



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:59 AM UTC

PDB ID : 1TEE / pdb_00001tee
Title : Crystal structure of C205F mutant of PKS18 from Mycobacterium tuberculosis
Authors : Sankaranarayanan, R.; Shanmugam, V.M.; Rukmini, R.
Deposited on : 2004-05-25
Resolution : 2.90 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

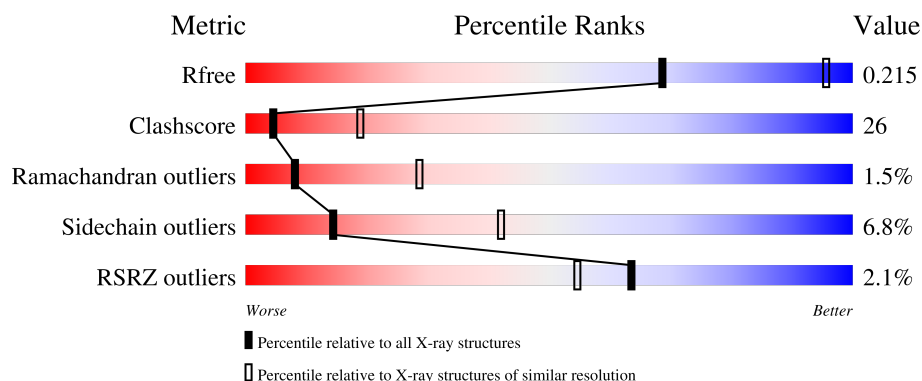
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	393	 2% 57% 31% 5% • 6%
1	B	393	 2% 49% 37% 5% 9%
1	C	393	 2% 55% 32% 5% • 6%
1	D	393	 2% 50% 37% 5% 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10876 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 pks18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2750	1749	474	514	13			
1	B	359	Total	C	N	O	S	0	0	0
			2688	1708	464	503	13			
1	C	368	Total	C	N	O	S	0	0	0
			2750	1749	474	514	13			
1	D	359	Total	C	N	O	S	0	0	0
			2688	1708	464	503	13			

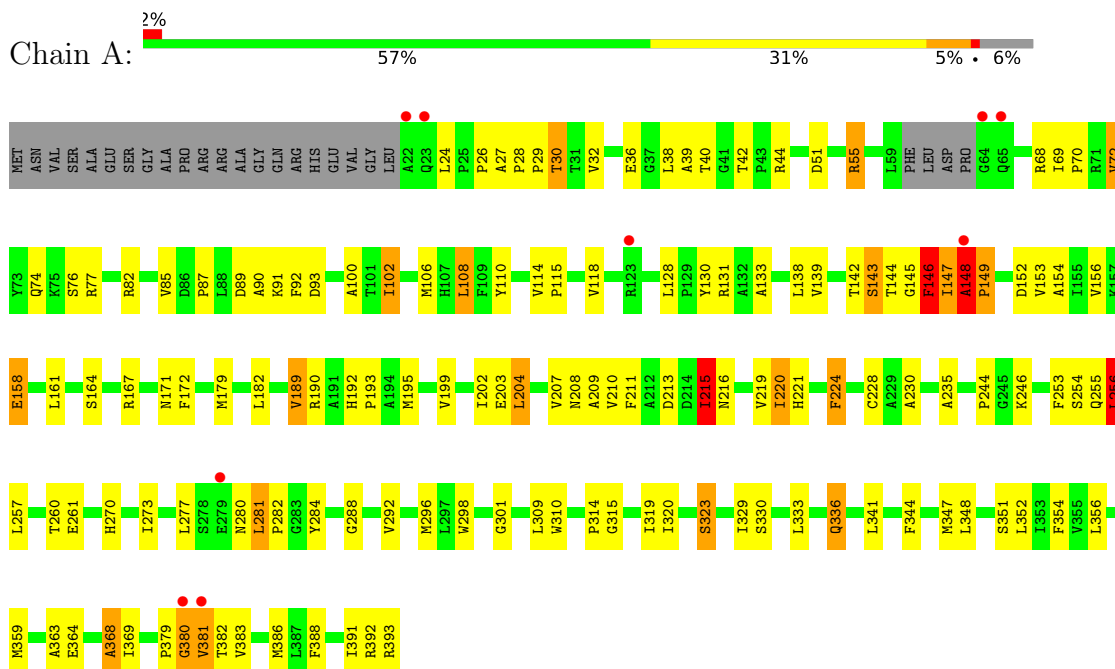
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	PHE	CYS	engineered mutation	UNP Q7D8I1
B	205	PHE	CYS	engineered mutation	UNP Q7D8I1
C	205	PHE	CYS	engineered mutation	UNP Q7D8I1
D	205	PHE	CYS	engineered mutation	UNP Q7D8I1

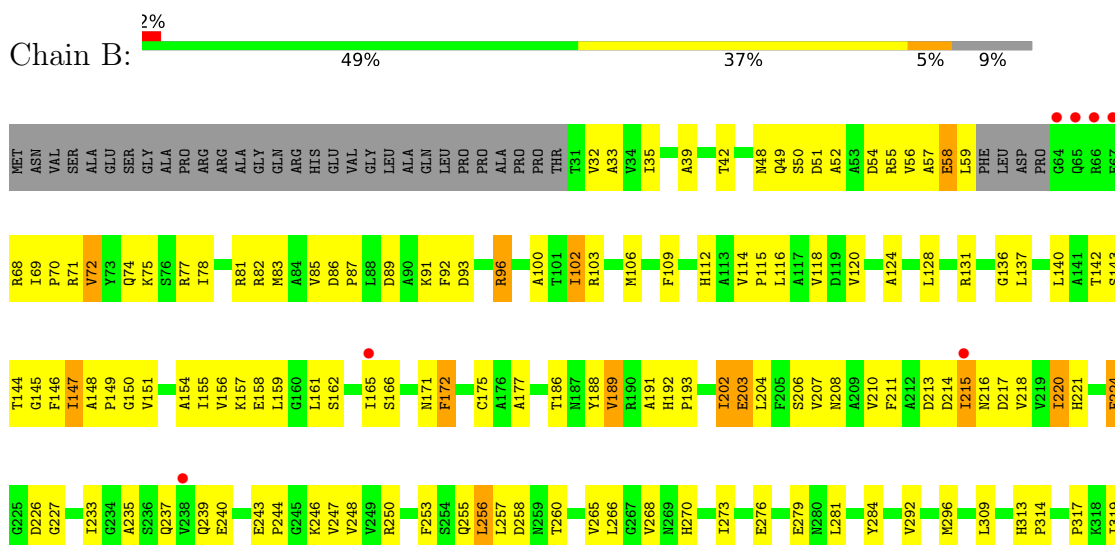
3 Residue-property plots

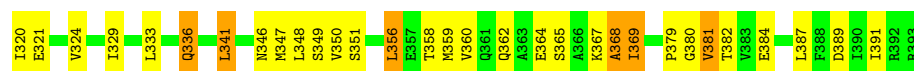
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: pks18

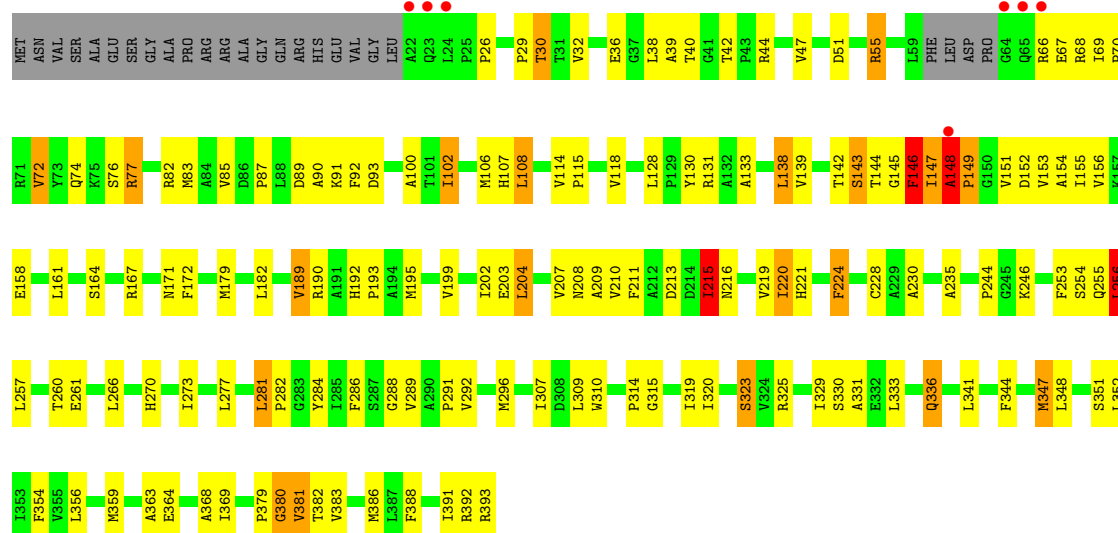


• Molecule 1: pks18

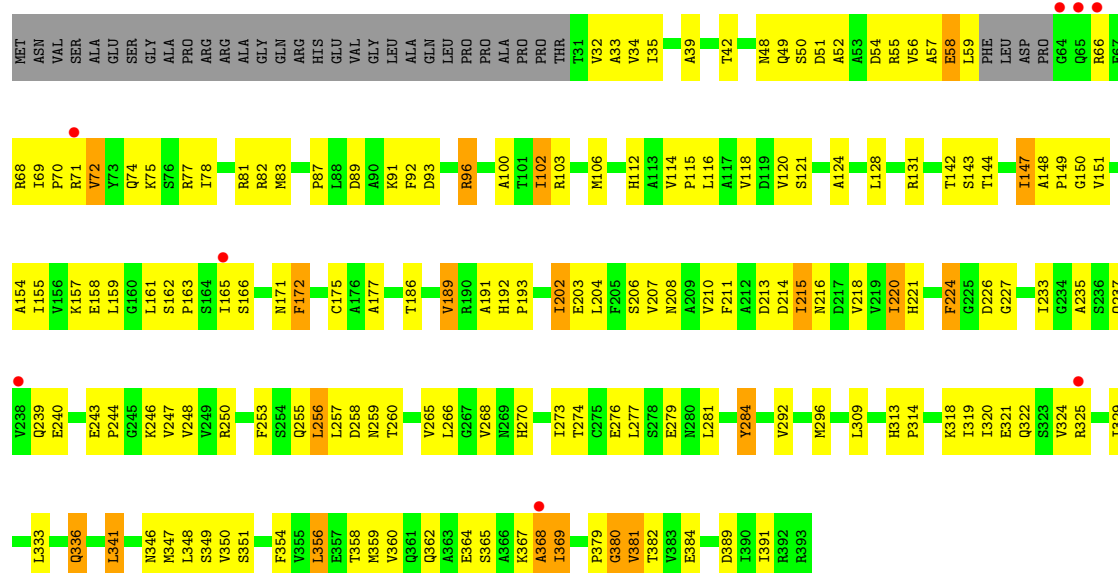




• Molecule 1: pks18



• Molecule 1: pks18



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.95Å 80.43Å 99.97Å 108.15° 93.14° 103.88°	Depositor
Resolution (Å)	24.95 – 2.90 24.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.6 (24.95-2.90) 96.5 (24.95-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.258 0.219 , 0.215	Depositor DCC
R_{free} test set	1798 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10876	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 [i](#)

5.1 Standard geometry [i](#)

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	0.51	0/2799	1.03	16/3812 (0.4%)
1	B	0.50	0/2733	0.98	7/3717 (0.2%)
1	C	0.50	0/2799	1.05	19/3812 (0.5%)
1	D	0.50	0/2733	1.00	11/3717 (0.3%)
All	All	0.51	0/11064	1.02	53/15058 (0.4%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	148	ALA	CA-C-N	-10.15	109.61	119.76
1	C	148	ALA	C-N-CA	-10.15	109.61	119.76
1	A	148	ALA	CA-C-N	-9.78	109.63	119.90
1	A	148	ALA	C-N-CA	-9.78	109.63	119.90
1	A	380	GLY	N-CA-C	-9.06	104.30	115.08
1	C	380	GLY	N-CA-C	-8.98	104.39	115.08
1	D	213	ASP	N-CA-C	8.63	120.31	111.07
1	B	213	ASP	N-CA-C	8.30	120.11	111.14
1	D	380	GLY	N-CA-C	-7.64	105.72	115.42
1	A	368	ALA	N-CA-C	-6.40	100.80	110.28
1	C	368	ALA	N-CA-C	-6.33	100.91	110.28
1	B	368	ALA	N-CA-C	-6.27	99.65	109.25
1	A	213	ASP	N-CA-C	6.22	120.06	112.23
1	C	213	ASP	N-CA-C	6.21	120.05	112.23
1	D	368	ALA	N-CA-C	-6.19	99.78	109.25
1	C	192	HIS	CA-C-N	6.16	127.54	119.84
1	C	192	HIS	C-N-CA	6.16	127.54	119.84
1	A	192	HIS	CA-C-N	6.15	127.52	119.84
1	A	192	HIS	C-N-CA	6.15	127.52	119.84
1	D	172	PHE	N-CA-C	6.14	120.00	111.90
1	D	192	HIS	CA-C-N	6.02	126.19	119.32
1	D	192	HIS	C-N-CA	6.02	126.19	119.32
1	B	224	PHE	N-CA-C	6.00	119.69	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	PRO	N-CA-C	-5.99	102.05	111.34
1	D	224	PHE	N-CA-C	5.93	119.56	110.20
1	B	172	PHE	N-CA-C	5.90	119.69	111.90
1	B	192	HIS	CA-C-N	5.85	125.99	119.32
1	B	192	HIS	C-N-CA	5.85	125.99	119.32
1	C	29	PRO	N-CA-C	-5.81	102.34	111.34
1	A	224	PHE	N-CA-C	5.77	119.31	110.20
1	C	224	PHE	N-CA-C	5.72	119.24	110.20
1	C	44	ARG	N-CA-C	5.71	117.58	111.36
1	C	256	LEU	N-CA-C	-5.71	99.83	108.67
1	C	149	PRO	N-CA-C	-5.69	102.26	111.19
1	C	215	ILE	CB-CA-C	-5.68	104.60	112.04
1	A	44	ARG	N-CA-C	5.54	117.40	111.36
1	A	215	ILE	CB-CA-C	-5.49	104.85	112.04
1	C	76	SER	N-CA-C	5.46	117.99	111.71
1	A	149	PRO	N-CA-C	-5.44	102.58	110.80
1	C	143	SER	N-CA-C	-5.43	104.61	113.19
1	A	76	SER	N-CA-C	5.42	117.94	111.71
1	C	107	HIS	N-CA-C	-5.40	105.30	111.14
1	A	256	LEU	N-CA-C	-5.40	100.30	108.67
1	C	320	ILE	N-CA-C	-5.32	105.53	110.53
1	A	143	SER	N-CA-C	-5.25	104.89	113.19
1	A	320	ILE	N-CA-C	-5.21	105.63	110.53
1	C	66	ARG	N-CA-C	-5.17	106.83	112.72
1	D	66	ARG	N-CA-C	-5.12	107.05	113.15
1	D	34	VAL	N-CA-C	5.09	115.80	108.48
1	D	284	TYR	N-CA-C	-5.07	105.64	111.07
1	D	354	PHE	N-CA-C	-5.04	105.68	111.07
1	C	307	ILE	N-CA-C	5.04	115.94	108.23
1	B	387	LEU	N-CA-C	-5.03	101.50	109.76

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	2750	0	2780	156	0
1	B	2688	0	2716	154	0
1	C	2750	0	2780	165	0
1	D	2688	0	2716	158	0
All	All	10876	0	10992	570	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 26.

All (570) 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:D:203:GLU:HG2	1:D:348:LEU:HB2	1.40	1.03
1:B:203:GLU:HG2	1:B:348:LEU:HB2	1.38	1.02
1:B:336:GLN:H	1:B:336:GLN:NE2	1.61	0.99
1:D:227:GLY:HA3	1:D:347:MET:HE2	1.44	0.98
1:B:227:GLY:HA3	1:B:347:MET:HE2	1.46	0.97
1:D:336:GLN:H	1:D:336:GLN:NE2	1.63	0.95
1:D:336:GLN:H	1:D:336:GLN:HE21	1.06	0.95
1:D:100:ALA:H	1:D:270:HIS:HD2	1.04	0.95
1:B:336:GLN:H	1:B:336:GLN:HE21	1.02	0.94
1:D:210:VAL:H	1:D:221:HIS:HE1	1.14	0.93
1:B:210:VAL:H	1:B:221:HIS:HE1	1.16	0.93
1:B:100:ALA:H	1:B:270:HIS:HD2	1.04	0.92
1:B:100:ALA:H	1:B:270:HIS:CD2	1.87	0.92
1:D:100:ALA:H	1:D:270:HIS:CD2	1.88	0.92
1:D:215:ILE:HD12	1:D:215:ILE:H	1.34	0.91
1:A:203:GLU:HG2	1:A:348:LEU:HB2	1.53	0.90
1:D:208:ASN:HD22	1:D:273:ILE:H	1.17	0.90
1:C:203:GLU:HG2	1:C:348:LEU:HB2	1.54	0.90
1:B:215:ILE:HD12	1:B:215:ILE:H	1.33	0.89
1:C:208:ASN:HD22	1:C:273:ILE:H	1.20	0.89
1:A:142:THR:HG22	1:A:144:THR:H	1.37	0.88
1:A:148:ALA:HB2	1:B:266:LEU:N	1.90	0.87
1:A:148:ALA:HB2	1:B:266:LEU:H	1.39	0.87
1:C:142:THR:HG22	1:C:144:THR:H	1.38	0.86
1:A:148:ALA:CB	1:B:266:LEU:H	1.88	0.86
1:B:208:ASN:HD22	1:B:273:ILE:H	1.24	0.86
1:A:208:ASN:HD22	1:A:273:ILE:H	1.20	0.85
1:A:261:GLU:HG3	1:B:157:LYS:HZ1	1.43	0.84
1:D:208:ASN:ND2	1:D:273:ILE:H	1.75	0.84
1:B:336:GLN:HE21	1:B:336:GLN:N	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:GLU:HG3	1:D:157:LYS:HZ1	1.41	0.83
1:D:142:THR:HG22	1:D:144:THR:H	1.43	0.83
1:C:148:ALA:HB1	1:C:149:PRO:HD3	1.62	0.82
1:C:91:LYS:HG3	1:C:92:PHE:H	1.45	0.82
1:B:142:THR:HG22	1:B:144:THR:H	1.42	0.81
1:B:208:ASN:ND2	1:B:273:ILE:H	1.78	0.81
1:C:148:ALA:HB2	1:D:266:LEU:N	1.96	0.81
1:C:148:ALA:HB2	1:D:266:LEU:H	1.46	0.81
1:A:179:MET:HE3	1:A:352:LEU:HD23	1.63	0.81
1:C:189:VAL:HG13	1:C:235:ALA:HB2	1.63	0.81
1:A:189:VAL:HG13	1:A:235:ALA:HB2	1.63	0.80
1:A:208:ASN:ND2	1:A:273:ILE:H	1.80	0.80
1:B:379:PRO:C	1:B:381:VAL:H	1.86	0.80
1:A:336:GLN:H	1:A:336:GLN:NE2	1.80	0.80
1:D:379:PRO:C	1:D:381:VAL:H	1.87	0.80
1:D:336:GLN:HE21	1:D:336:GLN:N	1.78	0.79
1:C:208:ASN:ND2	1:C:273:ILE:H	1.81	0.79
1:C:148:ALA:CB	1:D:266:LEU:H	1.94	0.79
1:A:91:LYS:HG3	1:A:92:PHE:H	1.47	0.79
1:C:216:ASN:HD21	1:C:277:LEU:H	1.30	0.79
1:D:329:ILE:HB	1:D:333:LEU:HD12	1.66	0.78
1:A:148:ALA:HB1	1:A:149:PRO:HD3	1.63	0.78
1:C:210:VAL:H	1:C:221:HIS:CE1	2.00	0.78
1:C:179:MET:HE3	1:C:352:LEU:HD23	1.66	0.77
1:B:71:ARG:O	1:B:74:GLN:HG2	1.85	0.77
1:D:161:LEU:HB3	1:D:165:ILE:HD12	1.66	0.77
1:A:51:ASP:O	1:A:55:ARG:HD2	1.83	0.77
1:B:161:LEU:HB3	1:B:165:ILE:HD12	1.66	0.77
1:A:27:ALA:HB3	1:C:325:ARG:HD3	1.68	0.76
1:B:257:LEU:HD12	1:B:381:VAL:HG12	1.67	0.76
1:C:336:GLN:H	1:C:336:GLN:NE2	1.81	0.76
1:A:210:VAL:H	1:A:221:HIS:CE1	2.03	0.76
1:A:69:ILE:HB	1:A:70:PRO:HD3	1.66	0.75
1:B:329:ILE:HB	1:B:333:LEU:HD12	1.69	0.75
1:D:71:ARG:O	1:D:74:GLN:HG2	1.87	0.74
1:C:220:ILE:HG13	1:C:224:PHE:CE2	2.23	0.74
1:A:216:ASN:HD21	1:A:277:LEU:H	1.33	0.74
1:D:257:LEU:HD12	1:D:381:VAL:HG12	1.68	0.74
1:C:51:ASP:O	1:C:55:ARG:HD2	1.87	0.74
1:C:220:ILE:HG13	1:C:224:PHE:HE2	1.52	0.73
1:A:298:TRP:CZ3	1:C:215:ILE:HG23	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:PRO:O	1:C:74:GLN:HG2	1.89	0.73
1:C:257:LEU:HD12	1:C:381:VAL:HG12	1.70	0.73
1:C:329:ILE:HG22	1:C:330:SER:N	2.04	0.73
1:A:220:ILE:HG13	1:A:224:PHE:HE2	1.53	0.73
1:A:329:ILE:HG22	1:A:330:SER:N	2.04	0.73
1:A:329:ILE:HG21	1:A:333:LEU:HD12	1.71	0.72
1:B:100:ALA:N	1:B:270:HIS:HD2	1.86	0.72
1:D:114:VAL:HB	1:D:115:PRO:HD3	1.71	0.72
1:C:38:LEU:HD23	1:C:39:ALA:N	2.05	0.72
1:C:329:ILE:HG21	1:C:333:LEU:HD12	1.72	0.71
1:B:114:VAL:HB	1:B:115:PRO:HD3	1.71	0.71
1:A:220:ILE:HG13	1:A:224:PHE:CE2	2.24	0.71
1:B:87:PRO:HA	1:B:92:PHE:CD2	2.25	0.71
1:C:69:ILE:HB	1:C:70:PRO:HD3	1.70	0.71
1:A:70:PRO:O	1:A:74:GLN:HG2	1.90	0.71
1:C:270:HIS:N	1:D:102:ILE:HD11	2.05	0.71
1:A:149:PRO:HG3	1:B:380:GLY:H	1.55	0.71
1:A:257:LEU:HD12	1:A:381:VAL:HG12	1.73	0.71
1:B:96:ARG:HH21	1:B:211:PHE:HB2	1.57	0.70
1:C:329:ILE:HG22	1:C:330:SER:H	1.56	0.70
1:D:91:LYS:HG3	1:D:92:PHE:H	1.56	0.70
1:C:100:ALA:H	1:C:270:HIS:HD2	1.39	0.70
1:A:171:ASN:HD22	1:B:171:ASN:HB2	1.55	0.70
1:A:38:LEU:HD23	1:A:39:ALA:N	2.06	0.70
1:D:87:PRO:HA	1:D:92:PHE:CD2	2.27	0.70
1:C:171:ASN:HD22	1:D:171:ASN:HB2	1.56	0.69
1:D:96:ARG:HH21	1:D:211:PHE:HB2	1.57	0.69
1:A:329:ILE:HG22	1:A:330:SER:H	1.56	0.69
1:B:91:LYS:HG3	1:B:92:PHE:H	1.57	0.69
1:C:148:ALA:CB	1:C:149:PRO:CD	2.71	0.69
1:D:211:PHE:H	1:D:221:HIS:CE1	2.11	0.69
1:B:96:ARG:NH2	1:B:211:PHE:HB2	2.08	0.69
1:A:329:ILE:CG2	1:A:333:LEU:HD12	2.23	0.69
1:B:320:ILE:O	1:B:324:VAL:HG23	1.92	0.69
1:B:93:ASP:HA	1:B:96:ARG:HD2	1.75	0.68
1:A:270:HIS:N	1:B:102:ILE:HD11	2.08	0.68
1:C:336:GLN:H	1:C:336:GLN:HE21	1.41	0.68
1:C:149:PRO:HG3	1:D:380:GLY:H	1.59	0.68
1:D:96:ARG:NH2	1:D:211:PHE:HB2	2.08	0.68
1:D:161:LEU:HB3	1:D:165:ILE:CD1	2.23	0.68
1:C:148:ALA:HB1	1:D:265:VAL:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:VAL:H	1:C:221:HIS:HE1	1.40	0.67
1:D:320:ILE:O	1:D:324:VAL:HG23	1.94	0.67
1:C:329:ILE:CG2	1:C:333:LEU:HD12	2.24	0.67
1:D:210:VAL:H	1:D:221:HIS:CE1	2.06	0.67
1:A:100:ALA:H	1:A:270:HIS:HD2	1.40	0.67
1:D:189:VAL:HG13	1:D:235:ALA:HB2	1.76	0.67
1:C:257:LEU:HD12	1:C:381:VAL:CG1	2.24	0.67
1:A:148:ALA:HB1	1:B:265:VAL:HA	1.76	0.66
1:A:336:GLN:H	1:A:336:GLN:HE21	1.40	0.66
1:B:161:LEU:HB3	1:B:165:ILE:CD1	2.25	0.66
1:B:189:VAL:HG13	1:B:235:ALA:HB2	1.76	0.66
1:A:148:ALA:CB	1:A:149:PRO:CD	2.73	0.66
1:A:210:VAL:H	1:A:221:HIS:HE1	1.43	0.66
1:D:255:GLN:HG3	1:D:292:VAL:HG22	1.78	0.65
1:D:93:ASP:HA	1:D:96:ARG:HD2	1.77	0.65
1:D:215:ILE:H	1:D:215:ILE:CD1	2.10	0.65
1:B:211:PHE:H	1:B:221:HIS:CE1	2.14	0.65
1:C:148:ALA:CB	1:C:149:PRO:HD3	2.26	0.64
1:A:288:GLY:O	1:A:292:VAL:HG23	1.97	0.64
1:A:148:ALA:CB	1:A:149:PRO:HD3	2.27	0.64
1:B:215:ILE:H	1:B:215:ILE:CD1	2.08	0.64
1:D:250:ARG:HD2	1:D:389:ASP:OD2	1.98	0.64
1:D:91:LYS:CG	1:D:92:PHE:H	2.10	0.64
1:B:250:ARG:HD2	1:B:389:ASP:OD2	1.98	0.64
1:D:309:LEU:HB3	1:D:359:MET:CE	2.28	0.64
1:B:91:LYS:CG	1:B:92:PHE:H	2.11	0.63
1:A:209:ALA:HA	1:A:221:HIS:HE1	1.63	0.63
1:D:56:VAL:HG12	1:D:69:ILE:HD13	1.80	0.63
1:C:108:LEU:HB3	1:C:207:VAL:CG2	2.27	0.63
1:B:56:VAL:HG12	1:B:69:ILE:HD13	1.81	0.63
1:C:209:ALA:HA	1:C:221:HIS:HE1	1.64	0.63
1:D:154:ALA:O	1:D:158:GLU:HB2	1.97	0.63
1:B:239:GLN:HE22	1:C:331:ALA:H	1.47	0.62
1:B:154:ALA:O	1:B:158:GLU:HB2	1.98	0.62
1:D:258:ASP:O	1:D:260:THR:HG23	1.99	0.62
1:D:89:ASP:OD1	1:D:91:LYS:HG2	1.99	0.62
1:B:33:ALA:HB1	1:B:186:THR:HG22	1.81	0.62
1:C:102:ILE:O	1:C:106:MET:HG2	1.99	0.62
1:D:100:ALA:N	1:D:270:HIS:HD2	1.86	0.62
1:D:257:LEU:HD12	1:D:381:VAL:CG1	2.29	0.62
1:A:102:ILE:O	1:A:106:MET:HG2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:HD12	1:A:381:VAL:CG1	2.28	0.62
1:C:114:VAL:O	1:C:118:VAL:HG23	2.00	0.62
1:B:309:LEU:HB3	1:B:359:MET:CE	2.30	0.62
1:D:106:MET:HE2	1:D:106:MET:HA	1.82	0.62
1:D:92:PHE:O	1:D:96:ARG:HG3	2.00	0.61
1:C:261:GLU:HG3	1:D:157:LYS:NZ	2.15	0.61
1:B:210:VAL:H	1:B:221:HIS:CE1	2.07	0.61
1:D:91:LYS:HG3	1:D:92:PHE:N	2.15	0.61
1:B:257:LEU:HD12	1:B:381:VAL:CG1	2.30	0.61
1:A:42:THR:OG1	1:A:82:ARG:HG3	2.01	0.60
1:B:255:GLN:HG3	1:B:292:VAL:HG22	1.82	0.60
1:C:100:ALA:H	1:C:270:HIS:CD2	2.19	0.60
1:C:288:GLY:O	1:C:292:VAL:HG23	2.01	0.60
1:B:89:ASP:OD1	1:B:91:LYS:HG2	2.00	0.60
1:C:319:ILE:O	1:C:323:SER:HB2	2.02	0.60
1:D:365:SER:OG	1:D:367:LYS:HG2	2.01	0.60
1:A:106:MET:SD	1:A:145:GLY:O	2.58	0.60
1:A:108:LEU:HB3	1:A:207:VAL:CG2	2.31	0.60
1:A:301:GLY:HA2	1:C:215:ILE:HD11	1.83	0.60
1:B:91:LYS:HG3	1:B:92:PHE:N	2.15	0.60
1:A:344:PHE:HB3	1:A:347:MET:CE	2.31	0.60
1:B:48:ASN:OD1	1:B:50:SER:HB2	2.02	0.60
1:B:106:MET:HA	1:B:106:MET:HE2	1.84	0.60
1:C:114:VAL:HB	1:C:115:PRO:HD3	1.82	0.60
1:D:253:PHE:CE2	1:D:296:MET:HE2	2.37	0.60
1:B:102:ILE:HD12	1:B:103:ARG:H	1.67	0.59
1:B:258:ASP:O	1:B:260:THR:HG23	2.02	0.59
1:D:33:ALA:HB1	1:D:186:THR:HG22	1.84	0.59
1:B:365:SER:OG	1:B:367:LYS:HG2	2.03	0.59
1:C:42:THR:OG1	1:C:82:ARG:HG3	2.02	0.59
1:A:261:GLU:HG3	1:B:157:LYS:NZ	2.16	0.59
1:B:379:PRO:C	1:B:381:VAL:N	2.59	0.59
1:A:114:VAL:O	1:A:118:VAL:HG23	2.01	0.59
1:B:253:PHE:CE2	1:B:296:MET:HE2	2.37	0.59
1:C:106:MET:SD	1:C:145:GLY:O	2.61	0.59
1:A:149:PRO:HG3	1:B:380:GLY:N	2.18	0.59
1:D:348:LEU:N	1:D:348:LEU:HD12	2.18	0.59
1:A:146:PHE:CD1	1:A:146:PHE:N	2.71	0.59
1:C:379:PRO:C	1:C:381:VAL:H	2.10	0.59
1:B:92:PHE:O	1:B:96:ARG:HG3	2.02	0.58
1:A:179:MET:HE2	1:A:179:MET:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:THR:OG1	1:C:381:VAL:HB	2.04	0.58
1:D:89:ASP:CG	1:D:91:LYS:HG2	2.29	0.58
1:A:253:PHE:CE1	1:A:296:MET:HE2	2.38	0.58
1:A:319:ILE:O	1:A:323:SER:HB2	2.02	0.58
1:A:379:PRO:C	1:A:381:VAL:H	2.10	0.58
1:B:313:HIS:HE1	1:B:348:LEU:O	1.85	0.58
1:C:179:MET:HA	1:C:179:MET:HE2	1.85	0.58
1:C:344:PHE:HB3	1:C:347:MET:CE	2.33	0.58
1:D:313:HIS:HE1	1:D:348:LEU:O	1.87	0.58
1:D:68:ARG:O	1:D:72:VAL:HG12	2.04	0.58
1:A:24:LEU:HD22	1:C:77:ARG:NH2	2.19	0.57
1:A:114:VAL:HB	1:A:115:PRO:HD3	1.85	0.57
1:C:51:ASP:HB3	1:C:55:ARG:NH1	2.18	0.57
1:C:171:ASN:HB2	1:D:171:ASN:HB2	1.85	0.57
1:A:100:ALA:H	1:A:270:HIS:CD2	2.20	0.57
1:A:260:THR:OG1	1:A:381:VAL:HB	2.04	0.57
1:C:146:PHE:CD1	1:C:146:PHE:N	2.72	0.57
1:D:314:PRO:HB2	1:D:341:LEU:HB2	1.86	0.57
1:A:30:THR:HB	1:C:325:ARG:HH21	1.69	0.57
1:C:91:LYS:HG3	1:C:92:PHE:N	2.18	0.57
1:C:348:LEU:N	1:C:348:LEU:HD12	2.19	0.57
1:A:298:TRP:CH2	1:C:215:ILE:HG23	2.40	0.57
1:C:253:PHE:CE1	1:C:296:MET:HE2	2.38	0.57
1:A:215:ILE:O	1:A:219:VAL:HG23	2.05	0.57
1:D:102:ILE:HD12	1:D:103:ARG:H	1.70	0.57
1:A:102:ILE:O	1:A:102:ILE:HD13	2.04	0.57
1:A:128:LEU:H	1:A:128:LEU:HD22	1.70	0.56
1:A:281:LEU:N	1:A:282:PRO:HD2	2.20	0.56
1:A:102:ILE:HB	1:A:270:HIS:O	2.05	0.56
1:B:244:PRO:HA	1:B:391:ILE:HG22	1.87	0.56
1:B:89:ASP:CG	1:B:91:LYS:HG2	2.30	0.56
1:D:48:ASN:OD1	1:D:50:SER:HB2	2.06	0.56
1:A:301:GLY:CA	1:C:215:ILE:HD11	2.36	0.56
1:B:314:PRO:HB2	1:B:341:LEU:HB2	1.87	0.56
1:B:253:PHE:CD2	1:B:296:MET:HG3	2.40	0.56
1:D:253:PHE:CD2	1:D:296:MET:HG3	2.41	0.56
1:A:202:ILE:CD1	1:A:228:CYS:HB2	2.36	0.56
1:A:348:LEU:N	1:A:348:LEU:HD12	2.21	0.56
1:B:49:GLN:HG3	1:B:78:ILE:O	2.06	0.55
1:A:147:ILE:O	1:A:148:ALA:O	2.24	0.55
1:C:281:LEU:N	1:C:282:PRO:HD2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LEU:H	1:C:128:LEU:HD22	1.71	0.55
1:A:171:ASN:HB2	1:B:171:ASN:HB2	1.89	0.55
1:A:386:MET:HE3	1:A:388:PHE:CD2	2.41	0.55
1:B:215:ILE:HD12	1:B:215:ILE:N	2.14	0.55
1:C:102:ILE:O	1:C:102:ILE:HD13	2.06	0.55
1:A:89:ASP:OD1	1:A:91:LYS:HG2	2.07	0.55
1:D:260:THR:OG1	1:D:381:VAL:HB	2.07	0.55
1:A:208:ASN:HD22	1:A:273:ILE:N	1.99	0.55
1:C:149:PRO:HG3	1:D:380:GLY:N	2.20	0.55
1:C:261:GLU:CG	1:D:157:LYS:HZ1	2.16	0.55
1:B:348:LEU:HD12	1:B:348:LEU:N	2.21	0.54
1:C:202:ILE:CD1	1:C:228:CYS:HB2	2.37	0.54
1:C:154:ALA:O	1:C:158:GLU:HB2	2.07	0.54
1:C:244:PRO:HG3	1:C:393:ARG:HA	1.90	0.54
1:D:142:THR:HG22	1:D:143:SER:N	2.22	0.54
1:C:386:MET:HE3	1:C:388:PHE:CD2	2.42	0.54
1:C:215:ILE:O	1:C:219:VAL:HG23	2.07	0.54
1:B:319:ILE:HD12	1:B:319:ILE:H	1.72	0.53
1:B:203:GLU:HG2	1:B:348:LEU:CB	2.26	0.53
1:C:147:ILE:O	1:C:148:ALA:O	2.26	0.53
1:A:220:ILE:HG22	1:A:221:HIS:N	2.23	0.53
1:D:215:ILE:HD12	1:D:215:ILE:N	2.16	0.53
1:A:154:ALA:O	1:A:158:GLU:HB2	2.08	0.53
1:B:91:LYS:CG	1:B:92:PHE:N	2.72	0.53
1:C:315:GLY:C	1:C:319:ILE:HD12	2.33	0.53
1:A:255:GLN:O	1:A:382:THR:HA	2.09	0.53
1:A:315:GLY:C	1:A:319:ILE:HD12	2.34	0.53
1:D:91:LYS:CG	1:D:92:PHE:N	2.71	0.53
1:B:131:ARG:HH11	1:B:131:ARG:HG3	1.73	0.53
1:C:36:GLU:HA	1:C:246:LYS:HE2	1.91	0.53
1:C:199:VAL:O	1:C:230:ALA:HA	2.09	0.53
1:D:49:GLN:HG3	1:D:78:ILE:O	2.08	0.53
1:A:244:PRO:HG3	1:A:393:ARG:HA	1.90	0.53
1:A:336:GLN:HE21	1:A:336:GLN:N	2.06	0.53
1:B:68:ARG:O	1:B:72:VAL:HG12	2.09	0.53
1:C:255:GLN:O	1:C:382:THR:HA	2.09	0.53
1:D:379:PRO:C	1:D:381:VAL:N	2.61	0.53
1:B:260:THR:OG1	1:B:381:VAL:HB	2.09	0.52
1:C:89:ASP:O	1:C:93:ASP:HB2	2.10	0.52
1:D:244:PRO:HA	1:D:391:ILE:HG22	1.91	0.52
1:C:203:GLU:CG	1:C:348:LEU:HD22	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ILE:HG22	1:C:221:HIS:N	2.24	0.52
1:B:102:ILE:CD1	1:B:103:ARG:H	2.22	0.52
1:A:91:LYS:HG3	1:A:92:PHE:N	2.20	0.52
1:B:142:THR:HG22	1:B:143:SER:N	2.23	0.52
1:D:131:ARG:HG3	1:D:131:ARG:HH11	1.74	0.52
1:A:36:GLU:HA	1:A:246:LYS:HE2	1.91	0.52
1:C:171:ASN:HD22	1:D:171:ASN:CB	2.23	0.52
1:A:89:ASP:O	1:A:93:ASP:HB2	2.09	0.51
1:C:189:VAL:CG1	1:C:235:ALA:HB2	2.38	0.51
1:C:363:ALA:HA	1:C:392:ARG:NH2	2.24	0.51
1:A:30:THR:HB	1:C:325:ARG:NH2	2.24	0.51
1:A:146:PHE:HZ	1:A:172:PHE:CD1	2.28	0.51
1:A:171:ASN:HD22	1:B:171:ASN:CB	2.23	0.51
1:D:114:VAL:O	1:D:118:VAL:HG23	2.09	0.51
1:A:215:ILE:HD12	1:A:215:ILE:N	2.25	0.51
1:A:260:THR:HG22	1:A:284:TYR:CD1	2.45	0.51
1:C:202:ILE:HD12	1:C:228:CYS:HB2	1.92	0.51
1:D:147:ILE:O	1:D:147:ILE:HD12	2.11	0.51
1:A:203:GLU:CG	1:A:348:LEU:HD22	2.40	0.51
1:D:102:ILE:HD12	1:D:102:ILE:N	2.26	0.51
1:C:102:ILE:HB	1:C:270:HIS:O	2.10	0.51
1:B:54:ASP:O	1:B:58:GLU:HG3	2.11	0.51
1:C:138:LEU:HD12	1:C:139:VAL:N	2.25	0.51
1:C:260:THR:HG22	1:C:284:TYR:CD1	2.46	0.51
1:D:319:ILE:H	1:D:319:ILE:HD12	1.76	0.51
1:A:51:ASP:HB3	1:A:55:ARG:NH1	2.25	0.51
1:C:89:ASP:OD1	1:C:90:ALA:N	2.44	0.50
1:A:189:VAL:CG1	1:A:235:ALA:HB2	2.38	0.50
1:C:89:ASP:OD1	1:C:91:LYS:HG2	2.11	0.50
1:C:106:MET:HE2	1:C:106:MET:HA	1.93	0.50
1:D:102:ILE:CD1	1:D:103:ARG:H	2.24	0.50
1:A:138:LEU:HD12	1:A:139:VAL:N	2.26	0.50
1:D:208:ASN:HD22	1:D:273:ILE:N	1.97	0.50
1:A:199:VAL:O	1:A:230:ALA:HA	2.12	0.50
1:B:102:ILE:HD12	1:B:102:ILE:N	2.26	0.50
1:C:329:ILE:CG2	1:C:330:SER:N	2.73	0.50
1:A:254:SER:HA	1:A:383:VAL:O	2.12	0.50
1:C:209:ALA:HA	1:C:221:HIS:CE1	2.46	0.50
1:C:254:SER:HA	1:C:383:VAL:O	2.12	0.50
1:D:54:ASP:O	1:D:58:GLU:HG3	2.11	0.50
1:A:40:THR:HB	1:A:354:PHE:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:PRO:HG3	1:B:237:GLN:CG	2.42	0.49
1:A:128:LEU:HD22	1:A:128:LEU:N	2.27	0.49
1:A:209:ALA:HA	1:A:221:HIS:CE1	2.45	0.49
1:A:363:ALA:HA	1:A:392:ARG:NH2	2.27	0.49
1:C:131:ARG:HG3	1:C:131:ARG:HH11	1.76	0.49
1:C:146:PHE:HZ	1:C:172:PHE:CD1	2.30	0.49
1:C:215:ILE:HD12	1:C:215:ILE:N	2.27	0.49
1:D:356:LEU:O	1:D:360:VAL:HG23	2.12	0.49
1:C:336:GLN:HE21	1:C:336:GLN:N	2.07	0.49
1:C:128:LEU:HD22	1:C:128:LEU:N	2.27	0.49
1:D:49:GLN:HE22	1:D:81:ARG:HH21	1.61	0.49
1:D:118:VAL:HG13	1:D:159:LEU:CD1	2.43	0.49
1:A:142:THR:HG22	1:A:143:SER:N	2.28	0.49
1:B:35:ILE:HB	1:B:247:VAL:HB	1.95	0.49
1:B:356:LEU:O	1:B:360:VAL:HG23	2.12	0.49
1:A:89:ASP:OD1	1:A:90:ALA:N	2.46	0.48
1:A:344:PHE:HB3	1:A:347:MET:HE3	1.94	0.48
1:C:164:SER:HB3	1:D:255:GLN:HE21	1.77	0.48
1:D:162:SER:O	1:D:165:ILE:HG13	2.13	0.48
1:B:83:MET:HG2	1:B:206:SER:HB3	1.95	0.48
1:B:116:LEU:O	1:B:120:VAL:HG23	2.13	0.48
1:A:24:LEU:HD22	1:C:77:ARG:HH21	1.76	0.48
1:A:202:ILE:HD12	1:A:228:CYS:HB2	1.94	0.48
1:A:329:ILE:CG2	1:A:330:SER:N	2.74	0.48
1:B:118:VAL:HG13	1:B:159:LEU:CD1	2.42	0.48
1:C:380:GLY:N	1:D:149:PRO:HG3	2.29	0.48
1:D:128:LEU:HD22	1:D:128:LEU:N	2.28	0.48
1:A:148:ALA:HB3	1:A:149:PRO:CD	2.44	0.48
1:B:147:ILE:HD12	1:B:147:ILE:O	2.13	0.48
1:D:32:VAL:CG1	1:D:248:VAL:HG13	2.43	0.48
1:A:380:GLY:N	1:B:149:PRO:HG3	2.28	0.48
1:D:77:ARG:HG2	1:D:77:ARG:HH11	1.79	0.48
1:B:203:GLU:CG	1:B:348:LEU:HB2	2.27	0.48
1:D:83:MET:HG2	1:D:206:SER:HB3	1.95	0.48
1:A:314:PRO:HB2	1:A:341:LEU:HB2	1.95	0.48
1:B:32:VAL:CG1	1:B:248:VAL:HG13	2.44	0.48
1:B:142:THR:HG23	1:B:202:ILE:O	2.13	0.48
1:C:190:ARG:NH1	1:D:191:ALA:HB1	2.29	0.48
1:C:148:ALA:HB3	1:C:149:PRO:CD	2.42	0.47
1:C:244:PRO:HA	1:C:391:ILE:HG22	1.96	0.47
1:D:203:GLU:HG2	1:D:348:LEU:CB	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:GLU:H	1:D:364:GLU:CD	2.22	0.47
1:D:35:ILE:HB	1:D:247:VAL:HB	1.96	0.47
1:C:204:LEU:O	1:C:207:VAL:HG12	2.14	0.47
1:C:314:PRO:HB2	1:C:341:LEU:HB2	1.96	0.47
1:A:106:MET:HE2	1:A:106:MET:HA	1.95	0.47
1:A:156:VAL:HA	1:A:161:LEU:HD12	1.97	0.47
1:B:114:VAL:O	1:B:118:VAL:HG23	2.15	0.47
1:B:128:LEU:N	1:B:128:LEU:HD22	2.30	0.47
1:B:319:ILE:HD12	1:B:319:ILE:N	2.29	0.47
1:C:26:PRO:HG3	1:D:237:GLN:CG	2.44	0.47
1:C:87:PRO:HB2	1:C:211:PHE:HE2	1.79	0.47
1:C:148:ALA:HB1	1:C:149:PRO:CD	2.34	0.47
1:A:26:PRO:HG3	1:B:237:GLN:HG2	1.97	0.47
1:C:40:THR:HB	1:C:354:PHE:CE1	2.50	0.47
1:C:329:ILE:CG2	1:C:330:SER:H	2.26	0.47
1:D:314:PRO:HA	1:D:320:ILE:HD11	1.97	0.47
1:D:151:VAL:O	1:D:155:ILE:HG13	2.14	0.47
1:B:243:GLU:HG3	1:B:246:LYS:HD3	1.96	0.47
1:B:364:GLU:H	1:B:364:GLU:CD	2.22	0.47
1:C:310:TRP:NE1	1:C:329:ILE:HD13	2.30	0.47
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.80	0.46
1:A:87:PRO:HB2	1:A:211:PHE:HE2	1.79	0.46
1:A:329:ILE:CG2	1:A:330:SER:H	2.26	0.46
1:A:344:PHE:O	1:A:347:MET:HE3	2.15	0.46
1:A:148:ALA:CB	1:B:265:VAL:HG13	2.45	0.46
1:A:152:ASP:OD2	1:A:167:ARG:NH1	2.48	0.46
1:C:210:VAL:N	1:C:221:HIS:HE1	2.11	0.46
1:B:162:SER:O	1:B:165:ILE:HG13	2.15	0.46
1:C:364:GLU:CD	1:C:364:GLU:H	2.23	0.46
1:A:26:PRO:HD2	1:B:193:PRO:HB3	1.97	0.46
1:A:216:ASN:ND2	1:A:277:LEU:H	2.08	0.46
1:C:26:PRO:HG3	1:D:237:GLN:HG2	1.97	0.46
1:D:143:SER:N	1:D:203:GLU:OE2	2.47	0.46
1:D:177:ALA:HB3	1:D:349:SER:HB3	1.96	0.46
1:A:244:PRO:HA	1:A:391:ILE:HG22	1.96	0.46
1:B:208:ASN:HD22	1:B:273:ILE:N	2.02	0.46
1:B:313:HIS:CE1	1:B:351:SER:HB2	2.51	0.46
1:C:26:PRO:HD2	1:D:193:PRO:HB3	1.98	0.46
1:C:148:ALA:CB	1:D:265:VAL:HG13	2.46	0.46
1:C:208:ASN:HD22	1:C:273:ILE:N	2.00	0.45
1:C:215:ILE:HD12	1:C:216:ASN:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:LEU:HD21	1:B:364:GLU:OE1	2.17	0.45
1:B:49:GLN:HE22	1:B:81:ARG:HH21	1.63	0.45
1:D:216:ASN:OD1	1:D:220:ILE:HD13	2.15	0.45
1:B:57:ALA:C	1:B:59:LEU:H	2.24	0.45
1:B:216:ASN:OD1	1:B:220:ILE:HD13	2.17	0.45
1:B:131:ARG:HG3	1:B:131:ARG:NH1	2.32	0.45
1:D:233:ILE:HD12	1:D:233:ILE:N	2.31	0.45
1:D:255:GLN:O	1:D:382:THR:HA	2.16	0.45
1:D:309:LEU:HD21	1:D:364:GLU:OE1	2.16	0.45
1:A:36:GLU:OE1	1:A:130:TYR:OH	2.30	0.45
1:A:215:ILE:HD12	1:A:216:ASN:H	1.82	0.45
1:A:310:TRP:NE1	1:A:329:ILE:HD13	2.31	0.45
1:B:314:PRO:HA	1:B:320:ILE:HD11	1.99	0.45
1:C:351:SER:O	1:C:352:LEU:C	2.60	0.45
1:D:147:ILE:HD13	1:D:150:GLY:HA2	1.97	0.45
1:A:146:PHE:N	1:A:146:PHE:HD1	2.14	0.45
1:B:42:THR:CG2	1:B:82:ARG:HG3	2.47	0.45
1:C:152:ASP:OD2	1:C:167:ARG:NH1	2.50	0.45
1:D:165:ILE:HG22	1:D:166:SER:O	2.17	0.45
1:D:214:ASP:O	1:D:218:VAL:HG23	2.16	0.45
1:C:133:ALA:O	1:C:195:MET:HE1	2.17	0.45
1:B:255:GLN:O	1:B:382:THR:HA	2.16	0.44
1:D:57:ALA:C	1:D:59:LEU:H	2.25	0.44
1:C:164:SER:HB3	1:D:255:GLN:NE2	2.32	0.44
1:B:147:ILE:HD13	1:B:150:GLY:HA2	1.98	0.44
1:B:214:ASP:O	1:B:218:VAL:HG23	2.17	0.44
1:B:265:VAL:O	1:B:276:GLU:N	2.50	0.44
1:D:313:HIS:CE1	1:D:351:SER:HB2	2.52	0.44
1:D:319:ILE:HD12	1:D:319:ILE:N	2.32	0.44
1:B:109:PHE:CZ	1:B:142:THR:HG21	2.52	0.44
1:C:131:ARG:HG3	1:C:131:ARG:NH1	2.32	0.44
1:D:142:THR:HG23	1:D:202:ILE:O	2.17	0.44
1:A:364:GLU:CD	1:A:364:GLU:H	2.24	0.44
1:B:57:ALA:O	1:B:59:LEU:N	2.51	0.44
1:B:151:VAL:O	1:B:155:ILE:HG13	2.17	0.44
1:C:146:PHE:N	1:C:146:PHE:HD1	2.15	0.44
1:D:243:GLU:HG3	1:D:246:LYS:HD3	1.98	0.44
1:A:204:LEU:O	1:A:207:VAL:HG12	2.17	0.44
1:B:148:ALA:HA	1:B:149:PRO:C	2.42	0.44
1:B:177:ALA:HB3	1:B:349:SER:HB3	1.99	0.44
1:B:279:GLU:CD	1:B:279:GLU:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:PHE:HB3	1:C:347:MET:HE3	1.99	0.44
1:C:344:PHE:O	1:C:347:MET:HE3	2.18	0.44
1:A:182:LEU:HD12	1:A:182:LEU:O	2.18	0.44
1:A:351:SER:O	1:A:352:LEU:C	2.59	0.44
1:C:182:LEU:HD12	1:C:182:LEU:O	2.18	0.44
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.83	0.44
1:B:206:SER:OG	1:B:226:ASP:OD2	2.35	0.44
1:C:142:THR:HG22	1:C:143:SER:N	2.33	0.44
1:D:118:VAL:HG13	1:D:159:LEU:HD11	2.00	0.44
1:D:131:ARG:HG3	1:D:131:ARG:NH1	2.32	0.44
1:A:309:LEU:HD22	1:A:359:MET:HE2	2.00	0.44
1:A:333:LEU:HD23	1:A:333:LEU:HA	1.80	0.44
1:D:42:THR:CG2	1:D:82:ARG:HG3	2.48	0.43
1:D:368:ALA:O	1:D:369:ILE:HB	2.18	0.43
1:A:210:VAL:N	1:A:221:HIS:HE1	2.15	0.43
1:B:165:ILE:HG22	1:B:166:SER:O	2.18	0.43
1:B:368:ALA:O	1:B:369:ILE:HB	2.18	0.43
1:C:142:THR:HG22	1:C:144:THR:N	2.20	0.43
1:C:145:GLY:C	1:C:146:PHE:CD1	2.96	0.43
1:A:145:GLY:C	1:A:146:PHE:CD1	2.96	0.43
1:B:317:PRO:O	1:B:321:GLU:HB2	2.18	0.43
1:C:156:VAL:HA	1:C:161:LEU:HD12	2.01	0.43
1:D:358:THR:O	1:D:362:GLN:HG2	2.17	0.43
1:A:110:TYR:O	1:A:114:VAL:HG23	2.18	0.43
1:C:189:VAL:HG13	1:C:235:ALA:CB	2.42	0.43
1:A:145:GLY:O	1:A:146:PHE:CB	2.67	0.43
1:A:280:ASN:O	1:A:281:LEU:C	2.61	0.43
1:C:36:GLU:HB3	1:C:246:LYS:HZ1	1.83	0.43
1:D:116:LEU:O	1:D:120:VAL:HG23	2.19	0.43
1:D:348:LEU:HD12	1:D:348:LEU:H	1.84	0.43
1:B:142:THR:HG22	1:B:143:SER:H	1.83	0.43
1:B:224:PHE:HD1	1:B:346:ASN:HB3	1.84	0.43
1:C:145:GLY:O	1:C:146:PHE:CB	2.66	0.43
1:C:148:ALA:CB	1:D:265:VAL:HA	2.48	0.43
1:D:265:VAL:O	1:D:276:GLU:N	2.47	0.43
1:D:39:ALA:HB3	1:D:124:ALA:HB2	2.00	0.43
1:D:318:LYS:HA	1:D:321:GLU:HB2	2.01	0.43
1:C:67:GLU:O	1:C:70:PRO:HD2	2.18	0.43
1:D:148:ALA:HA	1:D:149:PRO:C	2.44	0.43
1:D:203:GLU:CG	1:D:348:LEU:HB2	2.29	0.43
1:C:216:ASN:ND2	1:C:277:LEU:H	2.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLU:CG	1:B:157:LYS:HZ1	2.23	0.42
1:C:36:GLU:HB3	1:C:246:LYS:NZ	2.33	0.42
1:C:47:VAL:HG21	1:C:83:MET:SD	2.59	0.42
1:A:30:THR:HG21	1:C:286:PHE:HB3	2.02	0.42
1:A:314:PRO:HG2	1:A:351:SER:HB3	2.01	0.42
1:C:153:VAL:HG13	1:D:256:LEU:HD11	2.01	0.42
1:C:156:VAL:HG21	1:C:167:ARG:HD3	2.01	0.42
1:B:233:ILE:HD12	1:B:233:ILE:N	2.33	0.42
1:C:68:ARG:O	1:C:72:VAL:HG12	2.19	0.42
1:C:145:GLY:O	1:C:146:PHE:HB2	2.19	0.42
1:A:153:VAL:HG13	1:B:256:LEU:HD11	2.01	0.42
1:B:156:VAL:HG13	1:B:161:LEU:HB2	2.02	0.42
1:C:333:LEU:HD23	1:C:333:LEU:HA	1.80	0.42
1:D:56:VAL:O	1:D:59:LEU:HG	2.20	0.42
1:D:347:MET:O	1:D:350:VAL:HB	2.19	0.42
1:A:27:ALA:HA	1:A:28:PRO:HD3	1.92	0.42
1:A:133:ALA:O	1:A:195:MET:HE1	2.20	0.42
1:B:68:ARG:O	1:B:71:ARG:HB2	2.20	0.42
1:B:358:THR:O	1:B:362:GLN:HG2	2.19	0.42
1:C:102:ILE:HG23	1:D:268:VAL:O	2.20	0.42
1:A:171:ASN:HB2	1:B:171:ASN:HD22	1.85	0.42
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.91	0.42
1:B:260:THR:HG22	1:B:284:TYR:CD1	2.55	0.42
1:D:216:ASN:HD21	1:D:277:LEU:N	2.18	0.42
1:A:190:ARG:NH1	1:B:191:ALA:HB1	2.35	0.42
1:B:74:GLN:CG	1:B:75:LYS:N	2.83	0.42
1:B:136:GLY:HA3	1:B:188:TYR:OH	2.20	0.42
1:C:309:LEU:HD22	1:C:359:MET:HE2	2.01	0.42
1:C:314:PRO:HG2	1:C:351:SER:HB3	2.00	0.42
1:B:143:SER:N	1:B:203:GLU:OE2	2.51	0.42
1:C:190:ARG:HH12	1:D:191:ALA:HB1	1.84	0.42
1:C:348:LEU:N	1:C:348:LEU:CD1	2.82	0.42
1:B:93:ASP:HA	1:B:96:ARG:CD	2.49	0.41
1:D:57:ALA:HA	1:D:69:ILE:HD12	2.02	0.41
1:D:74:GLN:CG	1:D:75:LYS:N	2.82	0.41
1:A:255:GLN:HG3	1:A:292:VAL:HG22	2.02	0.41
1:B:118:VAL:HG13	1:B:159:LEU:HD11	2.00	0.41
1:B:140:LEU:HD13	1:B:140:LEU:C	2.45	0.41
1:B:151:VAL:HG21	1:B:202:ILE:CD1	2.50	0.41
1:D:57:ALA:O	1:D:59:LEU:N	2.52	0.41
1:D:77:ARG:HG2	1:D:77:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:THR:HG22	1:D:284:TYR:CD1	2.55	0.41
1:A:68:ARG:O	1:A:72:VAL:HG12	2.20	0.41
1:A:156:VAL:HG21	1:A:167:ARG:HD3	2.02	0.41
1:A:348:LEU:N	1:A:348:LEU:CD1	2.84	0.41
1:C:142:THR:HG23	1:C:202:ILE:O	2.20	0.41
1:C:288:GLY:O	1:C:291:PRO:HG2	2.20	0.41
1:A:148:ALA:CB	1:B:265:VAL:HA	2.47	0.41
1:A:164:SER:HB3	1:B:255:GLN:HE21	1.84	0.41
1:B:137:LEU:HD22	1:B:188:TYR:HB2	2.03	0.41
1:C:36:GLU:OE1	1:C:130:TYR:OH	2.31	0.41
1:C:352:LEU:HD12	1:C:352:LEU:HA	1.88	0.41
1:D:258:ASP:O	1:D:259:ASN:C	2.64	0.41
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.36	0.41
1:B:145:GLY:O	1:B:146:PHE:CD1	2.73	0.41
1:D:279:GLU:H	1:D:279:GLU:CD	2.29	0.41
1:A:368:ALA:HA	1:A:392:ARG:HB2	2.02	0.41
1:D:121:SER:HB2	1:D:159:LEU:HD21	2.02	0.41
1:A:102:ILE:HG23	1:B:268:VAL:O	2.20	0.41
1:A:145:GLY:O	1:A:146:PHE:HB2	2.21	0.41
1:B:51:ASP:O	1:B:52:ALA:C	2.64	0.41
1:B:112:HIS:O	1:B:115:PRO:HD2	2.21	0.41
1:B:217:ASP:O	1:B:221:HIS:CD2	2.74	0.41
1:C:266:LEU:HB2	1:D:148:ALA:HB3	2.03	0.41
1:D:216:ASN:HD21	1:D:277:LEU:H	1.69	0.41
1:D:322:GLN:HE22	1:D:325:ARG:NH1	2.19	0.41
1:D:364:GLU:O	1:D:365:SER:HB3	2.20	0.41
1:B:103:ARG:HD2	1:B:103:ARG:HA	1.87	0.41
1:D:69:ILE:HB	1:D:70:PRO:HD3	2.02	0.41
1:D:106:MET:HE2	1:D:106:MET:CA	2.50	0.41
1:A:40:THR:HB	1:A:354:PHE:CZ	2.56	0.40
1:B:39:ALA:HB3	1:B:124:ALA:HB2	2.02	0.40
1:B:347:MET:O	1:B:350:VAL:HB	2.20	0.40
1:C:270:HIS:CA	1:D:102:ILE:HD11	2.51	0.40
1:D:142:THR:HG22	1:D:143:SER:H	1.86	0.40
1:D:162:SER:HA	1:D:163:PRO:HD3	1.90	0.40
1:D:224:PHE:HD1	1:D:346:ASN:HB3	1.85	0.40
1:A:30:THR:O	1:A:30:THR:HG23	2.21	0.40
1:D:112:HIS:O	1:D:115:PRO:HD2	2.21	0.40
1:B:69:ILE:HB	1:B:70:PRO:HD3	2.03	0.40
1:C:148:ALA:CB	1:D:266:LEU:N	2.66	0.40
1:C:151:VAL:O	1:C:155:ILE:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:ASP:O	1:D:52:ALA:C	2.63	0.40
1:A:189:VAL:HG13	1:A:235:ALA:CB	2.42	0.40
1:B:85:VAL:HG12	1:B:86:ASP:N	2.36	0.40
1:C:30:THR:O	1:C:30:THR:HG23	2.20	0.40
1:D:189:VAL:CG1	1:D:235:ALA:HB2	2.49	0.40
1:D:206:SER:OG	1:D:226:ASP:OD2	2.35	0.40
1:C:256:LEU:HD23	1:C:256:LEU:HA	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	364/393 (93%)	342 (94%)	17 (5%)	5 (1%)	9	30
1	B	355/393 (90%)	320 (90%)	30 (8%)	5 (1%)	9	30
1	C	364/393 (93%)	344 (94%)	14 (4%)	6 (2%)	7	27
1	D	355/393 (90%)	318 (90%)	31 (9%)	6 (2%)	7	26
All	All	1438/1572 (92%)	1324 (92%)	92 (6%)	22 (2%)	8	28

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ALA
1	B	58	GLU
1	B	240	GLU
1	C	148	ALA
1	D	58	GLU
1	D	240	GLU
1	A	146	PHE
1	C	146	PHE

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Mol	Chain	Res	Type
1	B	175	CYS
1	D	175	CYS
1	A	369	ILE
1	C	369	ILE
1	B	369	ILE
1	B	381	VAL
1	D	369	ILE
1	D	381	VAL
1	A	381	VAL
1	C	381	VAL
1	D	239	GLN
1	C	193	PRO
1	A	193	PRO
1	C	289	VAL

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	293/316 (93%)	273 (93%)	20 (7%)	14	42
1	B	286/316 (90%)	267 (93%)	19 (7%)	15	43
1	C	293/316 (93%)	272 (93%)	21 (7%)	13	39
1	D	286/316 (90%)	267 (93%)	19 (7%)	15	43
All	All	1158/1264 (92%)	1079 (93%)	79 (7%)	14	42

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	32	VAL
1	A	55	ARG
1	A	72	VAL
1	A	77	ARG
1	A	85	VAL
1	A	102	ILE

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Mol	Chain	Res	Type
1	A	108	LEU
1	A	146	PHE
1	A	147	ILE
1	A	158	GLU
1	A	189	VAL
1	A	204	LEU
1	A	215	ILE
1	A	220	ILE
1	A	256	LEU
1	A	281	LEU
1	A	323	SER
1	A	336	GLN
1	A	356	LEU
1	B	55	ARG
1	B	72	VAL
1	B	96	ARG
1	B	102	ILE
1	B	147	ILE
1	B	172	PHE
1	B	189	VAL
1	B	202	ILE
1	B	203	GLU
1	B	204	LEU
1	B	207	VAL
1	B	215	ILE
1	B	220	ILE
1	B	256	LEU
1	B	281	LEU
1	B	336	GLN
1	B	341	LEU
1	B	356	LEU
1	B	384	GLU
1	C	30	THR
1	C	32	VAL
1	C	55	ARG
1	C	72	VAL
1	C	77	ARG
1	C	85	VAL
1	C	102	ILE
1	C	108	LEU
1	C	138	LEU
1	C	146	PHE

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Mol	Chain	Res	Type
1	C	147	ILE
1	C	189	VAL
1	C	204	LEU
1	C	215	ILE
1	C	220	ILE
1	C	256	LEU
1	C	281	LEU
1	C	323	SER
1	C	336	GLN
1	C	347	MET
1	C	356	LEU
1	D	55	ARG
1	D	72	VAL
1	D	96	ARG
1	D	102	ILE
1	D	147	ILE
1	D	172	PHE
1	D	189	VAL
1	D	202	ILE
1	D	204	LEU
1	D	207	VAL
1	D	215	ILE
1	D	220	ILE
1	D	256	LEU
1	D	274	THR
1	D	281	LEU
1	D	336	GLN
1	D	341	LEU
1	D	356	LEU
1	D	384	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	171	ASN
1	A	180	ASN
1	A	208	ASN
1	A	216	ASN
1	A	221	HIS
1	A	239	GLN
1	A	255	GLN

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Mol	Chain	Res	Type
1	A	270	HIS
1	A	280	ASN
1	A	336	GLN
1	A	346	ASN
1	B	49	GLN
1	B	112	HIS
1	B	171	ASN
1	B	208	ASN
1	B	216	ASN
1	B	221	HIS
1	B	237	GLN
1	B	239	GLN
1	B	255	GLN
1	B	270	HIS
1	B	280	ASN
1	B	313	HIS
1	B	336	GLN
1	C	112	HIS
1	C	171	ASN
1	C	180	ASN
1	C	208	ASN
1	C	216	ASN
1	C	221	HIS
1	C	255	GLN
1	C	270	HIS
1	C	280	ASN
1	C	336	GLN
1	C	346	ASN
1	D	49	GLN
1	D	171	ASN
1	D	208	ASN
1	D	216	ASN
1	D	221	HIS
1	D	255	GLN
1	D	270	HIS
1	D	280	ASN
1	D	313	HIS
1	D	336	GLN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	368/393 (93%)	-0.15	9 (2%) 59 50	13, 24, 43, 68	0
1	B	359/393 (91%)	-0.08	7 (1%) 66 58	11, 26, 47, 66	0
1	C	368/393 (93%)	-0.19	7 (1%) 66 58	13, 23, 44, 61	0
1	D	359/393 (91%)	-0.06	8 (2%) 62 53	14, 26, 44, 58	0
All	All	1454/1572 (92%)	-0.12	31 (2%) 63 54	11, 25, 46, 68	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	64	GLY	4.8
1	B	64	GLY	4.2
1	C	65	GLN	3.8
1	B	238	VAL	3.7
1	D	66	ARG	3.6
1	D	64	GLY	3.6
1	A	22	ALA	3.5
1	D	65	GLN	3.3
1	C	22	ALA	3.3
1	C	66	ARG	3.1
1	C	148	ALA	3.0
1	B	65	GLN	2.9
1	C	23	GLN	2.9
1	A	65	GLN	2.7
1	D	238	VAL	2.7
1	A	64	GLY	2.7
1	A	148	ALA	2.6
1	A	23	GLN	2.5
1	D	165	ILE	2.2
1	B	67	GLU	2.2
1	D	368	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	380	GLY	2.2
1	A	279	GLU	2.1
1	A	123	ARG	2.1
1	B	165	ILE	2.1
1	D	71	ARG	2.1
1	A	381	VAL	2.0
1	C	24	LEU	2.0
1	B	66	ARG	2.0
1	D	325	ARG	2.0
1	B	215	ILE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.