



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:43 PM UTC

PDB ID : 1URJ / pdb_00001urj
Title : Single stranded DNA-binding protein(ICP8) from Herpes simplex virus-1
Authors : Panjikar, S.; Mapelli, M.; Tucker, P.A.
Deposited on : 2003-10-30
Resolution : 3.00 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

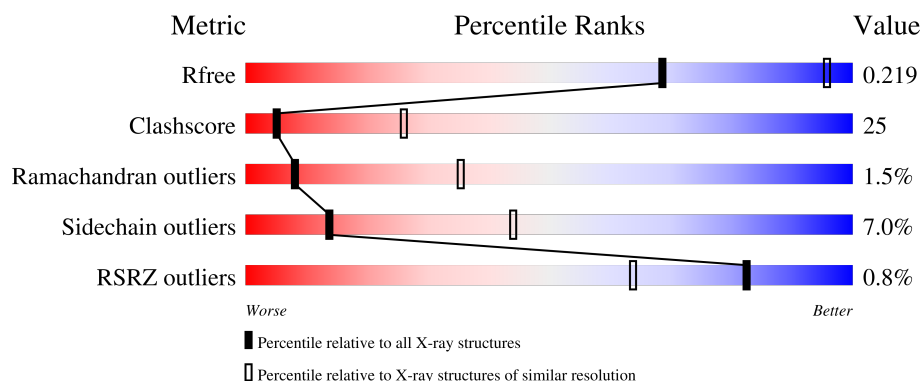
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	1136	
1	B	1136	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15798 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 MAJOR DNA-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1029	Total	C	N	O	S	0	0	1
			7840	4968	1384	1444	44			
1	B	1031	Total	C	N	O	S	0	0	1
			7853	4975	1386	1448	44			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	SER	CYS	engineered mutation	UNP P04296
A	455	SER	CYS	engineered mutation	UNP P04296
B	254	SER	CYS	engineered mutation	UNP P04296
B	455	SER	CYS	engineered mutation	UNP P04296

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Hg	0	0
			4	4		
3	B	4	Total	Hg	0	0
			4	4		

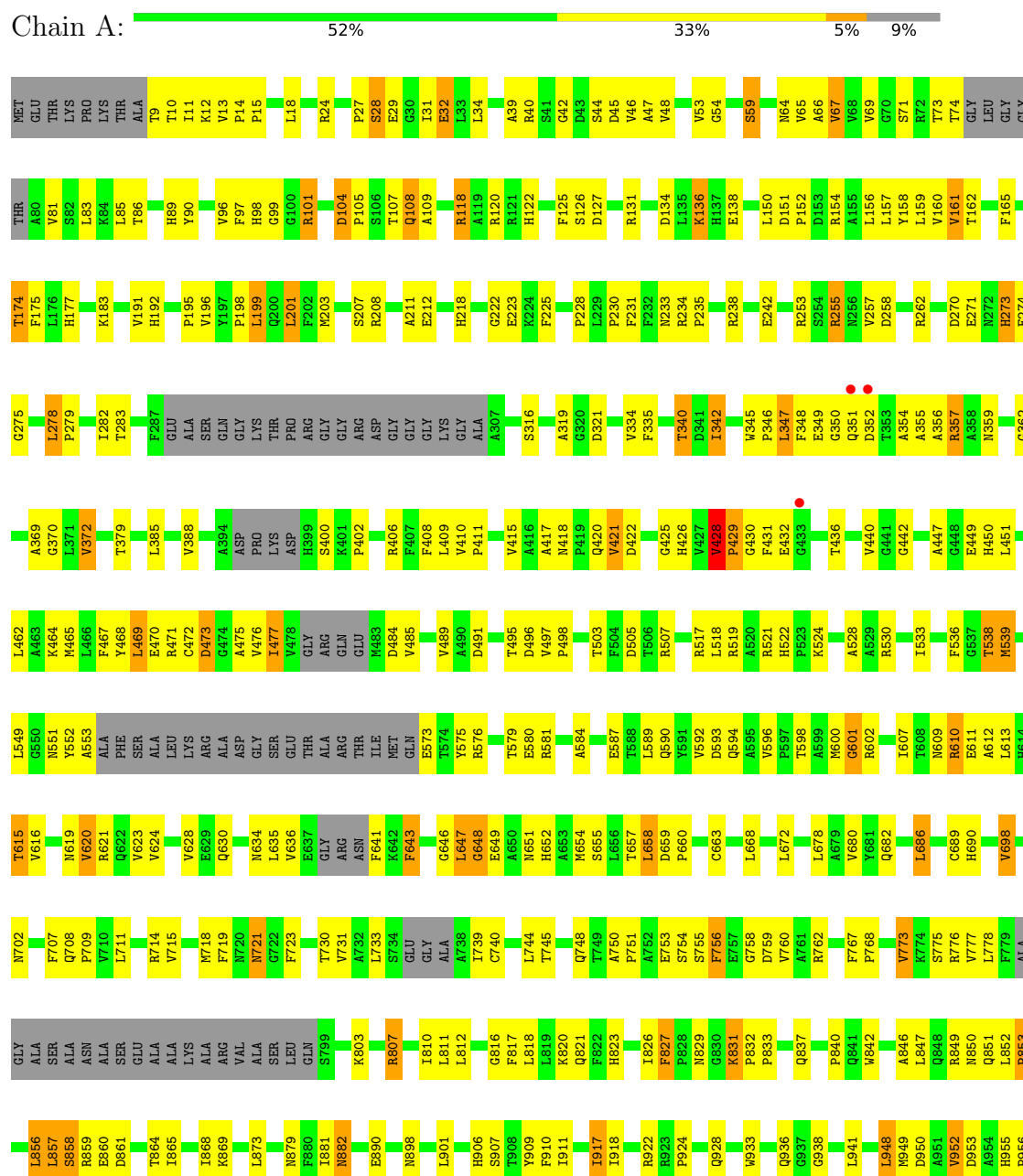
- Molecule 4 is water.

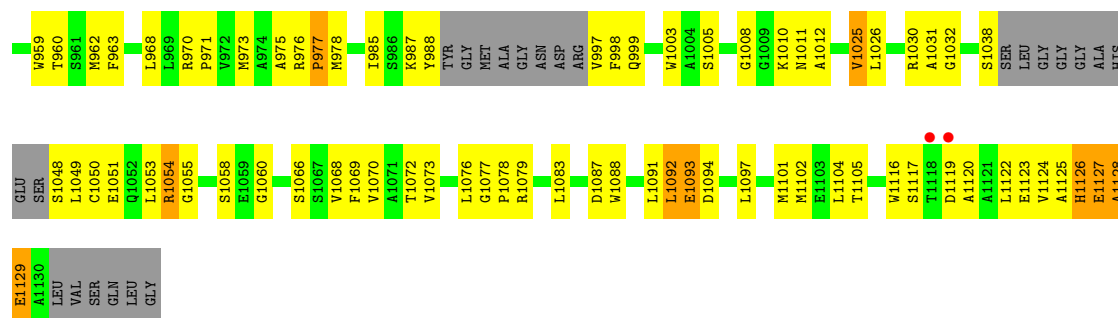
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total 50	O 50	0	0
4	B	45	Total 45	O 45	0	0

3 Residue-property plots

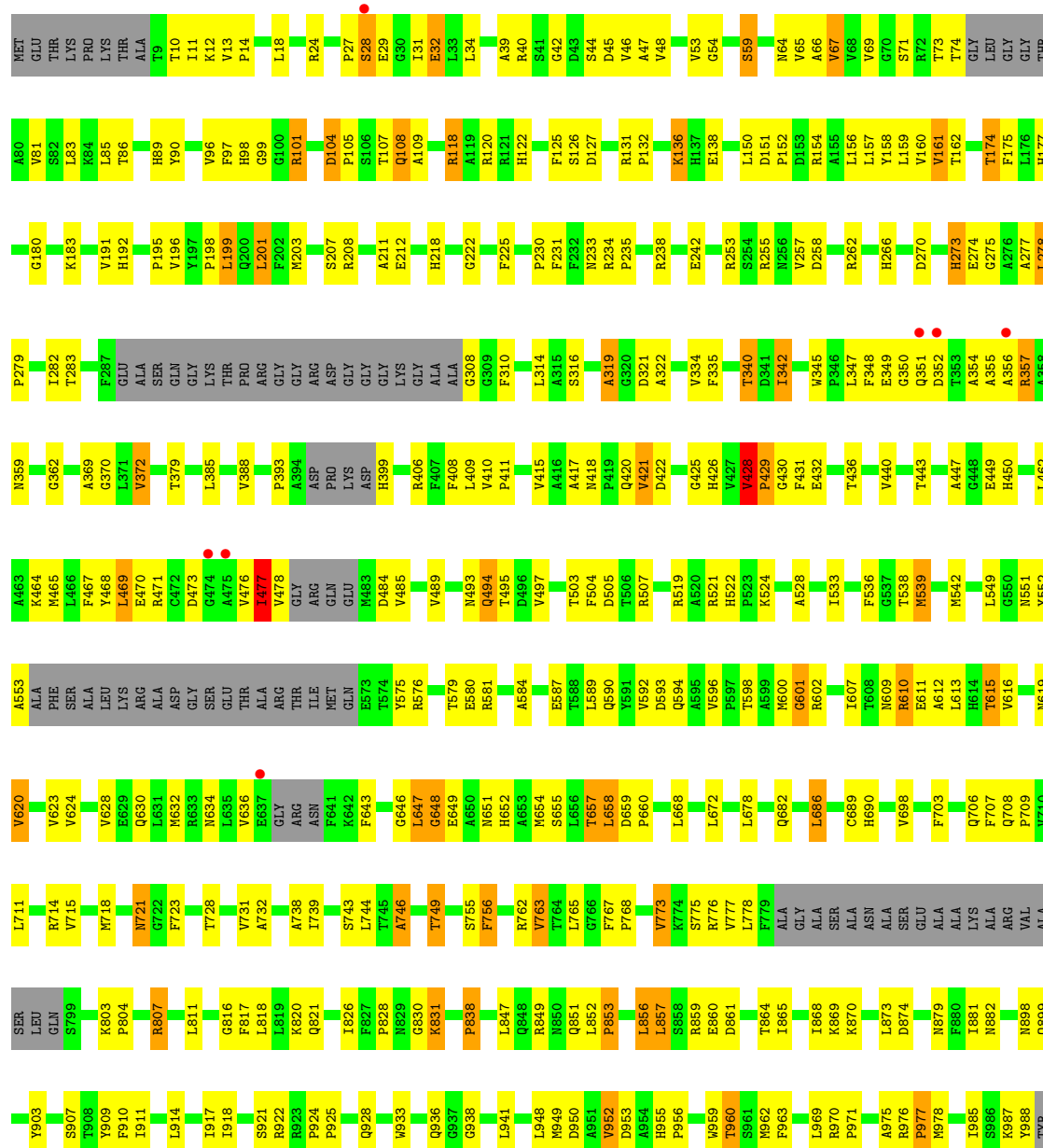
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





• Molecule 1: MAJOR DNA-BINDING PROTEIN



V1073	GLY
L1076	MET
G1077	ALA
P1078	GLY
R1079	ASN
	ASP
L1083	ARG
D1087	P997
W1088	P998
	P999
L1091	W1003
E1093	G1008
D1094	K1010
	N1011
L1097	A1012
	G1013
M1101	P1014
M1102	W1025
E1103	L1026
L1104	
T1105	R1030
	A1031
A1108	C1035
L1109	
W1116	S1038
S1117	SER
T1118	LEU
D1119	GLY
A1120	GLY
A1121	GLY
L1122	ALA
E1123	HIS
V1124	GLU
A1125	SER
H1126	S1048
E1127	L1049
A1128	C1050
E1129	E1051
A1130	P1052
LEU	L1053
VAL	R1054
SER	G1055
GLN	I1056
LEU	P1057
GLY	S1058
	E1059
	G1060
	S1066
	P1067
	F1068
	F1069
	V1070
	A1071
	T1072

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.91Å 145.37Å 162.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-3.00) 97.6 (20.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.286 0.217 , 0.219	Depositor DCC
R_{free} test set	1211 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.9	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	15798	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: HG, 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	0.50	1/8009 (0.0%)	0.99	34/10878 (0.3%)
1	B	0.51	1/8023 (0.0%)	0.99	31/10898 (0.3%)
All	All	0.51	2/16032 (0.0%)	0.99	65/21776 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1129	GLU	C-N	-5.36	1.25	1.33
1	B	1129	GLU	C-N	-5.06	1.26	1.33

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	ARG	N-CA-C	-12.39	97.87	113.23
1	B	357	ARG	N-CA-C	-12.37	97.89	113.23
1	A	827	PHE	CA-C-N	9.95	129.58	119.24
1	A	827	PHE	C-N-CA	9.95	129.58	119.24
1	B	428	VAL	CA-C-N	-8.37	109.38	119.84
1	B	428	VAL	C-N-CA	-8.37	109.38	119.84
1	A	428	VAL	CA-C-N	-7.71	110.20	119.84
1	A	428	VAL	C-N-CA	-7.71	110.20	119.84
1	B	1120	ALA	N-CA-C	-7.68	102.92	111.82
1	A	59	SER	N-CA-C	7.63	119.60	111.28
1	A	1120	ALA	N-CA-C	-7.61	102.99	111.82
1	B	59	SER	N-CA-C	7.31	119.25	111.28
1	B	731	VAL	N-CA-C	7.18	118.00	107.37
1	A	1026	LEU	N-CA-C	-7.16	97.58	109.46
1	B	658	LEU	N-CA-C	-7.12	102.90	112.94
1	A	909	TYR	N-CA-C	6.98	121.05	109.95
1	B	1026	LEU	N-CA-C	-6.94	97.93	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	658	LEU	N-CA-C	-6.85	103.29	112.94
1	B	1012	ALA	N-CA-C	-6.76	103.99	111.36
1	A	1012	ALA	N-CA-C	-6.65	104.11	111.36
1	B	909	TYR	N-CA-C	6.61	120.47	109.95
1	A	978	MET	N-CA-C	-6.59	98.88	109.96
1	B	978	MET	N-CA-C	-6.55	98.96	109.96
1	B	977	PRO	N-CA-C	6.45	121.37	111.57
1	A	977	PRO	N-CA-C	6.32	121.18	111.57
1	A	767	PHE	N-CA-C	6.28	113.87	108.22
1	B	648	GLY	N-CA-C	-6.28	107.76	114.67
1	B	767	PHE	N-CA-C	6.24	113.84	108.22
1	A	28	SER	N-CA-C	6.21	118.83	110.88
1	A	648	GLY	N-CA-C	-6.19	107.86	114.67
1	A	646	GLY	N-CA-C	6.16	120.12	112.73
1	B	856	LEU	N-CA-C	6.15	118.53	111.02
1	A	859	ARG	N-CA-C	-6.00	104.67	112.23
1	B	857	LEU	N-CA-C	5.96	119.23	109.76
1	B	108	GLN	N-CA-C	-5.95	105.98	113.18
1	A	400	SER	N-CA-C	-5.95	105.98	113.72
1	B	28	SER	N-CA-C	5.89	118.42	110.88
1	B	821	GLN	N-CA-C	5.89	117.70	111.28
1	A	442	GLY	N-CA-C	-5.81	105.36	112.68
1	A	108	GLN	N-CA-C	-5.77	106.20	113.18
1	A	211	ALA	N-CA-C	-5.76	100.90	110.17
1	A	257	VAL	N-CA-C	5.64	115.83	110.42
1	B	646	GLY	N-CA-C	5.59	119.44	112.73
1	A	756	PHE	N-CA-C	5.55	118.39	110.24
1	B	746	ALA	N-CA-C	5.48	119.22	112.54
1	B	274	GLU	N-CA-C	-5.44	101.86	109.69
1	B	749	THR	N-CA-C	-5.39	106.71	113.72
1	A	273	HIS	N-CA-C	5.39	117.50	109.25
1	A	472	CYS	N-CA-C	5.36	117.66	109.95
1	A	274	GLU	N-CA-C	-5.33	102.02	109.69
1	B	211	ALA	N-CA-C	-5.32	101.60	110.17
1	B	257	VAL	N-CA-C	5.32	115.53	110.42
1	A	917	ILE	N-CA-C	-5.31	99.31	106.85
1	A	689	CYS	N-CA-C	5.29	117.05	111.28
1	A	821	GLN	N-CA-C	5.28	117.72	111.33
1	B	319	ALA	N-CA-C	-5.22	105.76	111.82
1	B	1008	GLY	N-CA-C	-5.20	107.52	115.00
1	A	1008	GLY	N-CA-C	-5.17	107.55	115.00
1	B	689	CYS	N-CA-C	5.16	116.91	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	HIS	N-CA-C	5.14	117.12	109.25
1	A	907	SER	N-CA-C	5.12	116.59	108.96
1	A	812	LEU	N-CA-C	-5.12	105.75	112.41
1	B	907	SER	N-CA-C	5.10	116.56	108.96
1	B	542	MET	N-CA-C	-5.05	107.07	113.18
1	A	856	LEU	N-CA-C	-5.03	106.24	112.93

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	7840	0	7742	392	0
1	B	7853	0	7752	385	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	50	0	0	6	0
4	B	45	0	0	4	0
All	All	15798	0	15494	769	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 25.

All (769) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:GLN:HE21	1:B:494:GLN:HA	1.02	1.16
1:B:715:VAL:HA	1:B:718:MET:HE3	1.37	1.07
1:A:283:THR:HG23	1:A:420:GLN:HE21	1.21	1.04
1:A:715:VAL:HA	1:A:718:MET:HE3	1.39	1.03
1:A:1119:ASP:HB2	1:A:1122:LEU:HG	1.38	1.03
1:B:1119:ASP:HB2	1:B:1122:LEU:HG	1.39	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1070:VAL:HG22	1:B:1122:LEU:HD22	1.40	1.00
1:A:1070:VAL:HG22	1:A:1122:LEU:HD22	1.39	1.00
1:A:107:THR:HG22	1:A:109:ALA:H	1.30	0.95
1:B:613:LEU:HD12	1:B:826:ILE:HD13	1.48	0.93
1:B:107:THR:HG22	1:B:109:ALA:H	1.32	0.92
1:A:613:LEU:HD12	1:A:826:ILE:HD13	1.50	0.92
1:B:494:GLN:HA	1:B:494:GLN:NE2	1.83	0.91
1:B:159:LEU:HG	1:B:161:VAL:HG22	1.51	0.90
1:B:428:VAL:HB	1:B:429:PRO:HD3	1.52	0.90
1:B:447:ALA:H	1:B:450:HIS:HD2	1.18	0.89
1:A:988:TYR:CE1	1:A:998:PHE:HB2	2.08	0.89
1:B:283:THR:HG23	1:B:420:GLN:HE21	1.39	0.88
1:A:159:LEU:HG	1:A:161:VAL:HG22	1.55	0.88
1:A:739:ILE:HD12	1:A:758:GLY:H	1.40	0.85
1:A:651:ASN:HB3	1:A:776:ARG:HA	1.58	0.85
1:A:428:VAL:HB	1:A:429:PRO:HD3	1.55	0.85
1:A:651:ASN:HA	1:A:777:VAL:HG23	1.60	0.84
1:A:447:ALA:H	1:A:450:HIS:HD2	1.21	0.84
1:A:1070:VAL:HG22	1:A:1122:LEU:CD2	2.07	0.83
1:B:1070:VAL:HG22	1:B:1122:LEU:CD2	2.08	0.83
1:A:283:THR:HG23	1:A:420:GLN:NE2	1.93	0.83
1:B:651:ASN:HB3	1:B:776:ARG:HA	1.60	0.83
1:A:857:LEU:H	1:A:857:LEU:HD22	1.44	0.82
1:B:316:SER:HB3	1:B:388:VAL:HG21	1.61	0.81
1:A:316:SER:HB3	1:A:388:VAL:HG21	1.62	0.81
1:A:429:PRO:HG2	1:A:430:GLY:H	1.45	0.81
1:A:11:ILE:HD12	1:A:12:LYS:H	1.47	0.80
1:A:340:THR:HG22	1:A:345:TRP:HE1	1.47	0.80
1:B:494:GLN:HE21	1:B:494:GLN:CA	1.87	0.80
1:A:1053:LEU:HD12	1:A:1091:LEU:HD22	1.66	0.78
1:B:632:MET:HE3	1:B:903:TYR:CD1	2.19	0.78
1:B:428:VAL:CB	1:B:429:PRO:HD3	2.13	0.78
1:B:136:LYS:HB3	1:B:136:LYS:HZ2	1.49	0.78
1:B:651:ASN:HA	1:B:777:VAL:HG23	1.66	0.78
1:A:428:VAL:CB	1:A:429:PRO:HD3	2.14	0.76
1:B:447:ALA:H	1:B:450:HIS:CD2	2.04	0.76
1:B:429:PRO:HG2	1:B:430:GLY:H	1.49	0.76
1:A:64:ASN:CG	1:A:334:VAL:HG13	2.10	0.76
1:B:596:VAL:HG12	1:B:598:THR:HG22	1.68	0.76
1:B:1050:CYS:HB3	1:B:1054:ARG:HH21	1.49	0.76
1:A:348:PHE:O	1:A:352:ASP:HB2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:THR:HG22	1:B:345:TRP:HE1	1.51	0.75
1:A:1069:PHE:HA	1:A:1101:MET:HE1	1.69	0.75
1:B:428:VAL:HB	1:B:429:PRO:CD	2.15	0.75
1:A:1070:VAL:CG2	1:A:1122:LEU:HD22	2.16	0.74
1:B:352:ASP:OD1	1:B:357:ARG:NE	2.20	0.74
1:A:852:LEU:HD21	1:A:856:LEU:HD23	1.70	0.74
1:A:428:VAL:HB	1:A:429:PRO:CD	2.17	0.74
1:A:807:ARG:HH12	1:A:873:LEU:HD11	1.51	0.73
1:A:1050:CYS:HB3	1:A:1054:ARG:HH21	1.53	0.73
1:B:348:PHE:O	1:B:352:ASP:HB2	1.86	0.73
1:B:449:GLU:HG3	4:B:2006:HOH:O	1.87	0.73
1:B:225:PHE:CE2	1:B:744:LEU:HD13	2.23	0.73
1:B:1070:VAL:CG2	1:B:1122:LEU:HD22	2.17	0.73
1:B:1053:LEU:HD12	1:B:1091:LEU:HD22	1.69	0.73
1:A:18:LEU:HD23	1:A:198:PRO:HG3	1.71	0.73
1:B:1069:PHE:HA	1:B:1101:MET:HE1	1.71	0.72
1:A:473:ASP:HB3	1:A:517:ARG:HH12	1.53	0.72
1:A:136:LYS:HB3	1:A:136:LYS:HZ2	1.54	0.72
1:A:497:VAL:HG21	1:A:507:ARG:CZ	2.20	0.72
1:B:1053:LEU:HD22	1:B:1068:VAL:HG13	1.72	0.72
1:A:428:VAL:CG1	1:A:429:PRO:HD3	2.20	0.72
1:A:596:VAL:HG12	1:A:598:THR:HG22	1.72	0.71
1:A:1048:SER:N	1:B:477:ILE:HG21	2.05	0.71
1:A:678:LEU:O	1:A:682:GLN:HG3	1.91	0.71
1:B:18:LEU:HD23	1:B:198:PRO:HG3	1.72	0.71
1:B:283:THR:HG23	1:B:420:GLN:NE2	2.05	0.71
1:A:832:PRO:HB3	1:A:842:TRP:CD2	2.25	0.71
1:A:203:MET:HE3	1:A:218:HIS:HD2	1.55	0.71
1:A:199:LEU:HD21	1:A:230:PRO:HG3	1.72	0.70
1:A:1053:LEU:HD22	1:A:1068:VAL:HG13	1.73	0.70
1:A:447:ALA:H	1:A:450:HIS:CD2	2.06	0.70
1:B:549:LEU:HB2	1:B:575:TYR:CE2	2.26	0.70
1:B:1125:ALA:C	1:B:1127:GLU:H	1.98	0.70
1:A:352:ASP:OD1	1:A:357:ARG:NE	2.20	0.70
1:B:203:MET:HE3	1:B:218:HIS:HD2	1.56	0.70
1:B:497:VAL:HG21	1:B:507:ARG:CZ	2.21	0.70
1:A:573:GLU:CB	1:A:581:ARG:HH22	2.05	0.70
1:A:997:VAL:HG13	1:A:997:VAL:O	1.92	0.69
1:B:1127:GLU:O	1:B:1129:GLU:N	2.25	0.69
1:B:1066:SER:O	1:B:1070:VAL:HG23	1.93	0.69
1:A:340:THR:CG2	1:A:345:TRP:HE1	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:GLU:O	1:A:1129:GLU:N	2.25	0.68
1:B:428:VAL:CG1	1:B:429:PRO:HD3	2.22	0.68
1:A:852:LEU:HD13	1:A:857:LEU:HD21	1.76	0.68
1:B:120:ARG:HD3	1:B:126:SER:O	1.94	0.68
1:B:970:ARG:HB3	1:B:971:PRO:HD3	1.74	0.68
1:A:429:PRO:CG	1:A:430:GLY:H	2.06	0.68
1:B:199:LEU:HD21	1:B:230:PRO:HG3	1.74	0.68
1:B:678:LEU:O	1:B:682:GLN:HG3	1.92	0.68
1:A:621:ARG:HD3	4:A:2028:HOH:O	1.92	0.68
1:A:275:GLY:HA2	1:A:708:GLN:HB3	1.74	0.68
1:A:613:LEU:HD12	1:A:826:ILE:CD1	2.24	0.68
1:A:1125:ALA:C	1:A:1127:GLU:H	1.99	0.67
1:B:107:THR:HG23	1:B:470:GLU:OE2	1.94	0.67
1:B:238:ARG:O	1:B:242:GLU:HG3	1.95	0.67
1:B:658:LEU:HD12	1:B:768:PRO:HB2	1.77	0.67
1:B:715:VAL:HA	1:B:718:MET:CE	2.20	0.67
1:B:340:THR:CG2	1:B:345:TRP:HE1	2.08	0.67
1:B:46:VAL:HG12	1:B:97:PHE:HA	1.74	0.67
1:B:1050:CYS:CB	1:B:1054:ARG:HH21	2.07	0.67
1:A:89:HIS:CD2	1:A:660:PRO:HG3	2.30	0.67
1:A:970:ARG:HB3	1:A:971:PRO:HD3	1.77	0.66
1:A:406:ARG:HH11	1:A:690:HIS:HD2	1.42	0.66
1:A:1097:LEU:O	1:A:1101:MET:HG2	1.96	0.66
1:B:370:GLY:HA3	1:B:963:PHE:CZ	2.31	0.66
1:A:120:ARG:HD3	1:A:126:SER:O	1.94	0.66
1:B:11:ILE:HD13	1:B:334:VAL:HG11	1.76	0.66
1:B:275:GLY:HA2	1:B:708:GLN:HB3	1.78	0.66
1:A:107:THR:HG23	1:A:470:GLU:OE2	1.95	0.66
1:A:778:LEU:HD23	1:A:911:ILE:HG22	1.78	0.66
1:B:370:GLY:HA3	1:B:963:PHE:HZ	1.60	0.65
1:A:1066:SER:O	1:A:1070:VAL:HG23	1.96	0.65
1:B:136:LYS:HB3	1:B:136:LYS:NZ	2.10	0.65
1:A:46:VAL:HG12	1:A:97:PHE:HA	1.79	0.65
1:A:576:ARG:O	1:A:580:GLU:HG3	1.97	0.65
1:A:1072:THR:HG21	1:A:1088:TRP:CH2	2.32	0.65
1:A:203:MET:HE3	1:A:218:HIS:CD2	2.31	0.65
1:A:24:ARG:NH2	1:A:27:PRO:HB3	2.11	0.65
1:A:1003:TRP:HZ2	1:A:1025:VAL:HG22	1.61	0.65
1:B:18:LEU:HD12	1:B:18:LEU:C	2.21	0.65
1:A:1050:CYS:CB	1:A:1054:ARG:HH21	2.10	0.64
1:B:24:ARG:NH2	1:B:27:PRO:HB3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASP:OD1	1:A:101:ARG:HD2	1.96	0.64
1:A:238:ARG:O	1:A:242:GLU:HG3	1.96	0.64
1:A:54:GLY:HA3	1:A:342:ILE:HD11	1.80	0.64
1:B:118:ARG:HD2	1:B:449:GLU:OE2	1.98	0.64
1:A:136:LYS:HB3	1:A:136:LYS:NZ	2.13	0.64
1:A:610:ARG:HD3	1:A:864:THR:OG1	1.98	0.64
1:B:988:TYR:CE1	1:B:998:PHE:HB2	2.33	0.64
1:B:283:THR:HG22	4:B:2020:HOH:O	1.98	0.63
1:B:476:VAL:O	1:B:477:ILE:HG13	1.98	0.63
1:A:473:ASP:HB2	1:A:518:LEU:CD2	2.28	0.63
1:B:1072:THR:HG21	1:B:1088:TRP:CH2	2.33	0.63
1:A:283:THR:OG1	1:A:420:GLN:HB3	1.98	0.63
1:A:9:THR:HG23	1:A:10:THR:H	1.63	0.63
1:A:592:VAL:HG12	1:A:593:ASP:N	2.12	0.63
1:A:10:THR:HA	1:A:730:THR:HG23	1.80	0.63
1:B:429:PRO:CG	1:B:430:GLY:H	2.10	0.63
1:A:18:LEU:C	1:A:18:LEU:HD12	2.23	0.62
1:A:156:LEU:C	1:A:157:LEU:HD12	2.23	0.62
1:A:636:VAL:HG23	1:A:643:PHE:HZ	1.64	0.62
1:A:177:HIS:HB3	1:A:195:PRO:HG2	1.80	0.62
1:B:1097:LEU:O	1:B:1101:MET:HG2	1.99	0.62
1:B:1119:ASP:CB	1:B:1122:LEU:HG	2.24	0.62
1:A:778:LEU:CD2	1:A:911:ILE:HG22	2.30	0.62
1:B:406:ARG:HH11	1:B:690:HIS:HD2	1.47	0.62
1:B:592:VAL:HG12	1:B:593:ASP:N	2.14	0.62
1:B:156:LEU:C	1:B:157:LEU:HD12	2.25	0.62
1:B:177:HIS:HB3	1:B:195:PRO:HG2	1.80	0.62
1:B:807:ARG:HH12	1:B:873:LEU:HD11	1.65	0.62
1:B:1003:TRP:HZ2	1:B:1025:VAL:HG22	1.65	0.62
1:B:203:MET:HE3	1:B:218:HIS:CD2	2.35	0.61
1:A:90:TYR:CD2	1:A:160:VAL:HG12	2.35	0.61
1:B:420:GLN:HG2	1:B:431:PHE:CE2	2.35	0.61
1:B:647:LEU:HD23	1:B:648:GLY:N	2.14	0.61
1:B:861:ASP:O	1:B:865:ILE:HG12	2.01	0.61
1:A:739:ILE:CD1	1:A:758:GLY:H	2.11	0.61
1:A:1119:ASP:HB2	1:A:1122:LEU:CG	2.22	0.61
1:B:385:LEU:HD12	1:B:533:ILE:HG23	1.80	0.61
1:B:576:ARG:O	1:B:580:GLU:HG3	2.00	0.61
1:A:484:ASP:HA	1:A:928:GLN:NE2	2.16	0.61
1:A:810:ILE:HD11	1:A:869:LYS:HG2	1.82	0.61
1:A:420:GLN:HG2	1:A:431:PHE:CE2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:MET:HE2	1:A:655:SER:O	2.01	0.61
1:B:1010:LYS:H	1:B:1010:LYS:HD2	1.65	0.61
1:A:1069:PHE:CA	1:A:1101:MET:HE1	2.30	0.61
1:A:715:VAL:HA	1:A:718:MET:CE	2.24	0.61
1:B:90:TYR:CD2	1:B:160:VAL:HG12	2.36	0.61
1:A:385:LEU:HD12	1:A:533:ILE:HG23	1.83	0.61
1:B:45:ASP:OD1	1:B:101:ARG:HD2	2.00	0.61
1:B:1069:PHE:CA	1:B:1101:MET:HE1	2.30	0.61
1:B:613:LEU:HD12	1:B:826:ILE:CD1	2.27	0.61
1:A:807:ARG:NH1	1:A:873:LEU:HD11	2.16	0.60
1:A:832:PRO:HB3	1:A:842:TRP:CE2	2.36	0.60
1:A:610:ARG:HH11	1:A:610:ARG:HG2	1.66	0.60
1:B:1119:ASP:HB2	1:B:1122:LEU:CG	2.24	0.60
1:A:370:GLY:HA3	1:A:963:PHE:HZ	1.67	0.60
1:A:1083:LEU:HD22	1:A:1087:ASP:HB3	1.84	0.60
1:B:610:ARG:HG2	1:B:610:ARG:HH11	1.66	0.60
1:A:319:ALA:CB	1:A:686:LEU:HD13	2.32	0.60
1:B:253:ARG:NH2	1:B:682:GLN:OE1	2.35	0.60
1:A:1010:LYS:H	1:A:1010:LYS:HD2	1.67	0.60
1:B:54:GLY:HA3	1:B:342:ILE:HD11	1.83	0.60
1:B:104:ASP:OD2	1:B:104:ASP:N	2.35	0.60
1:A:484:ASP:HA	1:A:928:GLN:HE22	1.65	0.59
1:A:610:ARG:NH2	1:A:860:GLU:HB3	2.16	0.59
1:B:406:ARG:HH11	1:B:690:HIS:CD2	2.20	0.59
1:A:225:PHE:CE2	1:A:744:LEU:HD13	2.37	0.59
1:A:406:ARG:HH11	1:A:690:HIS:CD2	2.20	0.59
1:A:610:ARG:NH2	1:A:860:GLU:CB	2.65	0.59
1:A:651:ASN:HB2	1:A:775:SER:O	2.03	0.59
1:A:861:ASP:O	1:A:865:ILE:HG12	2.02	0.59
1:B:817:PHE:CE2	1:B:818:LEU:HG	2.37	0.59
1:B:350:GLY:O	1:B:352:ASP:N	2.35	0.59
1:A:370:GLY:HA3	1:A:963:PHE:CZ	2.36	0.59
1:A:647:LEU:HD23	1:A:648:GLY:N	2.18	0.59
1:B:1083:LEU:HD22	1:B:1087:ASP:HB3	1.84	0.59
1:A:753:GLU:HG2	1:A:755:SER:OG	2.03	0.59
1:B:83:LEU:HD12	1:B:739:ILE:HG22	1.85	0.58
1:B:476:VAL:HG22	1:B:1014:PRO:HB2	1.85	0.58
1:B:421:VAL:HG22	1:B:426:HIS:C	2.29	0.58
1:B:71:SER:HB2	1:B:81:VAL:CG1	2.33	0.58
1:A:233:ASN:OD1	1:A:235:PRO:HD2	2.04	0.58
1:A:1070:VAL:HG22	1:A:1122:LEU:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ARG:HD2	1:A:449:GLU:OE2	2.04	0.58
1:A:817:PHE:CE2	1:A:818:LEU:HG	2.38	0.58
1:A:827:PHE:CZ	1:A:865:ILE:HD13	2.39	0.58
1:A:278:LEU:HD22	1:A:321:ASP:OD1	2.04	0.57
1:A:847:LEU:HD23	1:A:852:LEU:HD12	1.84	0.57
1:A:1053:LEU:C	1:A:1055:GLY:H	2.12	0.57
1:A:1092:LEU:C	1:A:1094:ASP:H	2.13	0.57
1:B:616:VAL:O	1:B:620:VAL:HG13	2.05	0.57
1:A:1049:LEU:N	1:B:477:ILE:HG23	2.20	0.57
1:A:350:GLY:O	1:A:352:ASP:N	2.36	0.57
1:A:348:PHE:HB3	1:A:352:ASP:CG	2.30	0.57
1:B:1092:LEU:C	1:B:1094:ASP:H	2.12	0.57
1:A:11:ILE:HD12	1:A:12:LYS:N	2.17	0.57
1:A:271:GLU:HB2	1:A:762:ARG:NH1	2.20	0.57
1:B:131:ARG:HH12	1:B:212:GLU:CD	2.12	0.57
1:A:104:ASP:OD2	1:A:104:ASP:N	2.34	0.56
1:B:647:LEU:HD23	1:B:648:GLY:H	1.69	0.56
1:A:335:PHE:HB3	1:A:659:ASP:OD2	2.05	0.56
1:A:731:VAL:HG11	1:A:760:VAL:HG21	1.88	0.56
1:A:1053:LEU:CD1	1:A:1091:LEU:HD22	2.34	0.56
1:B:632:MET:HB3	1:B:903:TYR:CE2	2.40	0.56
1:B:1053:LEU:C	1:B:1055:GLY:H	2.12	0.56
1:B:266:HIS:CD2	4:B:2013:HOH:O	2.58	0.56
1:B:1068:VAL:HG12	1:B:1101:MET:HE2	1.87	0.56
1:A:428:VAL:HG12	1:A:429:PRO:HD3	1.86	0.56
1:A:922:ARG:HD3	1:A:962:MET:SD	2.45	0.56
1:B:658:LEU:CD1	1:B:768:PRO:HB2	2.34	0.56
1:B:987:LYS:N	1:B:987:LYS:HD2	2.21	0.56
1:B:428:VAL:CB	1:B:429:PRO:CD	2.81	0.56
1:B:258:ASP:O	1:B:262:ARG:HG3	2.06	0.55
1:B:440:VAL:HG21	1:B:528:ALA:HB2	1.87	0.55
1:A:157:LEU:HD12	1:A:157:LEU:N	2.21	0.55
1:A:636:VAL:CG2	1:A:643:PHE:HZ	2.19	0.55
1:B:1069:PHE:HD2	1:B:1122:LEU:HD23	1.71	0.55
1:A:519:ARG:HD2	1:A:519:ARG:O	2.06	0.55
1:A:987:LYS:HD2	1:A:987:LYS:N	2.21	0.55
1:A:1069:PHE:HD2	1:A:1122:LEU:HD23	1.71	0.55
1:A:447:ALA:N	1:A:450:HIS:HD2	1.98	0.55
1:A:477:ILE:HD12	1:A:477:ILE:N	2.21	0.55
1:A:610:ARG:CZ	1:A:860:GLU:HB3	2.36	0.55
1:B:420:GLN:O	1:B:428:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:GLN:O	1:A:428:VAL:HG23	2.06	0.55
1:A:610:ARG:C	1:A:610:ARG:HD2	2.32	0.55
1:B:552:TYR:CE1	1:B:647:LEU:HB3	2.41	0.55
1:B:708:GLN:N	1:B:709:PRO:CD	2.69	0.55
1:A:613:LEU:CD1	1:A:826:ILE:HD13	2.31	0.55
1:A:616:VAL:O	1:A:620:VAL:HG13	2.07	0.55
1:A:652:HIS:CE1	1:A:777:VAL:HG22	2.41	0.55
1:B:40:ARG:HG3	1:B:47:ALA:HB2	1.88	0.55
1:B:447:ALA:N	1:B:450:HIS:HD2	1.96	0.55
1:B:467:PHE:C	1:B:467:PHE:CD1	2.85	0.55
1:A:552:TYR:CE1	1:A:647:LEU:HB3	2.42	0.55
1:B:64:ASN:CG	1:B:334:VAL:HG13	2.31	0.54
1:A:1070:VAL:HG22	1:A:1122:LEU:CD1	2.37	0.54
1:B:647:LEU:HG	1:B:778:LEU:CD1	2.37	0.54
1:A:40:ARG:HG3	1:A:47:ALA:HB2	1.90	0.54
1:A:723:PHE:CB	1:A:999:GLN:HB2	2.37	0.54
1:B:879:ASN:HA	1:B:898:ASN:CG	2.33	0.54
1:A:421:VAL:HG22	1:A:426:HIS:C	2.32	0.54
1:B:1070:VAL:HG22	1:B:1122:LEU:HD13	1.88	0.54
1:B:948:LEU:HD22	1:B:955:HIS:CE1	2.43	0.54
1:B:1069:PHE:O	1:B:1073:VAL:HG23	2.08	0.54
1:A:592:VAL:CG1	1:A:593:ASP:N	2.71	0.54
1:A:708:GLN:N	1:A:709:PRO:CD	2.70	0.54
1:B:28:SER:O	1:B:29:GLU:HG3	2.08	0.54
1:B:348:PHE:HB3	1:B:352:ASP:CG	2.32	0.54
1:A:98:HIS:CD2	1:A:157:LEU:HD13	2.43	0.54
1:A:918:ILE:N	1:A:918:ILE:HD12	2.22	0.54
1:A:1119:ASP:CB	1:A:1122:LEU:HG	2.24	0.54
1:A:1068:VAL:HG12	1:A:1101:MET:HE2	1.89	0.54
1:A:1102:MET:HE3	1:A:1105:THR:HG21	1.90	0.54
1:B:408:PHE:HA	1:B:686:LEU:HD23	1.90	0.54
1:A:476:VAL:H	1:A:477:ILE:HD12	1.73	0.54
1:B:864:THR:O	1:B:868:ILE:HG12	2.08	0.54
1:B:610:ARG:HD2	1:B:610:ARG:C	2.33	0.53
1:A:467:PHE:CD1	1:A:467:PHE:C	2.86	0.53
1:A:647:LEU:HG	1:A:778:LEU:CD1	2.38	0.53
1:A:415:VAL:HG12	1:A:415:VAL:O	2.08	0.53
1:B:83:LEU:HD12	1:B:739:ILE:CG2	2.37	0.53
1:B:918:ILE:HD12	1:B:918:ILE:N	2.22	0.53
1:B:539:MET:HE2	1:B:655:SER:O	2.09	0.53
1:A:647:LEU:HD23	1:A:648:GLY:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ASN:HA	1:A:898:ASN:CG	2.34	0.53
1:B:1053:LEU:CD1	1:B:1091:LEU:HD22	2.37	0.53
1:A:29:GLU:C	1:A:31:ILE:H	2.17	0.53
1:A:39:ALA:HB3	1:A:48:VAL:HG13	1.91	0.53
1:B:29:GLU:C	1:B:31:ILE:H	2.17	0.53
1:A:64:ASN:OD1	1:A:334:VAL:HG13	2.08	0.53
1:B:1102:MET:HE3	1:B:1105:THR:HG21	1.90	0.53
1:A:316:SER:HB3	1:A:388:VAL:CG2	2.37	0.53
1:B:476:VAL:C	1:B:477:ILE:HG13	2.33	0.53
1:A:744:LEU:HG	1:A:756:PHE:HZ	1.75	0.52
1:B:362:GLY:HA3	1:B:956:PRO:O	2.09	0.52
1:A:201:LEU:HD22	1:A:744:LEU:HD21	1.91	0.52
1:A:1049:LEU:CB	1:B:477:ILE:HG23	2.39	0.52
1:B:174:THR:HG23	1:B:175:PHE:N	2.23	0.52
1:B:174:THR:HG22	1:B:231:PHE:HB3	1.91	0.52
1:B:519:ARG:HD2	1:B:519:ARG:O	2.10	0.52
1:A:711:LEU:O	1:A:715:VAL:HG23	2.10	0.52
1:A:1069:PHE:O	1:A:1073:VAL:HG23	2.09	0.52
1:B:922:ARG:HD3	1:B:962:MET:SD	2.49	0.52
1:A:28:SER:O	1:A:29:GLU:HG3	2.08	0.52
1:B:98:HIS:CD2	1:B:157:LEU:HD13	2.44	0.52
1:B:319:ALA:CB	1:B:686:LEU:HD13	2.39	0.52
1:A:131:ARG:HH12	1:A:212:GLU:CD	2.17	0.52
1:B:507:ARG:HG3	1:B:507:ARG:HH11	1.74	0.52
1:B:619:ASN:O	1:B:623:VAL:HG13	2.10	0.52
1:B:859:ARG:HG3	1:B:860:GLU:OE2	2.08	0.52
1:B:879:ASN:HD22	1:B:898:ASN:HD21	1.57	0.52
1:A:610:ARG:HH22	1:A:860:GLU:CB	2.23	0.52
1:A:635:LEU:HD13	1:A:641:PHE:CE2	2.45	0.52
1:A:359:ASN:OD1	1:A:956:PRO:HA	2.10	0.52
1:B:415:VAL:HG12	1:B:415:VAL:O	2.09	0.52
1:A:857:LEU:H	1:A:857:LEU:CD2	2.18	0.52
1:B:44:SER:OG	1:B:46:VAL:HG22	2.10	0.52
1:B:233:ASN:OD1	1:B:235:PRO:HD2	2.10	0.52
1:A:473:ASP:CB	1:A:517:ARG:HH12	2.21	0.52
1:B:90:TYR:HA	1:B:162:THR:HA	1.92	0.52
1:A:258:ASP:O	1:A:262:ARG:HG3	2.09	0.51
1:B:39:ALA:HB3	1:B:48:VAL:HG13	1.92	0.51
1:B:428:VAL:HG12	1:B:429:PRO:HD3	1.90	0.51
1:B:1127:GLU:OE2	1:B:1128:ALA:HA	2.10	0.51
1:A:31:ILE:HG23	1:A:32:GLU:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ARG:NH2	1:A:682:GLN:OE1	2.44	0.51
1:A:975:ALA:O	1:A:976:ARG:C	2.53	0.51
1:B:99:GLY:HA3	1:B:156:LEU:HD23	1.92	0.51
1:B:1070:VAL:HG13	1:B:1122:LEU:HD11	1.92	0.51
1:B:1123:GLU:HA	1:B:1126:HIS:HB3	1.93	0.51
1:A:612:ALA:O	1:A:615:THR:HG23	2.10	0.51
1:B:462:LEU:O	1:B:465:MET:HB3	2.10	0.51
1:A:372:VAL:HG11	1:A:468:TYR:CG	2.46	0.51
1:B:157:LEU:HD12	1:B:157:LEU:N	2.25	0.51
1:B:975:ALA:O	1:B:976:ARG:C	2.53	0.51
1:B:484:ASP:HA	1:B:928:GLN:NE2	2.25	0.51
1:A:847:LEU:HD13	1:A:847:LEU:C	2.36	0.51
1:A:831:LYS:HB3	1:A:837:GLN:C	2.36	0.51
1:B:611:GLU:O	1:B:615:THR:HG22	2.11	0.51
1:B:711:LEU:O	1:B:715:VAL:HG23	2.10	0.51
1:A:44:SER:OG	1:A:46:VAL:HG22	2.11	0.51
1:A:837:GLN:HA	1:A:837:GLN:NE2	2.26	0.51
1:B:316:SER:HB3	1:B:388:VAL:CG2	2.37	0.51
1:B:592:VAL:CG1	1:B:593:ASP:N	2.73	0.51
1:A:71:SER:HB2	1:A:81:VAL:CG1	2.41	0.51
1:A:90:TYR:HA	1:A:162:THR:HA	1.93	0.51
1:A:429:PRO:HD2	1:A:431:PHE:HD1	1.76	0.51
1:A:421:VAL:CG1	1:A:425:GLY:HA2	2.41	0.50
1:A:429:PRO:CG	1:A:430:GLY:N	2.71	0.50
1:A:744:LEU:HG	1:A:756:PHE:CZ	2.45	0.50
1:A:1123:GLU:HA	1:A:1126:HIS:HB3	1.92	0.50
1:B:138:GLU:OE2	1:B:234:ARG:HB2	2.11	0.50
1:B:372:VAL:HG11	1:B:468:TYR:CG	2.46	0.50
1:A:228:PRO:HB2	1:A:748:GLN:NE2	2.25	0.50
1:A:846:ALA:HB1	1:A:851:GLN:O	2.12	0.50
1:B:207:SER:HB2	1:B:208:ARG:CZ	2.41	0.50
1:B:421:VAL:CG1	1:B:425:GLY:HA2	2.41	0.50
1:B:429:PRO:CG	1:B:430:GLY:N	2.74	0.50
1:B:613:LEU:HD23	1:B:613:LEU:C	2.36	0.50
1:A:98:HIS:HB3	1:A:157:LEU:HB2	1.94	0.50
1:A:107:THR:HG22	1:A:108:GLN:N	2.27	0.50
1:A:207:SER:HB2	1:A:208:ARG:CZ	2.42	0.50
1:A:647:LEU:HD12	1:A:901:LEU:HD23	1.94	0.50
1:B:73:THR:O	1:B:74:THR:HB	2.12	0.50
1:B:651:ASN:HB2	1:B:775:SER:O	2.11	0.50
1:B:484:ASP:HA	1:B:928:GLN:HE22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1076:LEU:HB3	1:B:1079:ARG:HB2	1.94	0.50
1:B:1125:ALA:O	1:B:1127:GLU:N	2.45	0.50
1:A:151:ASP:HB3	1:A:154:ARG:HB2	1.93	0.50
1:A:521:ARG:HD2	1:A:1011:ASN:O	2.11	0.50
1:A:651:ASN:HB2	1:A:775:SER:C	2.37	0.50
1:A:733:LEU:HD22	1:A:759:ASP:HB3	1.94	0.50
1:A:849:ARG:O	1:A:850:ASN:HB2	2.10	0.50
1:A:948:LEU:HD22	1:A:955:HIS:CE1	2.46	0.50
1:B:108:GLN:O	1:B:109:ALA:C	2.54	0.50
1:B:421:VAL:HG11	1:B:425:GLY:HA2	1.94	0.50
1:B:1070:VAL:HG22	1:B:1122:LEU:CD1	2.41	0.50
1:B:1127:GLU:C	1:B:1127:GLU:CD	2.80	0.50
1:A:1049:LEU:H	1:B:477:ILE:HG23	1.77	0.49
1:B:151:ASP:HB3	1:B:154:ARG:HB2	1.94	0.49
1:B:415:VAL:HG13	1:B:418:ASN:CG	2.37	0.49
1:A:108:GLN:O	1:A:109:ALA:C	2.55	0.49
1:A:421:VAL:HG11	1:A:425:GLY:HA2	1.94	0.49
1:A:495:THR:HG22	1:A:495:THR:O	2.13	0.49
1:B:107:THR:HG22	1:B:108:GLN:N	2.28	0.49
1:A:99:GLY:HA3	1:A:156:LEU:HD23	1.92	0.49
1:A:174:THR:HG23	1:A:175:PHE:N	2.25	0.49
1:A:415:VAL:HG13	1:A:418:ASN:CG	2.38	0.49
1:A:1070:VAL:HG13	1:A:1122:LEU:HD11	1.94	0.49
1:B:277:ALA:HB3	1:B:321:ASP:OD1	2.12	0.49
1:A:174:THR:HG22	1:A:231:PHE:HB3	1.95	0.49
1:A:536:PHE:CD1	1:A:536:PHE:C	2.89	0.49
1:A:647:LEU:HG	1:A:778:LEU:HD11	1.94	0.49
1:B:31:ILE:HG23	1:B:32:GLU:N	2.26	0.49
1:B:539:MET:CE	1:B:655:SER:H	2.25	0.49
1:B:647:LEU:HG	1:B:778:LEU:HD11	1.95	0.49
1:B:853:PRO:HB2	1:B:856:LEU:HB2	1.93	0.49
1:A:613:LEU:C	1:A:613:LEU:HD23	2.38	0.49
1:A:619:ASN:O	1:A:623:VAL:HG13	2.12	0.49
1:A:654:MET:HE3	1:A:973:MET:SD	2.53	0.49
1:B:612:ALA:O	1:B:615:THR:HG23	2.12	0.49
1:B:857:LEU:HD22	1:B:861:ASP:HB3	1.95	0.49
1:B:739:ILE:HG22	1:B:739:ILE:O	2.11	0.49
1:A:879:ASN:HD22	1:A:898:ASN:HD21	1.60	0.49
1:B:471:ARG:HE	1:B:933:TRP:HZ2	1.60	0.49
1:A:125:PHE:CD2	1:A:255:ARG:HA	2.47	0.49
1:A:283:THR:CG2	1:A:420:GLN:HE21	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:ALA:HB2	1:A:575:TYR:H	1.78	0.49
1:A:680:VAL:HG13	1:A:985:ILE:HD11	1.95	0.49
1:B:807:ARG:NH1	1:B:873:LEU:HD11	2.27	0.49
1:A:975:ALA:HA	1:A:1031:ALA:HB3	1.93	0.49
1:A:428:VAL:CB	1:A:429:PRO:CD	2.81	0.48
1:A:1127:GLU:OE2	1:A:1128:ALA:HA	2.13	0.48
1:B:847:LEU:HD23	1:B:852:LEU:HD12	1.95	0.48
1:A:67:VAL:HG22	1:A:86:THR:HG22	1.95	0.48
1:B:107:THR:CG2	1:B:470:GLU:OE2	2.60	0.48
1:A:203:MET:CE	1:A:218:HIS:HD2	2.23	0.48
1:A:1076:LEU:HB3	1:A:1079:ARG:HB2	1.94	0.48
1:A:1125:ALA:C	1:A:1127:GLU:N	2.67	0.48
1:B:89:HIS:CD2	1:B:660:PRO:HG3	2.48	0.48
1:A:73:THR:O	1:A:74:THR:HB	2.11	0.48
1:A:1127:GLU:CD	1:A:1127:GLU:C	2.82	0.48
1:B:1050:CYS:O	1:B:1054:ARG:HB2	2.13	0.48
1:A:107:THR:CG2	1:A:470:GLU:OE2	2.62	0.48
1:B:283:THR:CG2	1:B:420:GLN:HE21	2.19	0.48
1:B:632:MET:HE2	1:B:903:TYR:HB3	1.96	0.48
1:B:1091:LEU:O	1:B:1092:LEU:HD23	2.13	0.48
1:A:611:GLU:O	1:A:615:THR:HG22	2.13	0.48
1:A:630:GLN:HG2	1:A:634:ASN:ND2	2.29	0.48
1:B:429:PRO:HD2	1:B:431:PHE:HD1	1.78	0.48
1:B:98:HIS:HB3	1:B:157:LEU:HB2	1.96	0.47
1:A:654:MET:O	1:A:773:VAL:HG13	2.14	0.47
1:B:125:PHE:CD2	1:B:255:ARG:HA	2.49	0.47
1:B:354:ALA:C	1:B:356:ALA:H	2.20	0.47
1:B:471:ARG:NE	1:B:933:TRP:CZ2	2.82	0.47
1:A:385:LEU:HB3	1:A:409:LEU:HB3	1.96	0.47
1:A:440:VAL:HG21	1:A:528:ALA:HB2	1.96	0.47
1:B:778:LEU:HD23	1:B:911:ILE:HG22	1.97	0.47
1:A:1050:CYS:O	1:A:1054:ARG:HB2	2.14	0.47
1:B:24:ARG:HB3	1:B:191:VAL:HG22	1.96	0.47
1:B:174:THR:HG23	1:B:196:VAL:HG13	1.95	0.47
1:B:536:PHE:C	1:B:536:PHE:CD1	2.92	0.47
1:B:847:LEU:C	1:B:847:LEU:HD13	2.39	0.47
1:B:348:PHE:O	1:B:349:GLU:C	2.56	0.47
1:B:723:PHE:CB	1:B:999:GLN:HB2	2.45	0.47
1:A:503:THR:O	1:A:507:ARG:HG2	2.14	0.47
1:A:538:THR:HG21	1:A:663:CYS:HA	1.95	0.47
1:A:539:MET:CE	1:A:655:SER:H	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:THR:O	1:A:496:ASP:HB3	2.14	0.47
1:A:857:LEU:O	1:A:858:SER:O	2.33	0.47
1:A:1005:SER:HA	4:A:2048:HOH:O	2.15	0.47
1:B:278:LEU:HD22	1:B:321:ASP:OD1	2.15	0.47
1:B:632:MET:HB3	1:B:903:TYR:CZ	2.49	0.47
1:B:852:LEU:O	1:B:853:PRO:C	2.55	0.47
1:A:14:PRO:O	1:A:65:VAL:HG23	2.15	0.47
1:A:847:LEU:HD13	1:A:847:LEU:O	2.14	0.47
1:B:314:LEU:HD21	1:B:703:PHE:CD2	2.49	0.47
1:B:654:MET:O	1:B:773:VAL:HG13	2.15	0.47
1:B:775:SER:HB2	1:B:1003:TRP:HB3	1.96	0.47
1:B:1069:PHE:N	1:B:1101:MET:HE1	2.29	0.47
1:A:462:LEU:O	1:A:465:MET:HB3	2.15	0.47
1:A:1050:CYS:SG	1:B:476:VAL:CG2	3.03	0.47
1:B:352:ASP:CG	1:B:357:ARG:HE	2.18	0.47
1:B:652:HIS:CE1	1:B:777:VAL:HG22	2.50	0.47
1:B:975:ALA:HA	1:B:1031:ALA:HB3	1.97	0.47
1:A:24:ARG:HB3	1:A:191:VAL:HG22	1.97	0.47
1:A:718:MET:O	1:A:719:PHE:C	2.58	0.47
1:A:138:GLU:OE2	1:A:234:ARG:HB2	2.14	0.46
1:A:1076:LEU:HD22	1:A:1079:ARG:HD3	1.97	0.46
1:B:485:VAL:O	1:B:489:VAL:HG23	2.15	0.46
1:B:471:ARG:HD2	1:B:959:TRP:O	2.15	0.46
1:B:668:LEU:HD13	1:B:668:LEU:C	2.39	0.46
1:A:222:GLY:O	1:A:225:PHE:HB2	2.16	0.46
1:A:1049:LEU:C	1:A:1051:GLU:N	2.71	0.46
1:A:1125:ALA:O	1:A:1127:GLU:N	2.47	0.46
1:A:369:ALA:HA	1:A:468:TYR:CD1	2.50	0.46
1:A:1091:LEU:O	1:A:1092:LEU:HD23	2.15	0.46
1:A:348:PHE:O	1:A:349:GLU:C	2.58	0.46
1:A:864:THR:O	1:A:868:ILE:HG12	2.14	0.46
1:B:83:LEU:HG	1:B:756:PHE:HB3	1.98	0.46
1:B:707:PHE:C	1:B:709:PRO:HD2	2.40	0.46
1:A:590:GLN:O	1:A:601:GLY:O	2.34	0.46
1:B:69:VAL:HA	1:B:198:PRO:HG2	1.97	0.46
1:B:590:GLN:O	1:B:601:GLY:O	2.34	0.46
1:B:651:ASN:HB2	1:B:775:SER:C	2.41	0.46
1:A:352:ASP:CG	1:A:357:ARG:HE	2.19	0.46
1:B:14:PRO:O	1:B:65:VAL:HG23	2.15	0.46
1:B:1050:CYS:HB3	1:B:1054:ARG:NH2	2.26	0.46
1:A:415:VAL:C	1:A:417:ALA:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:TYR:O	1:B:553:ALA:HB2	2.15	0.46
1:A:183:LYS:HE3	1:A:192:HIS:NE2	2.31	0.46
1:A:319:ALA:HB2	1:A:686:LEU:CD1	2.46	0.46
1:B:122:HIS:ND1	1:B:449:GLU:OE1	2.48	0.46
1:A:69:VAL:HA	1:A:198:PRO:HG2	1.98	0.46
1:B:340:THR:HG22	1:B:345:TRP:NE1	2.28	0.46
1:A:473:ASP:HB2	1:A:518:LEU:HD21	1.98	0.45
1:A:816:GLY:O	1:A:820:LYS:HG3	2.15	0.45
1:B:1068:VAL:HG12	1:B:1101:MET:CE	2.46	0.45
1:A:65:VAL:HG22	1:A:66:ALA:N	2.29	0.45
1:A:354:ALA:C	1:A:356:ALA:H	2.23	0.45
1:A:507:ARG:HH11	1:A:507:ARG:HG3	1.80	0.45
1:B:150:LEU:O	1:B:152:PRO:HD3	2.17	0.45
1:B:708:GLN:HE22	1:B:711:LEU:HD23	1.82	0.45
1:B:1069:PHE:HD2	1:B:1122:LEU:CD2	2.29	0.45
1:A:32:GLU:H	1:A:32:GLU:HG3	1.43	0.45
1:A:340:THR:HG22	1:A:345:TRP:NE1	2.23	0.45
1:B:997:VAL:O	1:B:997:VAL:HG13	2.15	0.45
1:A:122:HIS:ND1	1:A:449:GLU:OE1	2.45	0.45
1:A:471:ARG:HD2	1:A:959:TRP:O	2.16	0.45
1:B:816:GLY:O	1:B:820:LYS:HG3	2.17	0.45
1:B:849:ARG:O	1:B:851:GLN:HG3	2.16	0.45
1:A:702:ASN:HB2	4:A:2031:HOH:O	2.17	0.45
1:B:354:ALA:C	1:B:356:ALA:N	2.74	0.45
1:B:630:GLN:HG2	1:B:634:ASN:ND2	2.32	0.45
1:B:718:MET:O	1:B:721:ASN:HB2	2.16	0.45
1:A:85:LEU:N	1:A:85:LEU:HD12	2.32	0.45
1:B:600:MET:HA	1:B:600:MET:HE2	1.98	0.45
1:A:471:ARG:NE	1:A:933:TRP:CZ2	2.84	0.45
1:A:485:VAL:O	1:A:489:VAL:HG23	2.16	0.45
1:B:415:VAL:C	1:B:417:ALA:H	2.24	0.45
1:B:743:SER:CB	1:B:746:ALA:HB3	2.46	0.45
1:A:718:MET:O	1:A:721:ASN:HB2	2.17	0.45
1:A:936:GLN:O	1:A:941:LEU:HA	2.16	0.45
1:B:18:LEU:C	1:B:18:LEU:CD1	2.90	0.45
1:B:952:VAL:CG1	1:B:953:ASP:N	2.80	0.45
1:A:609:ASN:OD1	1:A:612:ALA:N	2.48	0.45
1:A:707:PHE:C	1:A:709:PRO:HD2	2.42	0.45
1:A:1119:ASP:O	1:A:1122:LEU:HG	2.17	0.45
1:B:85:LEU:HD12	1:B:85:LEU:N	2.32	0.45
1:A:852:LEU:HD23	1:A:853:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1069:PHE:HD2	1:A:1122:LEU:CD2	2.30	0.45
1:B:385:LEU:HB3	1:B:409:LEU:HB3	1.98	0.45
1:B:706:GLN:HG2	4:B:2034:HOH:O	2.16	0.45
1:B:1119:ASP:OD1	1:B:1122:LEU:HD11	2.17	0.45
1:A:45:ASP:CG	1:A:45:ASP:O	2.59	0.44
1:A:319:ALA:CB	1:A:686:LEU:CD1	2.94	0.44
1:A:497:VAL:HA	1:A:498:PRO:HD3	1.83	0.44
1:A:624:VAL:O	1:A:628:VAL:HG23	2.16	0.44
1:A:723:PHE:HB3	1:A:999:GLN:HB2	1.99	0.44
1:B:335:PHE:HB3	1:B:659:ASP:OD2	2.16	0.44
1:B:519:ARG:HA	1:B:522:HIS:CD2	2.52	0.44
1:A:362:GLY:HA3	1:A:956:PRO:O	2.18	0.44
1:B:42:GLY:HA2	1:B:105:PRO:HG3	1.99	0.44
1:B:270:ASP:OD2	1:B:273:HIS:HB2	2.17	0.44
1:B:521:ARG:HD2	1:B:1011:ASN:O	2.17	0.44
1:A:596:VAL:CG1	1:A:598:THR:HG22	2.46	0.44
1:B:478:VAL:HG12	1:B:478:VAL:O	2.17	0.44
1:B:596:VAL:HG12	1:B:598:THR:CG2	2.44	0.44
1:A:31:ILE:CG2	1:A:32:GLU:N	2.80	0.44
1:B:477:ILE:N	1:B:477:ILE:HD12	2.33	0.44
1:B:847:LEU:HD23	1:B:852:LEU:CD1	2.48	0.44
1:B:857:LEU:HD22	1:B:861:ASP:CB	2.47	0.44
1:A:270:ASP:OD2	1:A:273:HIS:HB2	2.18	0.44
1:A:952:VAL:CG1	1:A:953:ASP:N	2.79	0.44
1:A:857:LEU:C	1:A:858:SER:O	2.60	0.44
1:A:976:ARG:O	1:A:1030:ARG:HB2	2.18	0.44
1:A:985:ILE:HG22	1:A:987:LYS:HE3	1.99	0.44
1:B:201:LEU:HD22	1:B:744:LEU:HD21	2.00	0.44
1:A:1101:MET:O	1:A:1105:THR:HG22	2.18	0.44
1:B:370:GLY:CA	1:B:963:PHE:HZ	2.30	0.44
1:B:467:PHE:O	1:B:471:ARG:HG2	2.17	0.44
1:B:652:HIS:CG	1:B:914:LEU:HD11	2.52	0.44
1:B:803:LYS:HA	1:B:910:PHE:CE2	2.52	0.44
1:B:948:LEU:C	1:B:948:LEU:HD13	2.43	0.44
1:A:346:PRO:HG2	1:A:1032:GLY:C	2.42	0.44
1:B:308:GLY:C	1:B:310:PHE:H	2.26	0.44
1:B:575:TYR:O	1:B:579:THR:HG23	2.17	0.44
1:B:1069:PHE:HA	1:B:1101:MET:CE	2.45	0.44
1:B:551:ASN:CG	1:B:551:ASN:O	2.61	0.44
1:B:612:ALA:HA	1:B:615:THR:CG2	2.48	0.44
1:A:42:GLY:HA2	1:A:105:PRO:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:LEU:HB2	1:A:575:TYR:CE2	2.53	0.43
1:A:917:ILE:HG22	1:A:963:PHE:CD2	2.53	0.43
1:B:831:LYS:H	1:B:831:LYS:HD2	1.83	0.43
1:A:408:PHE:HA	1:A:686:LEU:HD23	2.01	0.43
1:A:1058:SER:O	1:A:1060:GLY:N	2.51	0.43
1:A:1069:PHE:N	1:A:1101:MET:HE1	2.33	0.43
1:B:936:GLN:O	1:B:941:LEU:HA	2.18	0.43
1:A:600:MET:HE2	1:A:600:MET:HA	2.00	0.43
1:A:658:LEU:HD12	1:A:768:PRO:HB2	2.01	0.43
1:B:636:VAL:HG23	1:B:643:PHE:HZ	1.83	0.43
1:B:1078:PRO:HA	1:B:1116:TRP:CD1	2.53	0.43
1:A:67:VAL:HG21	1:A:165:PHE:CE1	2.53	0.43
1:B:524:LYS:HA	1:B:524:LYS:HD3	1.82	0.43
1:B:609:ASN:OD1	1:B:612:ALA:N	2.49	0.43
1:B:610:ARG:HG2	1:B:610:ARG:NH1	2.33	0.43
1:B:728:THR:HA	1:B:765:LEU:O	2.18	0.43
1:A:96:VAL:HA	1:A:158:TYR:HB3	2.01	0.43
1:A:1049:LEU:HB2	1:B:477:ILE:HG23	2.00	0.43
1:A:1070:VAL:CG2	1:A:1122:LEU:HD13	2.48	0.43
1:B:283:THR:OG1	1:B:420:GLN:HB3	2.17	0.43
1:B:869:LYS:O	1:B:873:LEU:HD23	2.19	0.43
1:B:969:LEU:O	1:B:970:ARG:C	2.60	0.43
1:A:473:ASP:C	1:A:475:ALA:H	2.26	0.43
1:A:708:GLN:HE22	1:A:711:LEU:HD23	1.83	0.43
1:A:1127:GLU:O	1:A:1129:GLU:HG2	2.18	0.43
1:B:96:VAL:HA	1:B:158:TYR:HB3	2.01	0.43
1:B:222:GLY:O	1:B:225:PHE:HB2	2.18	0.43
1:B:743:SER:HB3	1:B:746:ALA:HB3	2.00	0.43
1:B:976:ARG:O	1:B:1030:ARG:HB2	2.18	0.43
1:A:18:LEU:C	1:A:18:LEU:CD1	2.91	0.43
1:A:354:ALA:C	1:A:356:ALA:N	2.76	0.43
1:A:970:ARG:CD	4:A:2047:HOH:O	2.67	0.43
1:B:45:ASP:O	1:B:45:ASP:CG	2.62	0.43
1:B:64:ASN:OD1	1:B:334:VAL:HG13	2.18	0.43
1:B:199:LEU:HD12	1:B:199:LEU:HA	1.90	0.43
1:B:476:VAL:C	1:B:477:ILE:CG1	2.91	0.43
1:B:657:THR:HB	1:B:659:ASP:H	1.82	0.43
1:B:776:ARG:HG2	1:B:778:LEU:O	2.19	0.43
1:B:53:VAL:HG13	1:B:59:SER:HA	2.01	0.43
1:B:355:ALA:C	1:B:357:ARG:H	2.27	0.43
1:B:369:ALA:CB	1:B:471:ARG:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LEU:HD12	1:A:469:LEU:HA	1.75	0.43
1:A:881:ILE:HG12	1:A:911:ILE:HD11	1.99	0.43
1:B:183:LYS:HE3	1:B:192:HIS:NE2	2.33	0.43
1:B:778:LEU:CD2	1:B:911:ILE:HG22	2.49	0.43
1:A:740:CYS:HA	1:A:754:SER:HA	1.99	0.43
1:A:850:ASN:C	1:A:852:LEU:H	2.27	0.43
1:B:29:GLU:O	1:B:32:GLU:HG3	2.19	0.43
1:B:493:ASN:HB2	1:B:504:PHE:CE1	2.54	0.43
1:B:1076:LEU:HD22	1:B:1079:ARG:HD3	2.00	0.43
1:A:174:THR:HG23	1:A:196:VAL:HG13	2.00	0.42
1:A:467:PHE:O	1:A:471:ARG:HG2	2.18	0.42
1:A:471:ARG:HE	1:A:933:TRP:HZ2	1.66	0.42
1:A:581:ARG:O	1:A:584:ALA:HB3	2.19	0.42
1:A:610:ARG:HG2	1:A:610:ARG:NH1	2.33	0.42
1:B:12:LYS:HD3	1:B:732:ALA:HB3	2.01	0.42
1:A:53:VAL:HG13	1:A:59:SER:HA	2.01	0.42
1:A:150:LEU:O	1:A:152:PRO:HD3	2.20	0.42
1:B:828:PRO:C	1:B:830:GLY:H	2.25	0.42
1:A:410:VAL:HB	1:A:411:PRO:HD2	2.00	0.42
1:A:612:ALA:HA	1:A:615:THR:CG2	2.49	0.42
1:A:882:ASN:HB3	4:A:2043:HOH:O	2.18	0.42
1:B:13:VAL:HG22	1:B:65:VAL:HA	2.00	0.42
1:B:71:SER:HB2	1:B:81:VAL:HG13	2.01	0.42
1:B:359:ASN:OD1	1:B:956:PRO:HA	2.20	0.42
1:B:503:THR:O	1:B:507:ARG:HG2	2.19	0.42
1:B:985:ILE:HG22	1:B:987:LYS:HE3	2.02	0.42
1:B:65:VAL:HG22	1:B:66:ALA:N	2.33	0.42
1:A:89:HIS:NE2	1:A:660:PRO:HG3	2.34	0.42
1:A:90:TYR:CE2	1:A:160:VAL:HG12	2.55	0.42
1:A:355:ALA:C	1:A:357:ARG:H	2.28	0.42
1:A:587:GLU:CD	1:A:594:GLN:HG3	2.44	0.42
1:A:698:VAL:O	1:A:698:VAL:HG13	2.19	0.42
1:A:803:LYS:HA	1:A:910:PHE:CE2	2.54	0.42
1:B:596:VAL:CG1	1:B:598:THR:HG22	2.43	0.42
1:B:632:MET:HG3	1:B:903:TYR:CD2	2.54	0.42
1:B:847:LEU:HD13	1:B:847:LEU:O	2.19	0.42
1:B:881:ILE:HG12	1:B:911:ILE:HD11	2.01	0.42
1:B:917:ILE:HG22	1:B:963:PHE:CD2	2.54	0.42
1:A:54:GLY:CA	1:A:342:ILE:HD11	2.47	0.42
1:A:422:ASP:OD1	1:A:422:ASP:C	2.62	0.42
1:A:575:TYR:O	1:A:579:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1052:GLN:O	1:B:1056:ILE:HG13	2.19	0.42
1:A:279:PRO:HG2	1:A:282:ILE:HB	2.02	0.42
1:A:607:ILE:HA	1:A:612:ALA:CB	2.50	0.42
1:B:159:LEU:CG	1:B:161:VAL:HG22	2.37	0.42
1:B:581:ARG:O	1:B:584:ALA:HB3	2.20	0.42
1:B:31:ILE:CG2	1:B:32:GLU:N	2.82	0.42
1:B:410:VAL:HB	1:B:411:PRO:HD2	2.01	0.42
1:B:469:LEU:HA	1:B:469:LEU:HD12	1.75	0.42
1:B:924:PRO:HA	1:B:925:PRO:HD2	1.95	0.42
1:A:601:GLY:O	1:A:602:ARG:HB2	2.19	0.42
1:A:833:PRO:HD3	1:A:853:PRO:HG2	2.02	0.42
1:A:1104:LEU:O	1:A:1105:THR:C	2.61	0.42
1:B:279:PRO:HG2	1:B:282:ILE:HB	2.02	0.42
1:B:587:GLU:CD	1:B:594:GLN:HG3	2.44	0.42
1:B:707:PHE:O	1:B:708:GLN:C	2.63	0.42
1:B:762:ARG:HG3	1:B:762:ARG:HH11	1.85	0.42
1:A:668:LEU:C	1:A:668:LEU:HD13	2.44	0.42
1:A:948:LEU:HD13	1:A:948:LEU:C	2.45	0.42
1:B:67:VAL:HG23	1:B:69:VAL:HG13	2.02	0.42
1:B:804:PRO:HD2	1:B:910:PHE:CZ	2.55	0.42
1:B:1049:LEU:C	1:B:1051:GLU:N	2.73	0.42
1:B:1083:LEU:O	1:B:1102:MET:HE1	2.20	0.42
1:A:596:VAL:HG12	1:A:598:THR:CG2	2.48	0.41
1:A:707:PHE:O	1:A:708:GLN:C	2.63	0.41
1:A:1092:LEU:C	1:A:1094:ASP:N	2.77	0.41
1:A:1123:GLU:O	1:A:1126:HIS:HB3	2.20	0.41
1:B:406:ARG:CD	1:B:690:HIS:HD2	2.33	0.41
1:B:422:ASP:OD1	1:B:422:ASP:C	2.61	0.41
1:B:870:LYS:HE2	1:B:874:ASP:OD2	2.19	0.41
1:A:83:LEU:HG	1:A:756:PHE:HB3	2.02	0.41
1:A:1068:VAL:HG12	1:A:1101:MET:CE	2.49	0.41
1:B:589:LEU:O	1:B:590:GLN:HB2	2.20	0.41
1:B:607:ILE:HA	1:B:612:ALA:CB	2.50	0.41
1:B:778:LEU:HD23	1:B:778:LEU:HA	1.93	0.41
1:B:879:ASN:HA	1:B:898:ASN:OD1	2.20	0.41
1:A:29:GLU:O	1:A:32:GLU:HG3	2.20	0.41
1:A:602:ARG:HG2	1:B:443:THR:O	2.19	0.41
1:A:750:ALA:HB1	1:A:751:PRO:HD2	2.01	0.41
1:B:494:GLN:NE2	1:B:494:GLN:CA	2.59	0.41
1:B:601:GLY:O	1:B:602:ARG:HB2	2.21	0.41
1:B:948:LEU:HD13	1:B:948:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1101:MET:O	1:B:1105:THR:HG22	2.20	0.41
1:A:98:HIS:HD2	1:A:157:LEU:HD13	1.84	0.41
1:A:131:ARG:HB2	1:A:134:ASP:OD2	2.21	0.41
1:A:551:ASN:O	1:A:551:ASN:CG	2.64	0.41
1:A:823:HIS:HB2	1:A:840:PRO:HB3	2.03	0.41
1:A:846:ALA:HB1	1:A:851:GLN:C	2.45	0.41
1:A:1030:ARG:HH11	1:A:1030:ARG:HD3	1.76	0.41
1:B:1092:LEU:C	1:B:1094:ASP:N	2.77	0.41
1:A:408:PHE:HB3	1:A:530:ARG:HD2	2.02	0.41
1:A:924:PRO:O	1:A:949:MET:HE1	2.21	0.41
1:B:174:THR:CG2	1:B:175:PHE:N	2.83	0.41
1:B:421:VAL:HG22	1:B:425:GLY:C	2.46	0.41
1:B:714:ARG:HH11	1:B:714:ARG:HG2	1.85	0.41
1:B:1058:SER:O	1:B:1060:GLY:N	2.54	0.41
1:A:53:VAL:N	1:A:340:THR:O	2.47	0.41
1:A:778:LEU:HD22	1:A:906:HIS:CE1	2.56	0.41
1:B:32:GLU:HG3	1:B:32:GLU:H	1.44	0.41
1:B:831:LYS:HA	1:B:838:PRO:HA	2.03	0.41
1:A:67:VAL:HG23	1:A:69:VAL:HG13	2.02	0.41
1:A:1078:PRO:HA	1:A:1116:TRP:CD1	2.56	0.41
1:B:258:ASP:OD1	1:B:262:ARG:NH1	2.53	0.41
1:B:321:ASP:O	1:B:322:ALA:C	2.64	0.41
1:B:1124:VAL:O	1:B:1127:GLU:HB3	2.21	0.41
1:A:477:ILE:HD12	1:A:477:ILE:H	1.86	0.41
1:A:1050:CYS:SG	1:B:476:VAL:HG21	2.61	0.41
1:A:1124:VAL:O	1:A:1127:GLU:HB3	2.21	0.41
1:B:42:GLY:HA2	1:B:105:PRO:CG	2.50	0.41
1:B:90:TYR:CE2	1:B:160:VAL:HG12	2.54	0.41
1:B:266:HIS:CE1	1:B:273:HIS:CE1	3.08	0.41
1:B:1104:LEU:O	1:B:1105:THR:C	2.62	0.41
1:A:279:PRO:HA	4:A:2013:HOH:O	2.20	0.41
1:B:53:VAL:CG1	1:B:59:SER:HA	2.51	0.41
1:B:624:VAL:O	1:B:628:VAL:HG23	2.20	0.41
1:B:921:SER:HA	1:B:960:THR:O	2.20	0.41
1:A:723:PHE:HB2	1:A:999:GLN:HB2	2.02	0.41
1:A:776:ARG:HG2	1:A:778:LEU:O	2.21	0.41
1:A:890:GLU:HG2	1:A:968:LEU:HD13	2.02	0.41
1:B:39:ALA:HB3	1:B:48:VAL:CG1	2.50	0.41
1:B:177:HIS:CD2	1:B:180:GLY:HA3	2.56	0.41
1:B:415:VAL:C	1:B:417:ALA:N	2.79	0.41
1:B:1031:ALA:HA	1:B:1035:CYS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1119:ASP:O	1:B:1122:LEU:HG	2.20	0.41
1:A:13:VAL:O	1:A:13:VAL:HG13	2.20	0.40
1:A:524:LYS:HA	1:A:524:LYS:HD3	1.81	0.40
1:A:589:LEU:O	1:A:590:GLN:HB2	2.20	0.40
1:A:714:ARG:HH11	1:A:714:ARG:HG2	1.86	0.40
1:B:924:PRO:O	1:B:949:MET:HE1	2.21	0.40
1:B:1054:ARG:HD2	1:B:1093:GLU:OE1	2.21	0.40
1:A:71:SER:HB2	1:A:81:VAL:HG13	2.04	0.40
1:A:223:GLU:OE1	1:A:223:GLU:HA	2.21	0.40
1:A:451:LEU:HD12	1:A:451:LEU:HA	1.93	0.40
1:A:519:ARG:HA	1:A:522:HIS:CD2	2.55	0.40
1:A:1054:ARG:HD2	1:A:1093:GLU:OE1	2.20	0.40
1:B:899:GLN:OE1	1:B:899:GLN:HA	2.22	0.40
1:B:1109:LEU:HD12	1:B:1109:LEU:HA	1.98	0.40
1:A:24:ARG:HH21	1:A:27:PRO:HB3	1.85	0.40
1:A:345:TRP:C	1:A:347:LEU:N	2.79	0.40
1:B:86:THR:OG1	1:B:762:ARG:NH1	2.54	0.40
1:B:131:ARG:HA	1:B:132:PRO:HD3	1.95	0.40
1:B:225:PHE:CZ	1:B:744:LEU:HD13	2.55	0.40
1:B:539:MET:HE3	1:B:654:MET:HB2	2.02	0.40
1:A:15:PRO:HB3	1:A:85:LEU:CD2	2.51	0.40
1:B:203:MET:CE	1:B:218:HIS:HD2	2.28	0.40
1:B:507:ARG:HG3	1:B:507:ARG:NH1	2.37	0.40
1:B:98:HIS:HD2	1:B:157:LEU:HD13	1.84	0.40
1:B:393:PRO:HG3	1:B:399:HIS:CE1	2.56	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	1007/1136 (89%)	912 (91%)	81 (8%)	14 (1%)	9	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1011/1136 (89%)	912 (90%)	82 (8%)	17 (2%)	7	32
All	All	2018/2272 (89%)	1824 (90%)	163 (8%)	31 (2%)	8	35

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	428	VAL
1	A	429	PRO
1	A	858	SER
1	A	1128	ALA
1	B	428	VAL
1	B	429	PRO
1	B	1126	HIS
1	B	1128	ALA
1	A	601	GLY
1	A	1077	GLY
1	A	1117	SER
1	A	1126	HIS
1	B	477	ILE
1	B	601	GLY
1	B	755	SER
1	B	1077	GLY
1	B	1117	SER
1	A	473	ASP
1	A	882	ASN
1	B	473	ASP
1	B	756	PHE
1	B	882	ASN
1	A	1054	ARG
1	B	1054	ARG
1	B	738	ALA
1	A	491	ASP
1	A	643	PHE
1	A	938	GLY
1	B	938	GLY
1	B	763	VAL
1	B	838	PRO

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	818/887 (92%)	760 (93%)	58 (7%)	13	43
1	B	819/887 (92%)	763 (93%)	56 (7%)	14	45
All	All	1637/1774 (92%)	1523 (93%)	114 (7%)	14	44

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	34	LEU
1	A	67	VAL
1	A	101	ARG
1	A	104	ASP
1	A	118	ARG
1	A	127	ASP
1	A	136	LYS
1	A	161	VAL
1	A	174	THR
1	A	199	LEU
1	A	201	LEU
1	A	255	ARG
1	A	278	LEU
1	A	340	THR
1	A	342	ILE
1	A	347	LEU
1	A	351	GLN
1	A	372	VAL
1	A	379	THR
1	A	402	PRO
1	A	421	VAL
1	A	432	GLU
1	A	436	THR
1	A	464	LYS
1	A	469	LEU
1	A	477	ILE

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Mol	Chain	Res	Type
1	A	505	ASP
1	A	538	THR
1	A	539	MET
1	A	610	ARG
1	A	615	THR
1	A	620	VAL
1	A	647	LEU
1	A	649	GLU
1	A	657	THR
1	A	672	LEU
1	A	686	LEU
1	A	698	VAL
1	A	721	ASN
1	A	745	THR
1	A	773	VAL
1	A	807	ARG
1	A	811	LEU
1	A	829	ASN
1	A	831	LYS
1	A	853	PRO
1	A	857	LEU
1	A	948	LEU
1	A	950	ASP
1	A	952	VAL
1	A	960	THR
1	A	977	PRO
1	A	1025	VAL
1	A	1038	SER
1	A	1092	LEU
1	A	1093	GLU
1	A	1127	GLU
1	B	10	THR
1	B	32	GLU
1	B	34	LEU
1	B	67	VAL
1	B	101	ARG
1	B	104	ASP
1	B	118	ARG
1	B	127	ASP
1	B	136	LYS
1	B	161	VAL
1	B	174	THR

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Mol	Chain	Res	Type
1	B	199	LEU
1	B	201	LEU
1	B	278	LEU
1	B	340	THR
1	B	342	ILE
1	B	347	LEU
1	B	351	GLN
1	B	372	VAL
1	B	379	THR
1	B	421	VAL
1	B	432	GLU
1	B	436	THR
1	B	464	LYS
1	B	469	LEU
1	B	477	ILE
1	B	494	GLN
1	B	495	THR
1	B	505	ASP
1	B	538	THR
1	B	539	MET
1	B	610	ARG
1	B	615	THR
1	B	620	VAL
1	B	647	LEU
1	B	649	GLU
1	B	657	THR
1	B	672	LEU
1	B	686	LEU
1	B	698	VAL
1	B	721	ASN
1	B	749	THR
1	B	763	VAL
1	B	773	VAL
1	B	807	ARG
1	B	811	LEU
1	B	831	LYS
1	B	853	PRO
1	B	950	ASP
1	B	952	VAL
1	B	960	THR
1	B	977	PRO
1	B	1025	VAL

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Mol	Chain	Res	Type
1	B	1092	LEU
1	B	1093	GLU
1	B	1127	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	102	HIS
1	A	177	HIS
1	A	215	ASN
1	A	218	HIS
1	A	266	HIS
1	A	420	GLN
1	A	450	HIS
1	A	614	HIS
1	A	618	ASN
1	A	619	ASN
1	A	630	GLN
1	A	634	ASN
1	A	677	ASN
1	A	690	HIS
1	A	721	ASN
1	A	748	GLN
1	A	821	GLN
1	A	823	HIS
1	A	837	GLN
1	A	879	ASN
1	A	936	GLN
1	A	1011	ASN
1	A	1084	GLN
1	B	98	HIS
1	B	102	HIS
1	B	177	HIS
1	B	215	ASN
1	B	218	HIS
1	B	266	HIS
1	B	399	HIS
1	B	420	GLN
1	B	450	HIS
1	B	494	GLN
1	B	618	ASN

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Mol	Chain	Res	Type
1	B	630	GLN
1	B	634	ASN
1	B	677	ASN
1	B	690	HIS
1	B	721	ASN
1	B	821	GLN
1	B	837	GLN
1	B	841	GLN
1	B	879	ASN
1	B	936	GLN
1	B	1002	ASN
1	B	1011	ASN
1	B	1084	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1029/1136 (90%)	-0.23	5 (0%) 87 72	13, 34, 68, 79	0
1	B	1031/1136 (90%)	-0.26	11 (1%) 78 57	12, 33, 66, 80	0
All	All	2060/2272 (90%)	-0.24	16 (0%) 82 64	12, 34, 67, 80	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352	ASP	3.8
1	A	1118	THR	3.0
1	B	351	GLN	2.7
1	B	474	GLY	2.5
1	B	356	ALA	2.4
1	A	351	GLN	2.4
1	A	433	GLY	2.4
1	A	1119	ASP	2.4
1	B	1130	ALA	2.3
1	B	1108	ALA	2.3
1	A	352	ASP	2.2
1	B	475	ALA	2.1
1	B	28	SER	2.1
1	B	637	GLU	2.1
1	B	1118	THR	2.0
1	B	1121	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HG	A	2135	1/1	0.87	0.17	24,24,24,24	1
3	HG	A	2134	1/1	0.88	0.21	85,85,85,85	1
3	HG	B	2134	1/1	0.96	0.13	58,58,58,58	1
3	HG	B	2132	1/1	0.97	0.04	57,57,57,57	1
3	HG	A	2132	1/1	0.98	0.03	49,49,49,49	1
3	HG	B	2135	1/1	0.98	0.12	25,25,25,25	1
3	HG	B	2133	1/1	0.99	0.04	66,66,66,66	1
3	HG	A	2133	1/1	0.99	0.06	59,59,59,59	1
2	ZN	B	2131	1/1	0.99	0.02	29,29,29,29	0
2	ZN	A	2131	1/1	1.00	0.04	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.