN:HB2	1.90	0.72
1:E:311:TYR:C	1:E:313:VAL:H	1.98	0.71
1:G:230:ILE:H	1:G:230:ILE:CD1	2.02	0.71
1:E:230:ILE:H	1:E:230:ILE:CD1	2.03	0.71
2:D:144:ARG:O	2:D:148:ILE:HG12	1.90	0.71
1:A:429:THR:HG21	1:A:431:ASN:HD22	1.55	0.71
1:G:14:ALA:N	1:G:17:ASP:OD2	2.23	0.71
2:H:31:LEU:HD22	2:H:35:LEU:HD23	1.73	0.71
2:B:144:ARG:O	2:B:148:ILE:HG12	1.91	0.71
1:G:336:ILE:HG22	1:G:338:GLN:OE1	1.91	0.71
2:D:256:ARG:HG3	2:D:256:ARG:NH1	2.03	0.70
2:D:458:GLU:O	2:D:462:GLN:HB2	1.90	0.70
2:B:245:ARG:HE	2:B:245:ARG:HA	1.54	0.70
2:H:303:THR:HG22	2:H:305:SER:H	1.55	0.70
2:D:275:VAL:HG22	2:D:279:ALA:CB	2.22	0.70
1:E:336:ILE:HG22	1:E:338:GLN:OE1	1.92	0.69
1:G:99:ASN:ND2	1:G:101:MET:HE3	2.06	0.69
2:D:97:SER:OG	2:D:114:SER:HB3	1.92	0.69
2:D:303:THR:HG22	2:D:305:SER:H	1.56	0.69
1:C:62:HIS:CE1	1:C:66:ARG:HD2	2.26	0.69
2:B:350:ARG:NE	2:D:416:GLU:OE2	2.25	0.69
1:G:311:TYR:C	1:G:313:VAL:H	2.00	0.69
2:D:186:ASN:O	2:D:190:ILE:HG12	1.92	0.69
1:E:429:THR:HG21	1:E:431:ASN:HD22	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:TYR:C	1:G:313:VAL:N	2.48	0.69
2:F:186:ASN:O	2:F:190:ILE:HG12	1.93	0.69
1:G:246:PRO:HG3	1:G:448:GLY:HA2	1.75	0.69
2:B:97:SER:OG	2:B:114:SER:HB3	1.93	0.68
1:A:14:ALA:CB	1:A:404:PRO:HB3	2.23	0.68
2:D:31:LEU:HD22	2:D:35:LEU:HD23	1.75	0.68
1:A:175:PRO:HB3	1:E:175:PRO:HB3	1.75	0.68
1:A:290:SER:HB3	1:A:303:TYR:OH	1.94	0.68
2:H:23:ILE:HG13	2:H:23:ILE:O	1.94	0.68
2:F:236:GLU:C	2:F:238:PRO:HD3	2.19	0.68
1:A:99:ASN:ND2	1:A:101:MET:HE3	2.09	0.68
1:C:311:TYR:C	1:C:313:VAL:N	2.50	0.68
1:A:311:TYR:C	1:A:313:VAL:H	2.00	0.68
2:D:175:PRO:HA	2:D:178:ARG:NH1	2.09	0.68
1:A:99:ASN:HB2	1:A:101:MET:HE3	1.76	0.67
1:A:311:TYR:C	1:A:313:VAL:N	2.50	0.67
1:E:96:SER:HB3	1:E:99:ASN:OD1	1.93	0.67
1:C:33:SER:HB3	1:C:392:MET:CE	2.07	0.67
1:E:311:TYR:C	1:E:313:VAL:N	2.49	0.67
2:H:236:GLU:C	2:H:238:PRO:HD3	2.19	0.67
2:F:144:ARG:O	2:F:148:ILE:HG12	1.92	0.67
2:B:256:ARG:HG3	2:B:256:ARG:NH1	2.04	0.67
1:C:311:TYR:C	1:C:313:VAL:H	2.01	0.67
1:C:99:ASN:ND2	1:C:101:MET:HE3	2.11	0.66
2:B:31:LEU:HD22	2:B:35:LEU:HD23	1.76	0.66
1:C:99:ASN:HB2	1:C:101:MET:HE3	1.77	0.66
1:E:99:ASN:HB2	1:E:101:MET:HE3	1.77	0.66
2:B:303:THR:HG22	2:B:305:SER:H	1.61	0.65
1:A:19:PHE:CD1	1:A:392:MET:HE2	2.32	0.65
2:F:368:ILE:O	2:F:423:LYS:HE3	1.96	0.65
2:H:368:ILE:O	2:H:423:LYS:HE3	1.96	0.65
2:H:76:ALA:HB1	2:H:129:ILE:HG23	1.76	0.65
1:G:15:ARG:HG3	1:G:15:ARG:HH11	1.62	0.64
1:A:96:SER:HB3	1:A:99:ASN:OD1	1.96	0.64
2:H:245:ARG:HE	2:H:245:ARG:HA	1.63	0.64
2:H:439:VAL:HG22	2:H:453:VAL:HG13	1.77	0.64
2:B:439:VAL:HG22	2:B:453:VAL:HG13	1.77	0.64
1:E:99:ASN:ND2	1:E:101:MET:HE3	2.11	0.64
1:A:336:ILE:HG22	1:A:338:GLN:OE1	1.96	0.64
2:B:428:MET:HE2	2:B:428:MET:HA	1.78	0.64
2:H:275:VAL:HG22	2:H:279:ALA:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:204:LYS:HA	2:H:233:PRO:O	1.98	0.64
2:H:256:ARG:HG3	2:H:256:ARG:NH1	2.09	0.64
2:B:405:THR:HG22	2:B:407:LYS:H	1.62	0.64
2:B:61:GLU:HA	2:B:65:ASN:HD22	1.64	0.63
1:G:99:ASN:HB2	1:G:101:MET:HE3	1.80	0.63
2:B:368:ILE:O	2:B:423:LYS:HE3	1.99	0.63
1:C:336:ILE:HG22	1:C:338:GLN:OE1	1.97	0.63
2:D:136:ASP:OD2	2:D:138:SER:HB3	1.99	0.63
1:A:242:SER:OG	1:E:176:ARG:NH2	2.31	0.63
2:F:76:ALA:HB1	2:F:129:ILE:HG23	1.80	0.62
1:C:62:HIS:HE1	1:C:66:ARG:HD2	1.63	0.62
2:F:439:VAL:HG22	2:F:453:VAL:HG13	1.81	0.62
2:H:260:GLU:HG3	2:H:263:LEU:HG	1.81	0.62
1:G:268:ILE:HD13	1:G:268:ILE:N	2.14	0.62
1:C:379:LEU:HD13	2:D:46:SER:HB2	1.80	0.62
2:D:245:ARG:HA	2:D:245:ARG:HE	1.65	0.62
2:H:136:ASP:OD2	2:H:138:SER:HB3	2.00	0.62
2:H:90:LEU:HD13	2:H:94:ASN:ND2	2.15	0.62
2:F:441:MET:HE3	2:F:453:VAL:HG23	1.82	0.62
2:H:39:THR:HG21	2:H:218:HIS:HB2	1.81	0.62
1:A:294:PRO:HD2	2:B:99:LEU:HB3	1.81	0.61
2:B:236:GLU:C	2:B:238:PRO:HD3	2.25	0.61
2:F:275:VAL:HG22	2:F:279:ALA:CB	2.29	0.61
2:F:260:GLU:HG3	2:F:263:LEU:HG	1.81	0.61
2:F:136:ASP:OD2	2:F:138:SER:HB3	2.00	0.61
1:C:19:PHE:CD1	1:C:392:MET:HE2	2.35	0.61
2:D:76:ALA:HB1	2:D:129:ILE:HG23	1.81	0.61
2:D:236:GLU:C	2:D:238:PRO:HD3	2.25	0.61
2:D:368:ILE:O	2:D:423:LYS:HE3	1.99	0.61
2:D:260:GLU:HG3	2:D:263:LEU:HG	1.81	0.61
2:B:275:VAL:HG22	2:B:279:ALA:CB	2.30	0.61
1:C:342:GLN:O	1:C:346:VAL:HG23	2.00	0.61
1:C:122:VAL:O	1:C:191:ARG:NH2	2.33	0.61
2:H:401:GLN:O	2:H:405:THR:HB	2.01	0.61
1:G:268:ILE:HD13	1:G:268:ILE:H	1.65	0.60
1:G:19:PHE:HD1	1:G:392:MET:HE2	1.62	0.60
1:C:268:ILE:N	1:C:268:ILE:HD13	2.16	0.60
1:E:14:ALA:HB3	1:E:404:PRO:HB3	1.83	0.60
2:F:256:ARG:HG3	2:F:256:ARG:NH1	2.03	0.60
1:G:187:LEU:O	1:G:191:ARG:HG3	2.02	0.60
1:G:340:ALA:HB3	1:G:341:PRO:HD3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ALA:HB3	1:A:341:PRO:HD3	1.84	0.60
2:B:260:GLU:HG3	2:B:263:LEU:HG	1.83	0.60
2:F:192:ARG:NH1	2:F:196:LYS:HD2	2.17	0.60
1:A:289:PHE:CE2	1:A:291:ALA:HB2	2.37	0.59
2:D:441:MET:HE3	2:D:453:VAL:HG23	1.83	0.59
2:B:76:ALA:HB1	2:B:129:ILE:HG23	1.83	0.59
1:C:249:VAL:HG12	1:C:255:GLU:HB2	1.84	0.59
1:C:268:ILE:HD13	1:C:268:ILE:H	1.65	0.59
2:F:405:THR:HG22	2:F:407:LYS:H	1.67	0.59
1:G:296:LYS:HE2	1:G:298:MET:HE2	1.82	0.59
1:A:268:ILE:N	1:A:268:ILE:HD13	2.17	0.59
2:H:175:PRO:HA	2:H:178:ARG:NH1	2.18	0.59
1:A:268:ILE:HD13	1:A:268:ILE:H	1.67	0.59
2:B:39:THR:HG21	2:B:218:HIS:HB2	1.83	0.59
2:B:137:ASN:ND2	2:B:192:ARG:HD2	2.18	0.59
2:H:61:GLU:HA	2:H:65:ASN:HD22	1.66	0.59
2:H:405:THR:HG22	2:H:407:LYS:H	1.67	0.59
2:B:239:VAL:HG21	2:B:245:ARG:NH2	2.18	0.59
2:D:68:THR:HG23	2:D:195:LEU:HD23	1.83	0.59
2:H:375:ARG:NH2	2:H:379:GLN:OE1	2.36	0.59
1:A:187:LEU:O	1:A:191:ARG:HG3	2.03	0.58
2:D:61:GLU:HA	2:D:65:ASN:HD22	1.68	0.58
2:D:439:VAL:HG22	2:D:453:VAL:HG13	1.84	0.58
2:F:137:ASN:ND2	2:F:192:ARG:HD2	2.18	0.58
1:G:267:PRO:HD2	1:G:270:HIS:HB2	1.85	0.58
1:E:187:LEU:O	1:E:191:ARG:HG3	2.03	0.58
2:H:441:MET:HE3	2:H:453:VAL:HG23	1.84	0.58
2:F:97:SER:OG	2:F:114:SER:HB3	2.04	0.58
2:F:375:ARG:NH2	2:F:379:GLN:OE1	2.36	0.58
1:E:296:LYS:HE2	1:E:298:MET:CE	2.34	0.58
2:F:91:GLU:OE2	2:F:121:LYS:HD2	2.04	0.58
1:E:268:ILE:HD13	1:E:268:ILE:N	2.19	0.57
1:G:294:PRO:HB3	2:H:89:GLU:HA	1.86	0.57
2:H:204:LYS:HG3	2:H:235:SER:OG	2.04	0.57
1:E:256:LEU:CD1	1:E:314:GLU:HG2	2.34	0.57
2:H:91:GLU:OE2	2:H:121:LYS:HD2	2.05	0.57
1:C:267:PRO:HD2	1:C:270:HIS:HB2	1.85	0.57
2:F:401:GLN:O	2:F:405:THR:HB	2.04	0.56
1:G:67:LEU:HD13	1:G:135:GLN:HG3	1.86	0.56
1:A:287:GLY:C	1:A:289:PHE:H	2.13	0.56
1:A:373:GLN:NE2	2:B:93:GLU:OE1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:255:GLU:HB3	2:H:453:VAL:HG23	1.87	0.56
1:E:342:GLN:O	1:E:346:VAL:HG23	2.05	0.56
1:C:256:LEU:CD1	1:C:314:GLU:HG2	2.35	0.56
1:E:340:ALA:HB3	1:E:341:PRO:HD3	1.86	0.56
2:H:137:ASN:ND2	2:H:192:ARG:HD2	2.20	0.56
2:B:375:ARG:NH2	2:B:379:GLN:OE1	2.38	0.56
2:D:39:THR:HG21	2:D:218:HIS:HB2	1.87	0.56
2:F:255:GLU:HB3	2:F:453:VAL:HG23	1.87	0.56
2:H:97:SER:OG	2:H:114:SER:HB3	2.06	0.56
2:B:441:MET:HE3	2:B:453:VAL:HG23	1.88	0.56
2:H:311:VAL:O	2:H:315:GLN:HG3	2.05	0.56
2:D:311:VAL:O	2:D:315:GLN:HG3	2.06	0.56
2:B:245:ARG:HA	2:B:245:ARG:NE	2.19	0.55
2:D:350:ARG:O	2:D:354:ASN:ND2	2.39	0.55
1:E:268:ILE:HD13	1:E:268:ILE:H	1.70	0.55
1:C:67:LEU:HD13	1:C:135:GLN:HG3	1.88	0.55
2:F:61:GLU:HA	2:F:65:ASN:HD22	1.72	0.55
2:F:90:LEU:HD13	2:F:94:ASN:ND2	2.21	0.55
2:F:68:THR:HG23	2:F:195:LEU:HD23	1.88	0.55
2:F:175:PRO:HA	2:F:178:ARG:NH1	2.21	0.55
2:D:275:VAL:HG22	2:D:279:ALA:HB3	1.86	0.55
2:B:260:GLU:OE2	2:B:262:THR:HG23	2.07	0.55
2:D:255:GLU:HB3	2:D:453:VAL:HG23	1.88	0.55
1:A:67:LEU:HD13	1:A:135:GLN:HG3	1.88	0.55
1:C:187:LEU:O	1:C:191:ARG:HG3	2.06	0.55
2:B:275:VAL:HG22	2:B:279:ALA:HB3	1.88	0.55
1:G:249:VAL:HG12	1:G:255:GLU:HB2	1.89	0.55
1:G:256:LEU:CD1	1:G:314:GLU:HG2	2.36	0.55
1:E:122:VAL:O	1:E:191:ARG:NH2	2.40	0.54
1:E:256:LEU:HD11	1:E:314:GLU:HG2	1.89	0.54
1:E:267:PRO:HD2	1:E:270:HIS:HB2	1.88	0.54
2:D:119:ILE:N	2:D:120:PRO:HD2	2.23	0.54
2:F:275:VAL:HG22	2:F:279:ALA:HB3	1.89	0.54
2:H:144:ARG:HH21	2:H:188:LYS:C	2.15	0.54
1:C:256:LEU:HD11	1:C:314:GLU:HG2	1.89	0.54
1:G:14:ALA:N	1:G:19:PHE:HB3	2.22	0.54
2:F:144:ARG:HH21	2:F:188:LYS:C	2.16	0.54
2:H:192:ARG:NH1	2:H:196:LYS:HD2	2.23	0.54
2:F:116:GLN:O	2:F:119:ILE:HG12	2.08	0.53
2:B:136:ASP:OD2	2:B:138:SER:HB3	2.08	0.53
2:D:375:ARG:NH2	2:D:379:GLN:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:SER:HB3	1:E:392:MET:CE	2.06	0.53
1:E:249:VAL:HG12	1:E:255:GLU:HB2	1.91	0.53
1:A:176:ARG:NH2	1:E:242:SER:OG	2.41	0.53
2:H:141:GLU:O	2:H:144:ARG:HG3	2.08	0.53
1:G:296:LYS:HE2	1:G:298:MET:CE	2.38	0.53
2:H:27:ARG:HH11	2:H:27:ARG:HB3	1.73	0.53
2:F:260:GLU:OE2	2:F:262:THR:HG23	2.08	0.53
2:H:317:GLY:O	2:H:318:SER:OG	2.25	0.53
1:E:67:LEU:HD13	1:E:135:GLN:HG3	1.91	0.53
1:E:243:CYS:HA	1:E:446:MET:O	2.09	0.53
2:D:192:ARG:NH1	2:D:196:LYS:HD2	2.24	0.52
2:B:311:VAL:O	2:B:315:GLN:HG3	2.10	0.52
2:B:397:ASP:OD2	2:B:408:ARG:NH1	2.40	0.52
2:H:68:THR:HG23	2:H:195:LEU:HD23	1.91	0.52
2:B:401:GLN:O	2:B:405:THR:HB	2.10	0.52
1:C:114:MET:HE2	1:C:118:MET:HE3	1.92	0.52
2:D:405:THR:HG22	2:D:407:LYS:H	1.74	0.52
2:F:256:ARG:HH11	2:F:256:ARG:CG	2.15	0.52
1:E:45:TYR:OH	1:E:389:LEU:HG	2.09	0.52
2:F:40:GLU:OE1	2:F:408:ARG:NH2	2.43	0.52
1:A:256:LEU:CD1	1:A:314:GLU:HG2	2.40	0.51
1:A:429:THR:CG2	1:A:431:ASN:ND2	2.71	0.51
2:B:68:THR:HG23	2:B:195:LEU:HD23	1.91	0.51
2:F:119:ILE:N	2:F:120:PRO:HD2	2.26	0.51
2:H:119:ILE:N	2:H:120:PRO:HD2	2.25	0.51
1:A:267:PRO:HD2	1:A:270:HIS:HB2	1.92	0.51
2:H:40:GLU:OE1	2:H:408:ARG:NH2	2.43	0.51
1:A:246:PRO:HG3	1:A:448:GLY:HA2	1.93	0.51
1:E:241:GLU:HA	1:E:444:VAL:O	2.09	0.51
2:F:39:THR:HG21	2:F:218:HIS:HB2	1.92	0.51
2:H:234:LYS:HG2	2:H:235:SER:O	2.11	0.51
1:A:403:ILE:HG23	1:A:403:ILE:O	2.11	0.51
1:C:429:THR:CG2	1:C:431:ASN:ND2	2.70	0.51
2:F:311:VAL:O	2:F:315:GLN:HG3	2.10	0.51
1:G:140:GLU:HB3	1:G:176:ARG:NH1	2.25	0.51
1:C:45:TYR:OH	1:C:389:LEU:HG	2.11	0.51
2:D:401:GLN:O	2:D:405:THR:HB	2.11	0.51
2:H:260:GLU:OE2	2:H:262:THR:HG23	2.11	0.50
1:C:17:ASP:O	1:C:18:ASN:HB3	2.11	0.50
2:F:141:GLU:O	2:F:144:ARG:HG3	2.11	0.50
1:C:340:ALA:HB3	1:C:341:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:377:SER:O	1:G:381:ASN:HB2	2.12	0.50
1:C:467:ASN:O	1:C:468:SER:HB2	2.10	0.50
1:A:344:VAL:HG21	1:A:456:VAL:HG22	1.94	0.50
1:G:48:ALA:HB1	1:G:190:TYR:OH	2.11	0.50
1:A:296:LYS:HG2	1:A:298:MET:HE2	1.94	0.50
1:C:99:ASN:HD22	1:C:101:MET:CE	2.21	0.50
1:G:128:THR:OG1	1:G:131:GLU:HG3	2.12	0.50
1:A:377:SER:O	1:A:381:ASN:HB2	2.12	0.49
2:D:255:GLU:HB3	2:D:453:VAL:CG2	2.42	0.49
2:B:91:GLU:OE2	2:B:121:LYS:HD2	2.12	0.49
1:C:81:ALA:O	1:C:85:GLU:HG3	2.12	0.49
1:C:286:GLY:O	1:C:315:ASN:ND2	2.45	0.49
2:D:48:ALA:HB3	2:D:119:ILE:HD11	1.95	0.49
1:G:256:LEU:HD11	1:G:314:GLU:HG2	1.92	0.49
2:H:207:ARG:HH11	2:H:245:ARG:NH1	2.09	0.49
2:F:255:GLU:HB3	2:F:453:VAL:CG2	2.42	0.49
2:B:175:PRO:HA	2:B:178:ARG:NH1	2.27	0.49
1:A:35:THR:HB	1:A:36:PRO:CD	2.42	0.49
1:A:342:GLN:O	1:A:346:VAL:HG23	2.13	0.49
1:G:17:ASP:O	1:G:18:ASN:HB3	2.12	0.49
2:B:62:ASN:CG	2:B:65:ASN:HB2	2.37	0.49
2:B:90:LEU:HD13	2:B:94:ASN:ND2	2.27	0.49
2:B:62:ASN:OD1	2:B:65:ASN:HB2	2.13	0.49
2:B:373:VAL:O	2:B:377:LYS:HG3	2.13	0.48
1:C:246:PRO:HG3	1:C:448:GLY:CA	2.39	0.48
2:F:137:ASN:HD21	2:F:192:ARG:HD2	1.78	0.48
1:A:316:CYS:SG	1:A:333:LEU:HD23	2.54	0.48
2:H:90:LEU:CD1	2:H:94:ASN:HD21	2.27	0.48
2:B:144:ARG:HH21	2:B:188:LYS:C	2.21	0.48
2:D:90:LEU:HD13	2:D:94:ASN:ND2	2.29	0.48
2:F:441:MET:HE3	2:F:441:MET:HB3	1.74	0.48
1:G:268:ILE:H	1:G:268:ILE:CD1	2.27	0.48
2:H:428:MET:HA	2:H:428:MET:HE2	1.94	0.48
2:H:255:GLU:HB3	2:H:453:VAL:CG2	2.43	0.48
1:C:377:SER:O	1:C:381:ASN:HB2	2.14	0.48
1:A:128:THR:OG1	1:A:131:GLU:HG3	2.14	0.48
2:D:62:ASN:CG	2:D:65:ASN:HB2	2.39	0.48
1:G:342:GLN:O	1:G:346:VAL:HG23	2.14	0.48
1:C:235:ALA:O	1:C:436:GLY:HA3	2.14	0.48
2:D:91:GLU:OE2	2:D:121:LYS:HD2	2.13	0.48
1:A:19:PHE:HD1	1:A:392:MET:HE2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:428:MET:HA	2:B:428:MET:CE	2.44	0.47
1:C:19:PHE:HD1	1:C:392:MET:HE2	1.76	0.47
1:C:268:ILE:H	1:C:268:ILE:CD1	2.28	0.47
1:C:201:VAL:HG23	1:C:397:LEU:CD1	2.45	0.47
2:D:137:ASN:ND2	2:D:192:ARG:HD2	2.29	0.47
2:B:137:ASN:HD21	2:B:192:ARG:HD2	1.77	0.47
2:D:260:GLU:OE2	2:D:262:THR:HG23	2.13	0.47
1:E:377:SER:O	1:E:381:ASN:HB2	2.14	0.47
2:F:27:ARG:HB3	2:F:27:ARG:HH11	1.80	0.47
2:B:239:VAL:HG21	2:B:245:ARG:HH21	1.79	0.47
2:D:141:GLU:O	2:D:144:ARG:HG3	2.14	0.47
1:E:407:GLU:HG2	1:E:411:LYS:HE3	1.97	0.47
1:A:296:LYS:HE2	1:A:298:MET:HE2	1.97	0.47
1:E:333:LEU:HD13	1:E:334:SER:N	2.30	0.47
2:F:61:GLU:OE1	2:F:66:ASN:HA	2.14	0.47
2:F:253:ARG:HH21	2:F:457:GLU:CD	2.23	0.47
1:G:275:ALA:HB3	1:G:423:VAL:HG21	1.97	0.47
2:H:232:VAL:HG13	2:H:233:PRO:HD2	1.95	0.47
2:D:253:ARG:HH21	2:D:457:GLU:CD	2.23	0.47
1:E:114:MET:HE2	1:E:118:MET:HE3	1.97	0.47
2:F:245:ARG:HA	2:F:245:ARG:NE	2.24	0.47
2:F:295:TRP:CZ2	2:F:297:ARG:HA	2.49	0.47
2:F:317:GLY:O	2:F:318:SER:OG	2.33	0.47
2:H:370:ASP:OD1	2:H:423:LYS:NZ	2.46	0.47
1:C:45:TYR:N	1:C:45:TYR:CD1	2.82	0.46
2:H:147:ILE:HG22	2:H:187:ILE:HD13	1.97	0.46
1:E:467:ASN:O	1:E:468:SER:HB2	2.14	0.46
2:F:428:MET:HE2	2:F:428:MET:HA	1.98	0.46
2:H:62:ASN:CG	2:H:65:ASN:HB2	2.40	0.46
1:A:304:THR:HG22	1:A:305:HIS:ND1	2.29	0.46
1:G:310:TYR:HB3	1:G:312:PHE:CZ	2.51	0.46
2:F:218:HIS:O	2:F:222:VAL:HG23	2.16	0.46
2:F:52:ILE:HG23	2:F:52:ILE:O	2.16	0.46
1:G:72:THR:HG21	1:G:120:GLU:HB3	1.97	0.46
2:H:119:ILE:O	2:H:122:ALA:HB3	2.16	0.46
1:A:114:MET:HE2	1:A:118:MET:HE3	1.98	0.46
1:A:122:VAL:O	1:A:191:ARG:NH2	2.48	0.46
2:B:141:GLU:O	2:B:144:ARG:HG3	2.16	0.46
2:F:441:MET:HE3	2:F:453:VAL:CG2	2.46	0.46
1:G:62:HIS:CE1	1:G:66:ARG:HD2	2.50	0.46
2:F:398:ILE:HA	2:F:408:ARG:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:67:LEU:HD13	1:G:135:GLN:CG	2.46	0.46
1:G:407:GLU:HG2	1:G:411:LYS:HE3	1.98	0.46
1:G:429:THR:CG2	1:G:431:ASN:ND2	2.74	0.46
1:A:99:ASN:HD22	1:A:101:MET:CE	2.22	0.46
1:C:35:THR:HB	1:C:36:PRO:CD	2.46	0.46
2:D:370:ASP:OD1	2:D:423:LYS:NZ	2.47	0.46
1:E:81:ALA:O	1:E:85:GLU:HG3	2.16	0.46
1:E:270:HIS:O	1:E:273:ILE:HB	2.16	0.46
1:E:429:THR:CG2	1:E:431:ASN:ND2	2.75	0.46
2:H:317:GLY:O	2:H:318:SER:CB	2.63	0.46
2:F:192:ARG:HH12	2:F:196:LYS:HD2	1.80	0.45
1:G:114:MET:HE2	1:G:118:MET:HE3	1.98	0.45
1:A:72:THR:HG21	1:A:120:GLU:HB3	1.98	0.45
2:D:144:ARG:HH21	2:D:188:LYS:C	2.23	0.45
2:D:253:ARG:NH2	2:D:457:GLU:OE1	2.49	0.45
2:F:349:VAL:N	2:F:449:THR:OG1	2.49	0.45
1:E:140:GLU:HB3	1:E:176:ARG:NH1	2.31	0.45
1:A:268:ILE:H	1:A:268:ILE:CD1	2.30	0.45
1:C:201:VAL:HG23	1:C:397:LEU:HD13	1.98	0.45
2:H:439:VAL:HG13	2:H:457:GLU:HG2	1.98	0.45
1:G:344:VAL:HG21	1:G:456:VAL:HG22	1.98	0.45
2:H:90:LEU:HD13	2:H:94:ASN:HD21	1.77	0.45
1:A:45:TYR:OH	1:A:389:LEU:HG	2.16	0.45
2:H:253:ARG:HH21	2:H:457:GLU:CD	2.25	0.45
1:A:403:ILE:O	1:A:403:ILE:CG2	2.65	0.45
2:B:439:VAL:HG13	2:B:457:GLU:HG2	1.98	0.45
1:E:45:TYR:N	1:E:45:TYR:CD1	2.84	0.45
2:F:148:ILE:HD13	2:F:187:ILE:HG21	1.97	0.45
1:G:346:VAL:O	1:G:350:GLN:HG2	2.16	0.45
1:A:256:LEU:HD11	1:A:314:GLU:HG2	1.97	0.45
1:A:275:ALA:HB3	1:A:423:VAL:HG21	1.97	0.45
2:D:439:VAL:HG13	2:D:457:GLU:HG2	1.99	0.45
2:F:455:TYR:CD1	2:F:455:TYR:C	2.95	0.45
1:G:95:SER:HB3	1:G:100:LEU:HD13	1.98	0.45
2:H:61:GLU:OE1	2:H:66:ASN:HA	2.17	0.45
2:H:116:GLN:O	2:H:119:ILE:HG12	2.16	0.45
2:H:295:TRP:CZ2	2:H:297:ARG:HA	2.51	0.45
2:H:373:VAL:O	2:H:377:LYS:HG3	2.16	0.45
2:B:305:SER:HA	2:B:306:PRO:HD3	1.67	0.45
2:B:317:GLY:O	2:B:318:SER:OG	2.34	0.45
1:C:267:PRO:HA	1:C:323:TYR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:ALA:HA	1:E:105:SER:HA	1.99	0.45
2:F:62:ASN:CG	2:F:65:ASN:HB2	2.42	0.45
1:G:45:TYR:CD1	1:G:45:TYR:N	2.85	0.45
1:G:56:ASN:HD22	1:G:56:ASN:HA	1.57	0.45
2:B:61:GLU:OE1	2:B:66:ASN:HA	2.17	0.45
2:F:412:GLU:CD	2:F:412:GLU:H	2.24	0.45
1:G:304:THR:HG22	1:G:305:HIS:ND1	2.31	0.45
2:H:136:ASP:O	2:H:140:ILE:HG13	2.17	0.45
2:D:27:ARG:HB3	2:D:27:ARG:HH11	1.82	0.44
2:B:255:GLU:HB3	2:B:453:VAL:HG23	1.99	0.44
1:E:245:PRO:HA	1:E:246:PRO:HD3	1.80	0.44
1:E:336:ILE:HG22	1:E:337:PRO:HD2	1.98	0.44
1:G:127:ILE:HB	1:G:184:LYS:HE3	1.98	0.44
2:H:31:LEU:HD21	2:H:226:GLN:HA	1.98	0.44
2:H:218:HIS:O	2:H:222:VAL:HG23	2.17	0.44
2:F:305:SER:HA	2:F:306:PRO:HD3	1.67	0.44
2:F:317:GLY:O	2:F:318:SER:CB	2.64	0.44
1:G:122:VAL:O	1:G:191:ARG:NH2	2.50	0.44
2:H:397:ASP:OD2	2:H:408:ARG:NH1	2.49	0.44
2:H:441:MET:HE3	2:H:453:VAL:CG2	2.46	0.44
1:E:379:LEU:HD13	2:F:46:SER:HB2	1.98	0.44
1:G:386:LEU:HD12	1:G:386:LEU:HA	1.80	0.44
2:B:204:LYS:HG3	2:B:235:SER:OG	2.17	0.44
2:D:245:ARG:HA	2:D:245:ARG:NE	2.30	0.44
2:D:398:ILE:HA	2:D:408:ARG:HG3	2.00	0.44
1:E:17:ASP:O	1:E:18:ASN:HB3	2.17	0.44
1:E:253:LEU:HA	1:E:254:PRO:HD3	1.86	0.44
2:F:80:THR:C	2:F:82:ASN:H	2.25	0.44
2:B:119:ILE:N	2:B:120:PRO:HD2	2.33	0.44
2:B:207:ARG:HH11	2:B:245:ARG:NH1	2.15	0.44
2:B:458:GLU:CD	2:D:422:THR:HB	2.42	0.44
2:D:317:GLY:O	2:D:318:SER:CB	2.65	0.44
1:E:19:PHE:CD1	1:E:392:MET:HE2	2.53	0.44
1:E:67:LEU:HD13	1:E:135:GLN:CG	2.47	0.44
1:A:45:TYR:N	1:A:45:TYR:CD1	2.86	0.44
2:B:61:GLU:HA	2:B:65:ASN:ND2	2.31	0.44
2:H:207:ARG:NH1	2:H:245:ARG:NH1	2.65	0.44
1:A:287:GLY:O	1:A:289:PHE:N	2.51	0.44
2:B:255:GLU:HA	2:B:441:MET:O	2.18	0.44
1:E:32:THR:HG21	1:E:209:HIS:HA	2.00	0.44
2:H:398:ILE:HA	2:H:408:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LYS:HE2	1:A:298:MET:CE	2.48	0.44
1:C:333:LEU:HD13	1:C:334:SER:N	2.32	0.44
2:D:80:THR:C	2:D:82:ASN:H	2.25	0.44
1:E:95:SER:HB3	1:E:100:LEU:HD13	2.00	0.44
1:E:444:VAL:HG11	1:E:456:VAL:HG11	1.98	0.44
2:H:455:TYR:CD1	2:H:455:TYR:C	2.96	0.44
1:A:95:SER:HB3	1:A:100:LEU:HD13	2.00	0.43
1:A:294:PRO:HB3	2:B:89:GLU:HA	1.99	0.43
1:A:407:GLU:HG2	1:A:411:LYS:HE3	1.99	0.43
1:C:72:THR:HG21	1:C:120:GLU:HB3	2.00	0.43
2:D:303:THR:HG22	2:D:304:ASN:N	2.32	0.43
1:G:15:ARG:HG3	1:G:15:ARG:NH1	2.31	0.43
1:A:287:GLY:C	1:A:289:PHE:N	2.74	0.43
2:D:158:TYR:O	2:D:162:VAL:HG23	2.19	0.43
1:G:35:THR:HB	1:G:36:PRO:CD	2.48	0.43
2:H:39:THR:HG21	2:H:218:HIS:CB	2.48	0.43
2:H:148:ILE:HD13	2:H:187:ILE:HG21	2.00	0.43
2:H:303:THR:HG22	2:H:305:SER:N	2.29	0.43
2:B:97:SER:OG	2:B:114:SER:CB	2.64	0.43
1:C:444:VAL:HG11	1:C:456:VAL:HG11	2.00	0.43
2:D:253:ARG:HB3	2:D:438:PRO:HB2	2.00	0.43
1:E:101:MET:HE2	1:E:101:MET:HB3	1.89	0.43
1:G:263:PHE:CE2	1:G:442:ALA:HB2	2.53	0.43
2:B:429:TRP:CE2	2:B:433:ARG:HG3	2.54	0.43
2:B:439:VAL:CG2	2:B:453:VAL:HG13	2.47	0.43
1:C:67:LEU:HD13	1:C:135:GLN:CG	2.48	0.43
1:E:35:THR:HB	1:E:36:PRO:CD	2.48	0.43
2:D:97:SER:OG	2:D:114:SER:CB	2.63	0.43
2:D:236:GLU:O	2:D:238:PRO:HD3	2.18	0.43
1:E:268:ILE:H	1:E:268:ILE:CD1	2.31	0.43
2:H:137:ASN:HD21	2:H:192:ARG:HD2	1.80	0.43
2:H:268:ILE:HD12	2:H:268:ILE:N	2.33	0.43
2:B:398:ILE:HA	2:B:408:ARG:HG3	2.01	0.43
2:D:373:VAL:O	2:D:377:LYS:HG3	2.18	0.43
2:D:441:MET:HE3	2:D:453:VAL:CG2	2.48	0.43
1:E:62:HIS:CE1	1:E:66:ARG:HD2	2.54	0.43
1:G:41:ALA:HA	1:G:105:SER:HA	2.00	0.43
2:H:291:ILE:HD12	2:H:426:ILE:HD13	2.01	0.43
2:B:263:LEU:HA	2:B:264:PRO:HD3	1.82	0.43
2:B:350:ARG:NH2	2:D:419:ASP:OD2	2.46	0.43
2:D:441:MET:HE3	2:D:441:MET:HB3	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:PRO:HA	1:E:323:TYR:O	2.19	0.43
2:H:263:LEU:HA	2:H:264:PRO:HD3	1.79	0.43
2:F:119:ILE:O	2:F:122:ALA:HB3	2.18	0.43
2:H:92:ILE:HG23	2:H:97:SER:HB2	2.01	0.43
2:H:165:HIS:HD2	2:H:256:ARG:HE	1.67	0.43
1:A:311:TYR:O	1:A:313:VAL:N	2.51	0.43
1:G:151:GLU:CD	1:G:151:GLU:H	2.26	0.43
1:A:299:TYR:OH	2:B:86:GLN:HG2	2.19	0.43
2:B:412:GLU:H	2:B:412:GLU:CD	2.27	0.43
1:E:99:ASN:HD22	1:E:101:MET:CE	2.24	0.43
2:B:27:ARG:HH11	2:B:27:ARG:HB3	1.82	0.42
1:A:85:GLU:OE2	2:B:303:THR:HG23	2.17	0.42
1:A:167:THR:OG1	1:A:168:LEU:N	2.51	0.42
2:B:99:LEU:HD12	2:B:99:LEU:HA	1.91	0.42
2:B:207:ARG:NH1	2:B:245:ARG:NH1	2.66	0.42
2:B:441:MET:HE3	2:B:441:MET:HB3	1.79	0.42
1:C:311:TYR:O	1:C:313:VAL:N	2.52	0.42
1:G:403:ILE:HG23	1:G:403:ILE:O	2.17	0.42
2:H:232:VAL:HA	2:H:233:PRO:HD3	1.68	0.42
2:D:209:VAL:HG21	2:D:402:VAL:HG12	2.02	0.42
2:F:253:ARG:HB3	2:F:438:PRO:HB2	2.01	0.42
1:G:267:PRO:HA	1:G:323:TYR:O	2.19	0.42
2:H:441:MET:HE3	2:H:441:MET:HB3	1.78	0.42
1:C:392:MET:HE3	1:C:402:LYS:HD2	2.01	0.42
1:A:17:ASP:O	1:A:18:ASN:HB3	2.20	0.42
2:B:428:MET:HE2	2:B:428:MET:CA	2.48	0.42
1:E:302:LEU:HD23	1:E:302:LEU:HA	1.90	0.42
2:F:204:LYS:HG3	2:F:235:SER:OG	2.19	0.42
2:F:439:VAL:HG13	2:F:457:GLU:HG2	2.02	0.42
2:H:81:GLN:HG3	2:H:132:LYS:O	2.20	0.42
2:H:253:ARG:HB3	2:H:438:PRO:HB2	2.01	0.42
1:A:267:PRO:HA	1:A:323:TYR:O	2.19	0.42
2:B:148:ILE:HD13	2:B:187:ILE:HG21	2.00	0.42
2:D:255:GLU:HA	2:D:441:MET:O	2.20	0.42
1:G:84:LEU:HD13	1:G:91:TYR:CZ	2.55	0.42
1:G:315:ASN:OD1	1:G:316:CYS:N	2.52	0.42
2:H:326:PHE:CD1	2:H:326:PHE:C	2.98	0.42
1:A:270:HIS:O	1:A:273:ILE:HB	2.20	0.42
2:B:349:VAL:N	2:B:449:THR:OG1	2.53	0.42
2:B:455:TYR:CD1	2:B:455:TYR:C	2.97	0.42
2:D:204:LYS:HA	2:D:233:PRO:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:148:ILE:CD1	2:F:187:ILE:HG21	2.49	0.42
2:F:370:ASP:OD1	2:F:423:LYS:NZ	2.51	0.42
1:C:403:ILE:O	1:C:403:ILE:HG23	2.18	0.42
1:G:276:LEU:HD11	1:G:329:PHE:CD2	2.54	0.42
1:C:128:THR:OG1	1:C:131:GLU:HG3	2.19	0.41
1:C:310:TYR:CD1	1:C:312:PHE:CZ	3.08	0.41
2:D:305:SER:HA	2:D:306:PRO:HD3	1.68	0.41
1:A:35:THR:HB	1:A:36:PRO:HD2	2.02	0.41
2:B:166:LEU:HA	2:B:442:VAL:HG21	2.03	0.41
2:B:232:VAL:HA	2:B:233:PRO:HD3	1.73	0.41
2:D:23:ILE:HA	2:D:24:PRO:HD3	1.80	0.41
2:D:263:LEU:HA	2:D:264:PRO:HD3	1.78	0.41
2:D:428:MET:HE2	2:D:428:MET:HA	2.02	0.41
1:E:263:PHE:CE2	1:E:442:ALA:HB2	2.55	0.41
2:F:35:LEU:HA	2:F:205:GLY:O	2.20	0.41
2:H:357:LEU:O	2:H:361:LYS:HG3	2.20	0.41
2:B:253:ARG:HH21	2:B:457:GLU:CD	2.28	0.41
2:F:158:TYR:O	2:F:162:VAL:HG23	2.20	0.41
1:G:19:PHE:HD1	1:G:392:MET:CE	2.30	0.41
1:G:235:ALA:O	1:G:436:GLY:HA3	2.20	0.41
1:G:444:VAL:HG11	1:G:456:VAL:HG11	2.01	0.41
2:B:48:ALA:HB3	2:B:119:ILE:HD11	2.03	0.41
2:B:370:ASP:OD1	2:B:423:LYS:NZ	2.54	0.41
1:G:253:LEU:HA	1:G:254:PRO:HD3	1.93	0.41
1:E:403:ILE:O	1:E:403:ILE:HG23	2.20	0.41
2:F:90:LEU:CD1	2:F:94:ASN:HD21	2.34	0.41
1:A:32:THR:HG21	1:A:209:HIS:HA	2.02	0.41
1:A:114:MET:CE	1:A:118:MET:HG3	2.51	0.41
1:A:200:THR:HG22	1:A:201:VAL:N	2.35	0.41
2:D:116:GLN:O	2:D:119:ILE:HG12	2.20	0.41
1:G:34:ASN:OD1	1:G:35:THR:N	2.43	0.41
1:C:127:ILE:HB	1:C:184:LYS:HE3	2.03	0.41
1:C:151:GLU:CD	1:C:151:GLU:H	2.27	0.41
1:C:403:ILE:O	1:C:403:ILE:CG2	2.69	0.41
2:D:31:LEU:HD21	2:D:226:GLN:HA	2.02	0.41
2:F:303:THR:HG22	2:F:305:SER:N	2.28	0.41
2:H:412:GLU:CD	2:H:412:GLU:H	2.28	0.41
1:A:73:GLU:HG2	1:A:124:PHE:HB3	2.02	0.41
1:C:56:ASN:HD22	1:C:56:ASN:HA	1.55	0.41
1:C:311:TYR:O	1:C:312:PHE:C	2.61	0.41
1:C:333:LEU:HD13	1:C:333:LEU:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:LEU:HD13	1:E:333:LEU:C	2.45	0.41
1:E:429:THR:HG22	1:E:431:ASN:HD22	1.83	0.41
2:H:80:THR:C	2:H:82:ASN:H	2.29	0.41
1:A:47:ASP:HB3	1:A:199:ASN:OD1	2.21	0.41
1:C:16:THR:HG23	1:C:18:ASN:H	1.86	0.41
2:D:62:ASN:OD1	2:D:65:ASN:HB2	2.21	0.41
2:D:455:TYR:CD1	2:D:455:TYR:C	2.99	0.41
1:E:230:ILE:HD13	1:G:233:LYS:CE	2.50	0.41
2:F:147:ILE:HG22	2:F:187:ILE:HD13	2.03	0.41
1:G:268:ILE:N	1:G:268:ILE:CD1	2.82	0.41
2:H:52:ILE:HG23	2:H:52:ILE:O	2.21	0.41
2:H:255:GLU:HA	2:H:441:MET:O	2.20	0.41
2:H:439:VAL:CG2	2:H:453:VAL:HG13	2.49	0.41
2:B:136:ASP:O	2:B:140:ILE:HG13	2.21	0.41
1:C:263:PHE:CE2	1:C:442:ALA:HB2	2.56	0.41
1:E:204:PHE:CD1	1:E:204:PHE:N	2.88	0.41
2:F:222:VAL:O	2:F:225:ALA:HB3	2.21	0.41
2:F:397:ASP:OD2	2:F:408:ARG:NH1	2.50	0.41
1:G:333:LEU:HD13	1:G:334:SER:N	2.35	0.41
2:B:116:GLN:O	2:B:119:ILE:HG12	2.21	0.40
2:B:423:LYS:O	2:B:427:ILE:HG13	2.21	0.40
2:D:61:GLU:OE1	2:D:66:ASN:HA	2.22	0.40
2:D:317:GLY:O	2:D:318:SER:OG	2.36	0.40
2:F:373:VAL:O	2:F:377:LYS:HG3	2.21	0.40
1:G:45:TYR:OH	1:G:389:LEU:HG	2.21	0.40
1:G:63:ILE:HG22	1:G:67:LEU:HD22	2.02	0.40
2:H:80:THR:C	2:H:134:VAL:HG23	2.46	0.40
2:H:172:LYS:HD2	2:H:172:LYS:HA	1.88	0.40
1:A:67:LEU:HD13	1:A:135:GLN:CG	2.49	0.40
1:A:140:GLU:HB3	1:A:176:ARG:NH1	2.36	0.40
2:B:303:THR:HG22	2:B:305:SER:N	2.32	0.40
2:D:143:GLU:O	2:D:147:ILE:HG12	2.22	0.40
2:D:172:LYS:O	2:D:174:GLN:HG3	2.21	0.40
2:D:207:ARG:NH1	2:D:245:ARG:NH1	2.69	0.40
1:E:72:THR:HG21	1:E:120:GLU:HB3	2.02	0.40
1:E:275:ALA:HB3	1:E:423:VAL:HG21	2.03	0.40
1:E:296:LYS:CE	1:E:298:MET:HE2	2.44	0.40
1:G:237:TYR:CG	1:G:264:GLU:HB2	2.56	0.40
2:H:35:LEU:HA	2:H:205:GLY:O	2.22	0.40
2:H:148:ILE:CD1	2:H:187:ILE:HG21	2.52	0.40
1:C:48:ALA:HB1	1:C:190:TYR:OH	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:LEU:HD12	1:C:386:LEU:HA	1.91	0.40
2:D:99:LEU:HD12	2:D:99:LEU:HA	1.87	0.40
2:F:255:GLU:HA	2:F:441:MET:O	2.21	0.40
2:F:349:VAL:O	2:F:352:ILE:HG22	2.22	0.40
1:A:62:HIS:CD2	1:A:66:ARG:HD2	2.57	0.40
1:A:241:GLU:HA	1:A:444:VAL:O	2.20	0.40
1:A:336:ILE:HG22	1:A:337:PRO:HD2	2.04	0.40
1:C:140:GLU:HB3	1:C:176:ARG:NH1	2.37	0.40
2:D:232:VAL:HA	2:D:233:PRO:HD3	1.74	0.40
2:D:295:TRP:CZ2	2:D:297:ARG:HA	2.57	0.40
1:E:35:THR:HB	1:E:36:PRO:HD2	2.03	0.40
1:E:266:LEU:HA	1:E:267:PRO:HD3	1.89	0.40
2:F:159:ASP:OD1	2:F:159:ASP:N	2.54	0.40
2:F:253:ARG:NH2	2:F:457:GLU:OE1	2.55	0.40
2:D:218:HIS:O	2:D:222:VAL:HG23	2.21	0.40
1:E:56:ASN:HD22	1:E:56:ASN:HA	1.58	0.40
1:E:230:ILE:HD13	1:G:233:LYS:HE3	2.02	0.40
2:F:263:LEU:HA	2:F:264:PRO:HD3	1.79	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	455/475 (96%)	435 (96%)	16 (4%)	4 (1%)	14	20
1	C	440/475 (93%)	421 (96%)	17 (4%)	2 (0%)	24	34
1	E	444/475 (94%)	422 (95%)	20 (4%)	2 (0%)	24	34
1	G	446/475 (94%)	425 (95%)	19 (4%)	2 (0%)	30	39
2	B	437/443 (99%)	423 (97%)	12 (3%)	2 (0%)	24	34
2	D	439/443 (99%)	423 (96%)	15 (3%)	1 (0%)	43	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	438/443 (99%)	421 (96%)	16 (4%)	1 (0%)	43	56
2	H	438/443 (99%)	420 (96%)	16 (4%)	2 (0%)	24	34
All	All	3537/3672 (96%)	3390 (96%)	131 (4%)	16 (0%)	24	34

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	250	PHE
1	G	250	PHE
2	H	24	PRO
1	A	250	PHE
1	A	288	SER
2	B	318	SER
2	D	318	SER
1	E	250	PHE
2	F	318	SER
2	H	318	SER
1	A	290	SER
2	B	56	ALA
1	A	127	ILE
1	C	127	ILE
1	E	127	ILE
1	G	127	ILE

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	384/401 (96%)	362 (94%)	22 (6%)	18	28
1	C	376/401 (94%)	355 (94%)	21 (6%)	19	29
1	E	379/401 (94%)	357 (94%)	22 (6%)	18	27
1	G	378/401 (94%)	356 (94%)	22 (6%)	18	27
2	B	376/379 (99%)	354 (94%)	22 (6%)	18	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	378/379 (100%)	356 (94%)	22 (6%)	18	27
2	F	377/379 (100%)	355 (94%)	22 (6%)	18	27
2	H	377/379 (100%)	355 (94%)	22 (6%)	18	27
All	All	3025/3120 (97%)	2850 (94%)	175 (6%)	18	27

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	65	ASP
1	A	66	ARG
1	A	67	LEU
1	A	143	ILE
1	A	151	GLU
1	A	220	LEU
1	A	230	ILE
1	A	268	ILE
1	A	273	ILE
1	A	288	SER
1	A	305	HIS
1	A	307	LEU
1	A	311	TYR
1	A	314	GLU
1	A	361	ARG
1	A	381	ASN
1	A	382	LEU
1	A	386	LEU
1	A	429	THR
1	A	445	VAL
1	A	446	MET
2	B	27	ARG
2	B	31	LEU
2	B	39	THR
2	B	75	LEU
2	B	90	LEU
2	B	133	SER
2	B	149	ARG
2	B	176	LEU
2	B	181	LEU
2	B	219	GLU
2	B	250	VAL

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Mol	Chain	Res	Type
2	B	256	ARG
2	B	275	VAL
2	B	346	GLU
2	B	400	ARG
2	B	405	THR
2	B	408	ARG
2	B	424	ASP
2	B	428	MET
2	B	439	VAL
2	B	447	THR
2	B	449	THR
1	C	56	ASN
1	C	65	ASP
1	C	66	ARG
1	C	67	LEU
1	C	151	GLU
1	C	220	LEU
1	C	230	ILE
1	C	268	ILE
1	C	273	ILE
1	C	305	HIS
1	C	307	LEU
1	C	311	TYR
1	C	314	GLU
1	C	333	LEU
1	C	361	ARG
1	C	381	ASN
1	C	382	LEU
1	C	386	LEU
1	C	429	THR
1	C	445	VAL
1	C	446	MET
2	D	27	ARG
2	D	31	LEU
2	D	39	THR
2	D	75	LEU
2	D	90	LEU
2	D	149	ARG
2	D	176	LEU
2	D	181	LEU
2	D	219	GLU
2	D	250	VAL

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Mol	Chain	Res	Type
2	D	253	ARG
2	D	256	ARG
2	D	275	VAL
2	D	346	GLU
2	D	400	ARG
2	D	405	THR
2	D	408	ARG
2	D	424	ASP
2	D	439	VAL
2	D	441	MET
2	D	447	THR
2	D	449	THR
1	E	56	ASN
1	E	65	ASP
1	E	66	ARG
1	E	67	LEU
1	E	151	GLU
1	E	220	LEU
1	E	230	ILE
1	E	268	ILE
1	E	273	ILE
1	E	288	SER
1	E	305	HIS
1	E	307	LEU
1	E	311	TYR
1	E	314	GLU
1	E	333	LEU
1	E	361	ARG
1	E	381	ASN
1	E	382	LEU
1	E	386	LEU
1	E	429	THR
1	E	445	VAL
1	E	446	MET
2	F	27	ARG
2	F	31	LEU
2	F	39	THR
2	F	75	LEU
2	F	90	LEU
2	F	149	ARG
2	F	176	LEU
2	F	181	LEU

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Mol	Chain	Res	Type
2	F	219	GLU
2	F	250	VAL
2	F	256	ARG
2	F	275	VAL
2	F	346	GLU
2	F	400	ARG
2	F	405	THR
2	F	408	ARG
2	F	424	ASP
2	F	428	MET
2	F	439	VAL
2	F	441	MET
2	F	447	THR
2	F	449	THR
1	G	15	ARG
1	G	56	ASN
1	G	65	ASP
1	G	66	ARG
1	G	67	LEU
1	G	151	GLU
1	G	220	LEU
1	G	230	ILE
1	G	268	ILE
1	G	273	ILE
1	G	305	HIS
1	G	307	LEU
1	G	311	TYR
1	G	314	GLU
1	G	333	LEU
1	G	361	ARG
1	G	381	ASN
1	G	382	LEU
1	G	386	LEU
1	G	429	THR
1	G	445	VAL
1	G	446	MET
2	H	27	ARG
2	H	31	LEU
2	H	39	THR
2	H	75	LEU
2	H	90	LEU
2	H	149	ARG

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Mol	Chain	Res	Type
2	H	176	LEU
2	H	181	LEU
2	H	207	ARG
2	H	219	GLU
2	H	250	VAL
2	H	275	VAL
2	H	346	GLU
2	H	350	ARG
2	H	400	ARG
2	H	405	THR
2	H	408	ARG
2	H	424	ASP
2	H	439	VAL
2	H	441	MET
2	H	447	THR
2	H	449	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	62	HIS
1	A	99	ASN
1	A	320	ASN
1	A	349	GLN
1	A	381	ASN
1	A	406	ASN
1	A	431	ASN
2	B	44	ASN
2	B	65	ASN
2	B	66	ASN
2	B	85	GLN
2	B	137	ASN
2	B	165	HIS
2	B	223	GLN
2	B	304	ASN
2	B	315	GLN
2	B	374	ASN
2	B	436	ASN
2	B	462	GLN
1	C	56	ASN
1	C	315	ASN

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Mol	Chain	Res	Type
1	C	320	ASN
1	C	350	GLN
1	C	381	ASN
1	C	406	ASN
1	C	431	ASN
2	D	44	ASN
2	D	65	ASN
2	D	66	ASN
2	D	73	GLN
2	D	85	GLN
2	D	107	ASN
2	D	137	ASN
2	D	223	GLN
2	D	315	GLN
2	D	354	ASN
1	E	56	ASN
1	E	236	GLN
1	E	320	ASN
1	E	406	ASN
1	E	431	ASN
1	E	447	GLN
2	F	44	ASN
2	F	65	ASN
2	F	66	ASN
2	F	73	GLN
2	F	85	GLN
2	F	107	ASN
2	F	137	ASN
2	F	165	HIS
2	F	223	GLN
2	F	304	ASN
2	F	315	GLN
2	F	374	ASN
2	F	417	GLN
1	G	56	ASN
1	G	320	ASN
1	G	406	ASN
1	G	431	ASN
2	H	44	ASN
2	H	65	ASN
2	H	66	ASN
2	H	85	GLN

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Mol	Chain	Res	Type
2	H	107	ASN
2	H	137	ASN
2	H	165	HIS
2	H	223	GLN
2	H	304	ASN
2	H	315	GLN
2	H	374	ASN
2	H	462	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	457/475 (96%)	0.50	39 (8%)	16 16	31, 49, 83, 101	0
1	C	444/475 (93%)	0.45	23 (5%)	33 32	30, 50, 75, 101	0
1	E	448/475 (94%)	0.56	32 (7%)	22 21	34, 53, 80, 101	0
1	G	450/475 (94%)	0.63	38 (8%)	17 16	35, 54, 82, 101	0
2	B	439/443 (99%)	0.64	42 (9%)	13 13	30, 51, 76, 95	0
2	D	441/443 (99%)	0.74	34 (7%)	19 18	33, 58, 79, 97	0
2	F	440/443 (99%)	1.05	53 (12%)	9 8	44, 67, 86, 97	0
2	H	440/443 (99%)	1.58	127 (28%)	1 1	52, 75, 91, 99	0
All	All	3559/3672 (96%)	0.77	388 (10%)	10 10	30, 58, 85, 101	0

All (388) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	311	TYR	7.4
2	D	197	ASP	7.2
1	C	249	VAL	7.1
1	E	250	PHE	6.5
2	H	23	ILE	6.4
1	E	249	VAL	6.0
1	A	250	PHE	5.9
1	A	253	LEU	5.4
1	C	230	ILE	5.2
1	A	289	PHE	5.1
1	G	230	ILE	4.9
2	F	424	ASP	4.9
1	G	311	TYR	4.9
1	G	250	PHE	4.9
2	D	88	ILE	4.9
1	A	249	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	G	14	ALA	4.9
1	A	311	TYR	4.9
2	H	239	VAL	4.8
2	H	71	PHE	4.8
1	C	250	PHE	4.7
2	H	198	TYR	4.5
1	A	14	ALA	4.4
1	E	231	THR	4.4
1	G	294	PRO	4.2
1	C	253	LEU	4.2
1	C	303	TYR	4.2
2	D	245	ARG	4.2
1	C	311	TYR	4.2
2	D	449	THR	4.1
2	H	139	ALA	4.1
2	F	247	PRO	4.1
1	A	295	GLY	4.1
2	H	187	ILE	4.0
2	H	240	PRO	4.0
2	H	24	PRO	3.9
2	B	236	GLU	3.8
2	D	230	GLY	3.8
2	H	258	ILE	3.8
2	H	248	LEU	3.8
2	H	197	ASP	3.8
1	C	252	ASN	3.7
1	E	56	ASN	3.7
1	E	253	LEU	3.7
1	C	468	SER	3.7
1	A	17	ASP	3.7
1	G	399	HIS	3.6
2	F	60	ALA	3.6
2	H	234	LYS	3.6
2	H	233	PRO	3.6
1	C	312	PHE	3.6
1	E	16	THR	3.6
2	H	449	THR	3.6
1	A	290	SER	3.6
2	H	444	LEU	3.6
2	B	247	PRO	3.5
2	B	91	GLU	3.5
2	H	246	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	84	PRO	3.5
2	B	452	ASN	3.4
2	B	245	ARG	3.4
2	D	90	LEU	3.4
2	B	44	ASN	3.4
2	D	299	ILE	3.4
2	H	199	ILE	3.4
1	E	252	ASN	3.4
2	H	253	ARG	3.4
2	H	443	ALA	3.3
2	B	35	LEU	3.3
2	H	175	PRO	3.3
1	A	230	ILE	3.3
1	E	14	ALA	3.3
1	E	468	SER	3.3
1	E	312	PHE	3.3
2	F	127	SER	3.3
1	A	254	PRO	3.3
2	H	247	PRO	3.3
2	B	34	GLY	3.3
2	H	180	ILE	3.3
2	H	456	ILE	3.3
2	H	183	PRO	3.2
2	H	250	VAL	3.2
2	F	224	TYR	3.2
2	H	195	LEU	3.2
2	H	63	VAL	3.2
2	H	145	ASP	3.2
2	B	90	LEU	3.2
1	G	247	ALA	3.1
2	F	133	SER	3.1
1	G	252	ASN	3.1
2	F	198	TYR	3.1
1	A	399	HIS	3.1
2	H	244	PRO	3.1
1	G	253	LEU	3.1
1	A	231	THR	3.1
1	C	16	THR	3.1
2	H	190	ILE	3.1
2	H	200	THR	3.1
2	F	201	LYS	3.1
1	E	230	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	254	PRO	3.1
2	H	451	PRO	3.1
2	B	65	ASN	3.1
2	F	44	ASN	3.1
1	G	358	LYS	3.0
2	H	342	THR	3.0
2	B	24	PRO	3.0
2	H	206	ASP	3.0
2	H	226	GLN	3.0
2	H	181	LEU	3.0
1	E	288	SER	3.0
2	H	30	LYS	3.0
2	B	148	ILE	3.0
2	F	63	VAL	3.0
2	D	193	THR	3.0
2	H	254	GLY	3.0
2	D	236	GLU	2.9
1	E	248	PRO	2.9
1	C	307	LEU	2.9
1	G	249	VAL	2.9
1	G	248	PRO	2.9
1	E	303	TYR	2.9
2	H	138	SER	2.9
2	H	235	SER	2.9
2	B	27	ARG	2.9
1	A	145	GLU	2.9
1	A	288	SER	2.9
1	C	251	GLY	2.9
2	B	87	GLY	2.9
2	H	236	GLU	2.9
2	F	184	ILE	2.9
1	A	303	TYR	2.9
1	A	312	PHE	2.9
1	C	310	TYR	2.9
1	G	408	MET	2.9
1	E	377	SER	2.8
1	C	17	ASP	2.8
2	B	61	GLU	2.8
2	F	203	TYR	2.8
1	G	295	GLY	2.8
1	E	15	ARG	2.8
1	E	287	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	467	ASN	2.8
2	B	140	ILE	2.8
2	B	147	ILE	2.8
2	H	454	SER	2.8
1	A	291	ALA	2.8
2	H	428	MET	2.8
2	H	163	PHE	2.8
1	G	292	GLY	2.8
2	D	261	ASN	2.8
2	H	179	THR	2.8
2	H	269	ALA	2.8
2	H	142	ARG	2.8
2	H	299	ILE	2.7
1	G	231	THR	2.7
2	B	449	THR	2.7
2	H	72	LEU	2.7
2	H	64	LYS	2.7
1	E	378	LEU	2.7
2	B	428	MET	2.7
2	F	34	GLY	2.7
1	G	254	PRO	2.7
2	F	452	ASN	2.7
2	H	39	THR	2.7
1	G	407	GLU	2.7
2	H	61	GLU	2.7
2	H	332	ASP	2.7
1	A	34	ASN	2.7
2	B	172	LYS	2.7
2	D	64	LYS	2.6
2	D	71	PHE	2.6
1	E	400	GLY	2.6
2	F	42	ILE	2.6
2	F	261	ASN	2.6
2	H	209	VAL	2.6
2	D	448	SER	2.6
2	H	314	SER	2.6
2	H	211	ALA	2.6
1	A	310	TYR	2.6
1	A	358	LYS	2.6
2	D	246	GLY	2.6
2	H	182	GLY	2.6
2	F	71	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	28	THR	2.6
2	H	185	LYS	2.6
1	G	449	ASP	2.6
1	E	298	MET	2.6
1	G	403	ILE	2.6
1	G	360	LEU	2.6
1	G	378	LEU	2.6
2	B	241	LEU	2.6
2	F	239	VAL	2.6
2	H	261	ASN	2.6
2	F	237	SER	2.6
2	H	134	VAL	2.5
1	A	470	SER	2.5
1	A	15	ARG	2.5
2	F	302	GLY	2.5
2	F	23	ILE	2.5
2	D	81	GLN	2.5
1	G	406	ASN	2.5
2	H	156	LYS	2.5
2	H	450	VAL	2.5
2	H	59	ARG	2.5
2	D	87	GLY	2.5
1	E	408	MET	2.5
2	H	264	PRO	2.5
2	B	260	GLU	2.5
2	H	263	LEU	2.5
1	A	252	ASN	2.5
2	F	62	ASN	2.5
2	H	447	THR	2.5
1	A	248	PRO	2.4
1	C	359	ASP	2.4
2	H	37	ILE	2.4
2	H	171	TYR	2.4
2	H	455	TYR	2.4
2	H	107	ASN	2.4
2	H	348	ASN	2.4
1	G	462	ALA	2.4
1	A	411	LYS	2.4
1	G	461	LYS	2.4
2	H	130	LEU	2.4
2	B	253	ARG	2.4
2	F	146	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	208	MET	2.4
1	C	248	PRO	2.4
2	H	188	LYS	2.4
2	D	154	VAL	2.4
2	H	445	GLY	2.4
2	D	23	ILE	2.4
2	F	245	ARG	2.4
2	F	229	PHE	2.4
2	D	239	VAL	2.4
2	B	137	ASN	2.4
2	F	249	PRO	2.3
1	A	451	GLY	2.3
1	E	251	GLY	2.3
1	E	422	ARG	2.3
1	G	268	ILE	2.3
2	F	88	ILE	2.3
1	C	306	VAL	2.3
2	D	452	ASN	2.3
2	F	56	ALA	2.3
2	B	303	THR	2.3
2	F	81	GLN	2.3
2	F	187	ILE	2.3
2	D	118	ASP	2.3
2	D	252	CYS	2.3
1	E	241	GLU	2.3
2	F	348	ASN	2.3
1	A	468	SER	2.3
1	A	469	SER	2.3
2	B	37	ILE	2.3
2	H	128	ASP	2.3
2	H	349	VAL	2.3
2	F	202	ASN	2.3
1	A	16	THR	2.3
2	F	200	THR	2.3
2	B	246	GLY	2.3
2	D	242	GLY	2.3
2	H	99	LEU	2.3
1	G	298	MET	2.3
1	E	433	ASN	2.2
2	D	348	ASN	2.2
2	F	304	ASN	2.2
2	H	350	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	304	THR	2.2
1	C	148	MET	2.2
2	B	133	SER	2.2
2	H	133	SER	2.2
2	D	257	PHE	2.2
1	C	432	VAL	2.2
2	B	239	VAL	2.2
2	F	154	VAL	2.2
2	H	207	ARG	2.2
2	H	431	ASN	2.2
1	G	303	TYR	2.2
2	H	347	HIS	2.2
1	G	251	GLY	2.2
2	F	214	GLY	2.2
1	A	307	LEU	2.2
2	H	351	LEU	2.2
2	H	460	LEU	2.2
2	B	29	SER	2.2
1	A	129	GLU	2.2
2	H	154	VAL	2.2
2	B	316	ASN	2.2
2	H	313	ALA	2.2
2	H	165	HIS	2.2
2	H	203	TYR	2.2
2	H	220	LYS	2.2
2	H	108	THR	2.2
2	H	131	THR	2.2
2	H	252	CYS	2.2
2	F	181	LEU	2.2
1	G	269	ASP	2.2
2	H	245	ARG	2.2
2	F	251	PHE	2.2
2	B	64	LYS	2.2
1	A	406	ASN	2.2
1	G	56	ASN	2.2
2	F	428	MET	2.2
1	E	362	LEU	2.2
2	H	388	LEU	2.2
2	H	399	GLY	2.2
2	H	434	LEU	2.2
2	F	199	ILE	2.2
2	B	454	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	189	SER	2.2
1	G	255	GLU	2.2
2	D	173	ASP	2.2
2	D	84	PRO	2.2
2	H	204	LYS	2.2
1	C	408	MET	2.1
2	H	298	ALA	2.1
2	H	335	LEU	2.1
1	A	401	ARG	2.1
1	E	210	GLU	2.1
1	G	365	ASP	2.1
2	D	138	SER	2.1
2	H	424	ASP	2.1
2	F	172	LYS	2.1
1	A	432	VAL	2.1
2	D	222	VAL	2.1
2	F	232	VAL	2.1
2	F	208	MET	2.1
2	H	331	ALA	2.1
2	F	100	ASN	2.1
2	D	241	LEU	2.1
2	H	79	GLY	2.1
2	H	390	GLY	2.1
1	E	403	ILE	2.1
2	B	117	GLU	2.1
1	C	138	SER	2.1
2	H	237	SER	2.1
2	H	201	LYS	2.1
2	D	247	PRO	2.1
2	H	238	PRO	2.1
2	H	441	MET	2.1
2	H	186	ASN	2.1
1	A	464	GLY	2.1
2	H	28	THR	2.1
1	E	414	ASP	2.1
2	B	197	ASP	2.1
2	H	440	SER	2.1
2	B	183	PRO	2.1
1	C	399	HIS	2.1
2	H	44	ASN	2.1
1	A	251	GLY	2.1
2	F	246	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	242	GLY	2.1
2	F	449	THR	2.1
2	B	185	LYS	2.1
1	G	359	ASP	2.1
2	F	173	ASP	2.1
2	H	339	TYR	2.1
2	D	243	SER	2.1
2	H	243	SER	2.1
2	D	244	PRO	2.1
2	F	240	PRO	2.1
2	F	244	PRO	2.1
2	D	462	GLN	2.0
2	H	216	VAL	2.0
2	B	60	ALA	2.0
2	B	144	ARG	2.0
2	H	38	ALA	2.0
2	H	354	ASN	2.0
2	H	357	LEU	2.0
1	A	294	PRO	2.0
2	F	233	PRO	2.0
2	H	232	VAL	2.0
1	G	307	LEU	2.0
2	B	346	GLU	2.0
2	F	130	LEU	2.0
2	F	241	LEU	2.0
1	G	287	GLY	2.0
2	B	30	LYS	2.0
2	H	172	LYS	2.0
2	H	304	ASN	2.0
1	G	409	ILE	2.0
1	E	254	PRO	2.0
2	H	157	MET	2.0
2	H	249	PRO	2.0
1	A	141	TYR	2.0
2	F	98	HIS	2.0
2	H	58	SER	2.0

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

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	ZN	H	504	1/1	0.96	0.06	100,100,100,100	0
3	ZN	D	502	1/1	0.98	0.04	64,64,64,64	0
3	ZN	F	503	1/1	0.98	0.04	73,73,73,73	0
3	ZN	B	501	1/1	0.98	0.04	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.