



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:34 AM UTC

PDB ID : 6VR4 / pdb_00006vr4
Title : Virion-packaged DNA-dependent RNA polymerase of crAss-like phage phi14:2
Authors : Leiman, P.G.; Sokolova, M.L.
Deposited on : 2020-02-06
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

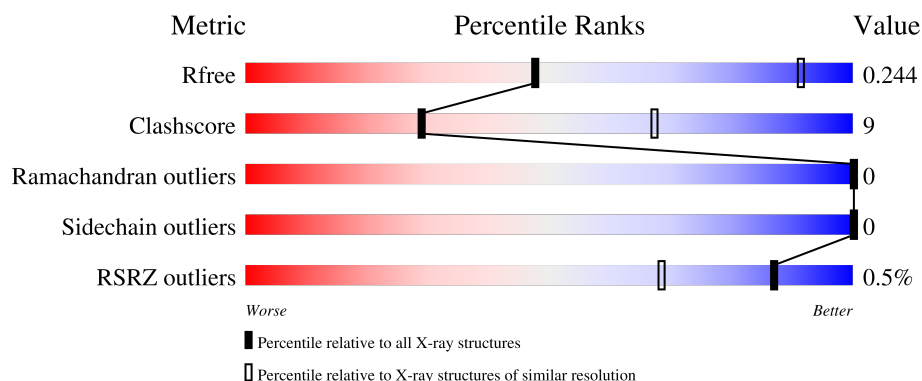
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	2194	 78% 21% .
1	B	2194	 % 78% 21% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34715 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 DNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	2166	Total	C	N	O	S	Se	0	0	0
			17344	11014	2859	3433	1	37			
1	B	2166	Total	C	N	O	S	Se	0	0	0
			17344	11014	2859	3433	1	37			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MSE	-	expression tag	UNP S0A2C3
A	-12	GLY	-	expression tag	UNP S0A2C3
A	-11	SER	-	expression tag	UNP S0A2C3
A	-10	SER	-	expression tag	UNP S0A2C3
A	-9	HIS	-	expression tag	UNP S0A2C3
A	-8	HIS	-	expression tag	UNP S0A2C3
A	-7	HIS	-	expression tag	UNP S0A2C3
A	-6	HIS	-	expression tag	UNP S0A2C3
A	-5	HIS	-	expression tag	UNP S0A2C3
A	-4	HIS	-	expression tag	UNP S0A2C3
A	-3	SER	-	expression tag	UNP S0A2C3
A	-2	GLN	-	expression tag	UNP S0A2C3
A	-1	ASP	-	expression tag	UNP S0A2C3
A	0	PRO	-	expression tag	UNP S0A2C3
B	-13	MSE	-	expression tag	UNP S0A2C3
B	-12	GLY	-	expression tag	UNP S0A2C3
B	-11	SER	-	expression tag	UNP S0A2C3
B	-10	SER	-	expression tag	UNP S0A2C3
B	-9	HIS	-	expression tag	UNP S0A2C3
B	-8	HIS	-	expression tag	UNP S0A2C3
B	-7	HIS	-	expression tag	UNP S0A2C3
B	-6	HIS	-	expression tag	UNP S0A2C3
B	-5	HIS	-	expression tag	UNP S0A2C3
B	-4	HIS	-	expression tag	UNP S0A2C3
B	-3	SER	-	expression tag	UNP S0A2C3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLN	-	expression tag	UNP S0A2C3
B	-1	ASP	-	expression tag	UNP S0A2C3
B	0	PRO	-	expression tag	UNP S0A2C3

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	11	Total Cl 11 11	0	0
2	B	10	Total Cl 10 10	0	0

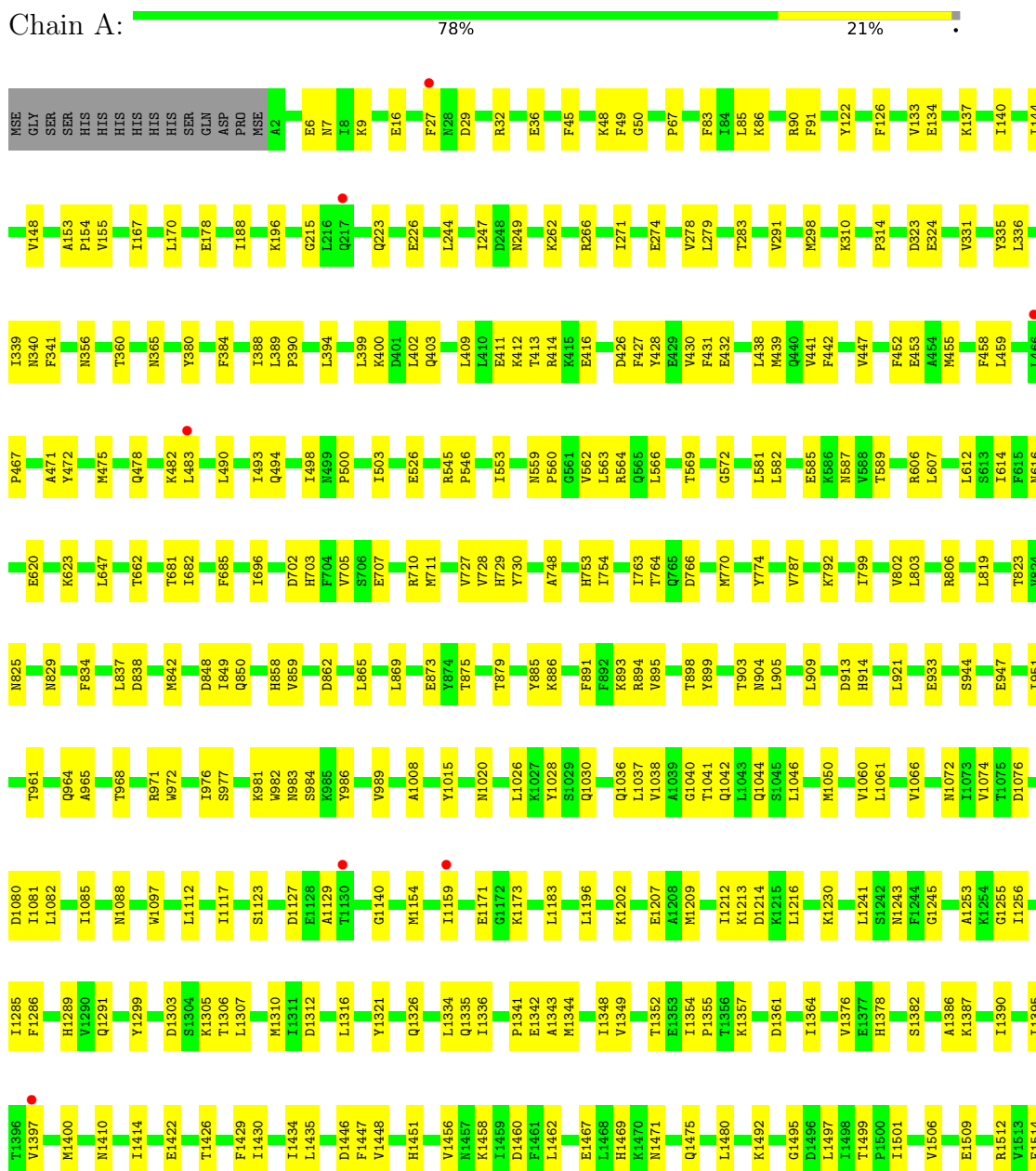
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

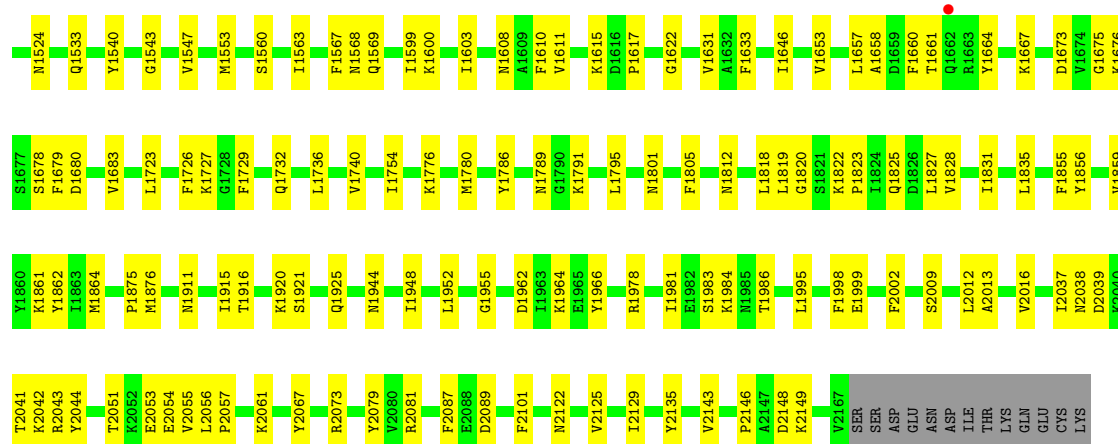
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Na 4 4	0	0
3	B	2	Total Na 2 2	0	0

3 Residue-property plots

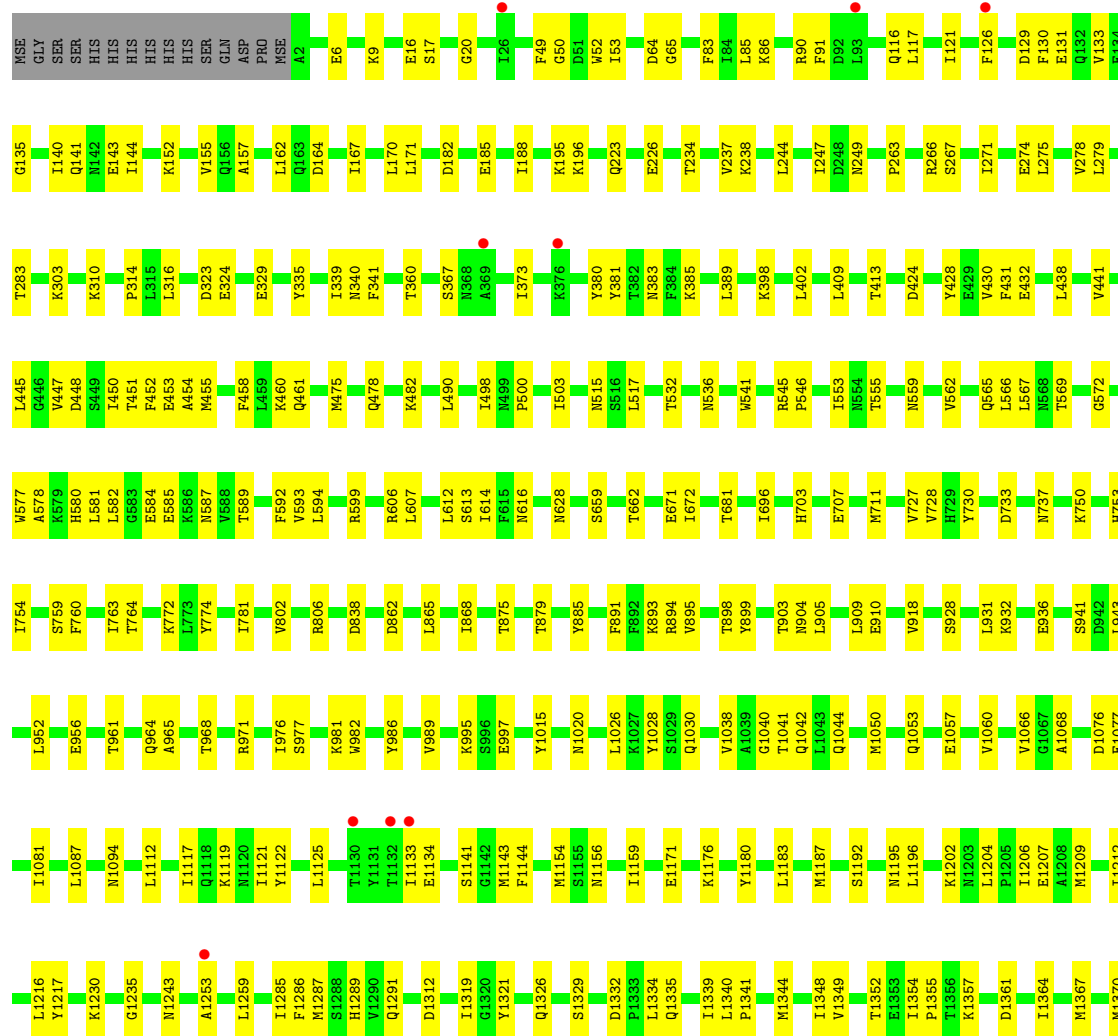
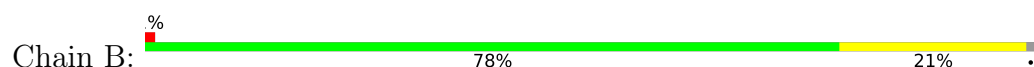
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





● Molecule 1: DNA-dependent RNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	266.44Å 297.18Å 92.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.93 – 3.50 31.93 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (31.93-3.50) 99.6 (31.93-3.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.192 , 0.239 0.199 , 0.244	Depositor DCC
R_{free} test set	4647 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	96.4	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34715	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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: CL, NA

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	0.14	0/17630	0.35	0/23740
1	B	0.14	0/17630	0.35	1/23740 (0.0%)
All	All	0.14	0/35260	0.35	1/47480 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1050	MSE	N-CA-C	-5.81	104.87	111.14

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	17344	0	17141	303	0
1	B	17344	0	17141	302	0
2	A	11	0	0	0	0
2	B	10	0	0	0	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
All	All	34715	0	34282	603	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 9.

All (603) 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:1286:PHE:HB2	1:B:1349:VAL:HB	1.51	0.91
1:A:707:GLU:OE1	1:A:710:ARG:NH2	2.12	0.81
1:A:1286:PHE:HB2	1:A:1349:VAL:HB	1.62	0.81
1:A:1015:TYR:HB3	1:A:1026:LEU:HB2	1.64	0.78
1:B:121:ILE:HG12	1:B:143:GLU:HG2	1.66	0.78
1:B:341:PHE:HB3	1:B:616:ASN:HB2	1.66	0.76
1:B:879:THR:HG21	1:B:891:PHE:HE1	1.50	0.75
1:A:710:ARG:NH1	1:A:748:ALA:O	2.20	0.74
1:A:1046:LEU:HG	1:A:1050:MSE:HE3	1.69	0.74
1:B:711:MSE:HE1	1:B:774:TYR:HE1	1.53	0.74
1:A:564:ARG:HG2	1:A:582:LEU:HD21	1.68	0.74
1:B:1410:ASN:HA	1:B:1418:GLU:HG3	1.70	0.72
1:B:1379:THR:HG22	1:B:1381:LYS:H	1.53	0.72
1:B:116:GLN:NE2	1:B:263:PRO:O	2.22	0.72
1:B:802:VAL:HG13	1:B:1524:ASN:HA	1.72	0.71
1:A:1827:LEU:HD22	1:A:1855:PHE:HE1	1.55	0.71
1:A:1397:VAL:HA	1:A:1400:MSE:HE3	1.72	0.70
1:B:1559:ARG:NH1	1:B:1795:LEU:HD12	2.07	0.69
1:B:727:VAL:HB	1:B:730:TYR:HB3	1.74	0.69
1:B:1015:TYR:HB3	1:B:1026:LEU:HB2	1.75	0.69
1:A:977:SER:HA	1:A:982:TRP:HB2	1.75	0.68
1:B:1171:GLU:O	1:B:1812:ASN:ND2	2.26	0.68
1:A:825:ASN:HD21	1:A:829:ASN:HB3	1.58	0.68
1:B:1827:LEU:HD22	1:B:1855:PHE:HE1	1.57	0.68
1:A:341:PHE:HB3	1:A:616:ASN:HB2	1.74	0.68
1:B:553:ILE:HD12	1:B:612:LEU:HD12	1.76	0.67
1:B:1285:ILE:HD12	1:B:1334:LEU:HD13	1.76	0.67
1:A:360:THR:HA	1:A:838:ASP:HB2	1.77	0.67
1:A:1540:TYR:HE1	1:A:1617:PRO:HG3	1.59	0.67
1:A:27:PHE:HE2	1:A:36:GLU:HG3	1.60	0.67
1:A:802:VAL:HG13	1:A:1524:ASN:HA	1.77	0.66
1:B:1187:MSE:HE3	1:B:1192:SER:HB2	1.77	0.66
1:A:711:MSE:HE1	1:A:774:TYR:HE1	1.60	0.66
1:A:1386:ALA:HB1	1:A:1430:ILE:HD12	1.77	0.66
1:A:553:ILE:HD12	1:A:612:LEU:HD12	1.78	0.66
1:A:1361:ASP:H	1:A:1364:ILE:HD12	1.61	0.65
1:B:303:LYS:HG3	1:B:316:LEU:HD11	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:LEU:HD22	1:B:441:VAL:HG23	1.78	0.65
1:B:977:SER:HA	1:B:982:TRP:HB2	1.77	0.65
1:A:244:LEU:HD12	1:A:271:ILE:HD13	1.79	0.65
1:B:1553:MSE:HG2	1:B:1633:PHE:HB3	1.79	0.65
1:A:490:LEU:HA	1:A:493:ILE:HG22	1.79	0.64
1:A:223:GLN:HB2	1:A:226:GLU:HG3	1.78	0.64
1:B:1332:ASP:OD1	1:B:1357:LYS:NZ	2.28	0.64
1:B:2021:ILE:HD11	1:B:2033:PHE:CD2	2.33	0.64
1:A:335:TYR:CE2	1:A:904:ASN:HB2	2.33	0.63
1:B:545:ARG:HD2	1:B:903:THR:HA	1.80	0.63
1:A:2055:VAL:HG11	1:A:2143:VAL:HG22	1.80	0.63
1:A:278:VAL:HG23	1:A:279:LEU:HD12	1.80	0.63
1:A:983:ASN:OD1	1:A:984:SER:N	2.31	0.63
1:A:1285:ILE:HD11	1:A:1348:ILE:HD11	1.81	0.63
1:A:1462:LEU:HD21	1:A:1475:GLN:HG2	1.81	0.63
1:B:244:LEU:HD12	1:B:271:ILE:HD13	1.80	0.62
1:A:1675:GLY:HA3	1:A:2043:ARG:HH12	1.64	0.62
1:B:90:ARG:NH1	1:B:1202:LYS:O	2.33	0.62
1:B:711:MSE:HE1	1:B:774:TYR:CE1	2.33	0.62
1:A:262:LYS:HD3	1:B:157:ALA:HB2	1.82	0.62
1:B:1028:TYR:CE2	1:B:1030:GLN:HG2	2.35	0.62
1:B:2055:VAL:HG11	1:B:2143:VAL:HG22	1.82	0.62
1:A:249:ASN:ND2	1:A:453:GLU:OE1	2.32	0.61
1:A:133:VAL:HG12	1:A:137:LYS:HD2	1.81	0.61
1:B:968:THR:HG23	1:B:971:ARG:H	1.64	0.61
1:A:879:THR:HG21	1:A:891:PHE:HE1	1.65	0.61
1:A:1117:ILE:HD12	1:A:1321:TYR:HB3	1.80	0.61
1:A:727:VAL:HB	1:A:730:TYR:HB3	1.82	0.61
1:A:1207:GLU:HG3	1:A:1818:LEU:HB3	1.83	0.61
1:B:9:LYS:HB2	1:B:53:ILE:HA	1.83	0.60
1:B:1506:VAL:HG23	1:B:1646:ILE:HD11	1.83	0.60
1:A:411:GLU:OE2	1:A:414:ARG:NH1	2.29	0.60
1:B:140:ILE:HG23	1:B:188:ILE:HD11	1.82	0.60
1:B:2155:SER:O	1:B:2159:ILE:HG12	2.02	0.60
1:B:1119:LYS:HE3	1:B:1555:VAL:HG21	1.83	0.60
1:A:335:TYR:HE2	1:A:904:ASN:HB2	1.67	0.60
1:B:1754:ILE:HD11	1:B:1820:GLY:HA2	1.84	0.60
1:B:339:ILE:HD11	1:B:614:ILE:HD12	1.83	0.59
1:A:339:ILE:HD11	1:A:614:ILE:HD12	1.84	0.59
1:B:140:ILE:O	1:B:144:ILE:HG12	2.03	0.59
1:B:2146:PRO:HA	1:B:2149:LYS:HE3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1117:ILE:HD12	1:B:1321:TYR:HB3	1.84	0.59
1:A:968:THR:HG23	1:A:971:ARG:H	1.67	0.59
1:B:1243:ASN:HD21	1:B:1352:THR:HB	1.67	0.59
1:A:1754:ILE:HD11	1:A:1820:GLY:HA2	1.85	0.58
1:A:1553:MSE:HG2	1:A:1633:PHE:HB3	1.85	0.58
1:B:1406:ASP:OD1	1:B:1407:HIS:N	2.36	0.58
1:B:587:ASN:HB3	1:B:593:VAL:HG12	1.85	0.58
1:A:1112:LEU:HD11	1:A:1230:LYS:HD2	1.84	0.58
1:B:244:LEU:HD22	1:B:314:PRO:HG2	1.85	0.58
1:A:1026:LEU:HB3	1:A:1028:TYR:CE1	2.39	0.58
1:A:215:GLY:HA3	1:A:1547:VAL:HG11	1.86	0.58
1:B:1112:LEU:HD11	1:B:1230:LYS:HD2	1.85	0.58
1:B:2016:VAL:HG22	1:B:2044:TYR:CZ	2.38	0.58
1:A:402:LEU:HD22	1:A:441:VAL:HG23	1.86	0.58
1:A:438:LEU:HA	1:A:441:VAL:HG12	1.86	0.57
1:A:986:TYR:HA	1:A:989:VAL:HG12	1.87	0.57
1:A:1154:MSE:HE1	1:A:1480:LEU:HB2	1.85	0.57
1:B:360:THR:HA	1:B:838:ASP:HB2	1.86	0.57
1:B:1285:ILE:HD11	1:B:1348:ILE:HD11	1.86	0.57
1:B:1742:LEU:HD13	1:B:1764:ILE:HD13	1.87	0.57
1:A:83:PHE:HB2	1:A:91:PHE:HB3	1.87	0.57
1:B:1259:LEU:HD11	1:B:1339:ILE:HG13	1.85	0.57
1:B:893:LYS:NZ	1:B:1615:LYS:O	2.30	0.57
1:A:1962:ASP:OD2	1:A:1964:LYS:NZ	2.37	0.57
1:A:442:PHE:CD2	1:A:455:MSE:HE1	2.40	0.57
1:A:587:ASN:HD21	1:A:589:THR:HG22	1.68	0.57
1:B:879:THR:HG21	1:B:891:PHE:CE1	2.38	0.57
1:B:283:THR:HA	1:B:335:TYR:HE1	1.69	0.56
1:B:1329:SER:O	1:B:1357:LYS:NZ	2.38	0.56
1:B:460:LYS:HG2	1:B:475:MSE:HE2	1.86	0.56
1:B:1699:SER:HB3	1:B:1724:LYS:HG3	1.86	0.56
1:B:2018:GLN:O	1:B:2021:ILE:HG22	2.05	0.56
1:A:681:THR:HG21	1:A:862:ASP:HA	1.86	0.56
1:A:167:ILE:HG12	1:B:162:LEU:HD22	1.87	0.56
1:B:126:PHE:CE2	1:B:133:VAL:HG11	2.41	0.56
1:A:879:THR:HG21	1:A:891:PHE:CE1	2.40	0.56
1:A:1256:ILE:H	1:A:1256:ILE:HD12	1.71	0.55
1:B:335:TYR:CE2	1:B:904:ASN:HB2	2.41	0.55
1:B:2062:VAL:HG12	1:B:2067:TYR:CE1	2.41	0.55
1:B:383:ASN:ND2	1:B:448:ASP:OD2	2.39	0.55
1:A:1915:ILE:HD12	1:A:1920:LYS:HE2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ILE:HG23	1:A:188:ILE:HD11	1.88	0.55
1:A:1944:ASN:O	1:A:1948:ILE:HG12	2.07	0.55
1:B:1026:LEU:HB3	1:B:1028:TYR:CE1	2.42	0.55
1:A:49:PHE:HB2	1:A:85:LEU:HD22	1.89	0.55
1:A:49:PHE:CZ	1:A:67:PRO:HB3	2.42	0.55
1:A:438:LEU:HD21	1:A:483:LEU:HD13	1.88	0.55
1:B:1682:ILE:HG22	1:B:1723:LEU:HD21	1.88	0.55
1:B:707:GLU:O	1:B:711:MSE:HG3	2.07	0.55
1:B:1683:VAL:HG12	1:B:1723:LEU:HD23	1.87	0.55
1:B:155:VAL:HG11	1:B:170:LEU:HD22	1.87	0.55
1:B:581:LEU:HD22	1:B:607:LEU:HD23	1.89	0.54
1:B:1196:LEU:HD12	1:B:1212:ILE:HG12	1.89	0.54
1:B:1539:THR:HG22	1:B:1617:PRO:HB2	1.89	0.54
1:B:1608:ASN:HA	1:B:1611:VAL:HG12	1.88	0.54
1:B:562:VAL:O	1:B:565:GLN:HG2	2.08	0.54
1:B:1183:LEU:HD23	1:B:1216:LEU:HG	1.88	0.54
1:A:696:ILE:HD13	1:A:865:LEU:HD13	1.90	0.54
1:A:1631:VAL:HG23	1:A:1729:PHE:HB3	1.90	0.54
1:B:452:PHE:O	1:B:455:MSE:HB2	2.08	0.54
1:A:1467:GLU:HB3	1:A:1469:HIS:CE1	2.43	0.54
1:B:566:LEU:O	1:B:569:THR:HG22	2.08	0.54
1:B:1042:GLN:HB3	1:B:1081:ILE:HG12	1.90	0.54
1:A:356:ASN:HB2	1:A:849:ILE:HD11	1.89	0.54
1:A:1171:GLU:HB3	1:A:1173:LYS:HE2	1.89	0.54
1:A:1028:TYR:CE2	1:A:1030:GLN:HG2	2.42	0.54
1:A:1916:THR:O	1:A:1920:LYS:NZ	2.35	0.54
1:B:1944:ASN:O	1:B:1948:ILE:HG12	2.08	0.54
1:B:587:ASN:HD21	1:B:589:THR:HG22	1.73	0.54
1:B:1864:MSE:HE1	1:B:1981:ILE:HD11	1.89	0.54
1:A:566:LEU:O	1:A:569:THR:HG22	2.07	0.53
1:A:1038:VAL:HB	1:A:1044:GLN:HA	1.90	0.53
1:A:1171:GLU:O	1:A:1812:ASN:ND2	2.41	0.53
1:A:707:GLU:O	1:A:711:MSE:HG3	2.08	0.53
1:B:1702:PHE:HB2	1:B:1707:LEU:HD11	1.89	0.53
1:B:931:LEU:HD21	1:B:956:GLU:HG2	1.89	0.53
1:A:2016:VAL:HG22	1:A:2044:TYR:CZ	2.44	0.53
1:B:681:THR:HG21	1:B:862:ASP:HA	1.89	0.53
1:A:1422:GLU:O	1:A:1426:THR:HG23	2.09	0.53
1:B:986:TYR:HA	1:B:989:VAL:HG12	1.91	0.53
1:B:1707:LEU:O	1:B:1711:ILE:HG13	2.09	0.53
1:B:1540:TYR:CE2	1:B:1617:PRO:HG3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2033:PHE:CE2	1:B:2079:TYR:HB2	2.44	0.53
1:A:560:PRO:O	1:A:563:LEU:HB2	2.08	0.53
1:A:1683:VAL:HG12	1:A:1723:LEU:HD23	1.91	0.53
1:B:130:PHE:O	1:B:133:VAL:HG12	2.10	0.52
1:A:2067:TYR:CE2	1:A:2081:ARG:HG3	2.44	0.52
1:A:155:VAL:HG11	1:A:170:LEU:HD22	1.90	0.52
1:A:2013:ALA:O	1:A:2061:LYS:NZ	2.39	0.52
1:B:9:LYS:NZ	1:B:64:ASP:O	2.33	0.52
1:B:753:HIS:ND1	1:B:754:ILE:HG13	2.24	0.52
1:A:1506:VAL:HG23	1:A:1646:ILE:HD11	1.92	0.52
1:A:1378:HIS:CG	1:A:1435:LEU:HD23	2.45	0.52
1:A:1661:THR:HG22	1:A:1678:SER:OG	2.10	0.52
1:B:1786:TYR:CD1	1:B:1795:LEU:HD22	2.44	0.52
1:B:2067:TYR:HB3	1:B:2079:TYR:HB3	1.92	0.52
1:A:662:THR:HG21	1:A:1533:GLN:O	2.10	0.52
1:A:1801:ASN:HA	1:A:1805:PHE:HB2	1.92	0.52
1:B:1040:GLY:HA3	1:B:1253:ALA:HA	1.90	0.52
1:B:1445:ASN:HA	1:B:1448:VAL:HG12	1.92	0.52
1:A:1448:VAL:HA	1:A:1451:HIS:O	2.10	0.52
1:A:1679:PHE:CE1	1:A:1727:LYS:HD2	2.45	0.51
1:B:895:VAL:O	1:B:898:THR:HG22	2.10	0.51
1:A:728:VAL:HG21	1:A:1061:LEU:HD11	1.93	0.51
1:B:1599:ILE:O	1:B:1603:ILE:HG13	2.09	0.51
1:A:885:TYR:CD2	1:A:1066:VAL:HG11	2.45	0.51
1:B:1341:PRO:HG2	1:B:1344:MSE:HG2	1.91	0.51
1:A:837:LEU:HD22	1:A:842:MSE:HB2	1.91	0.51
1:A:1243:ASN:HD21	1:A:1352:THR:HB	1.74	0.51
1:A:1037:LEU:O	1:A:1256:ILE:HD11	2.11	0.51
1:A:283:THR:HA	1:A:335:TYR:HE1	1.75	0.51
1:B:117:LEU:HD12	1:B:144:ILE:HD13	1.92	0.51
1:B:868:ILE:HG21	1:B:1525:LEU:HD23	1.93	0.51
1:B:1207:GLU:OE1	1:B:1819:LEU:HD23	2.11	0.51
1:B:1285:ILE:HG22	1:B:1335:GLN:O	2.11	0.51
1:A:1038:VAL:O	1:A:1044:GLN:HB2	2.11	0.51
1:A:1376:VAL:HB	1:A:1456:VAL:HG21	1.93	0.51
1:B:909:LEU:HD12	1:B:910:GLU:HG3	1.92	0.51
1:B:875:THR:HA	1:B:879:THR:HB	1.92	0.51
1:A:50:GLY:HA2	1:A:86:LYS:HE3	1.93	0.50
1:A:389:LEU:HD11	1:A:500:PRO:HB2	1.93	0.50
1:A:426:ASP:O	1:A:430:VAL:HG22	2.11	0.50
1:B:976:ILE:HG23	1:B:981:LYS:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1509:GLU:OE2	1:B:1512:ARG:NH1	2.44	0.50
1:A:442:PHE:HD2	1:A:455:MSE:HE1	1.75	0.50
1:A:1036:GLN:O	1:A:1255:GLY:HA3	2.11	0.50
1:B:249:ASN:ND2	1:B:453:GLU:OE2	2.43	0.50
1:B:455:MSE:HE2	1:B:517:LEU:HD11	1.93	0.50
1:B:1357:LYS:HE2	1:B:1497:LEU:O	2.12	0.50
1:A:498:ILE:HG23	1:A:503:ILE:HG23	1.92	0.50
1:A:1400:MSE:HG2	1:A:1429:PHE:CD2	2.47	0.50
1:A:2044:TYR:O	1:A:2057:PRO:HD3	2.11	0.50
1:A:2146:PRO:HA	1:A:2149:LYS:HE3	1.92	0.50
1:B:129:ASP:OD1	1:B:130:PHE:N	2.44	0.50
1:A:711:MSE:HE1	1:A:774:TYR:CE1	2.43	0.50
1:B:131:GLU:OE1	1:B:196:LYS:NZ	2.44	0.50
1:B:1235:GLY:HA2	1:B:1371:LEU:HD13	1.93	0.50
1:A:1471:ASN:HB3	1:A:1475:GLN:HB2	1.94	0.50
1:A:898:THR:HG23	1:A:899:TYR:HD1	1.77	0.50
1:A:1827:LEU:HD12	1:A:1995:LEU:HB3	1.94	0.50
1:A:6:GLU:HA	1:A:16:GLU:HA	1.94	0.50
1:A:1312:ASP:HB2	1:A:1460:ASP:HA	1.94	0.50
1:B:49:PHE:HB2	1:B:85:LEU:HD22	1.92	0.50
1:B:182:ASP:OD1	1:B:182:ASP:N	2.42	0.50
1:B:1026:LEU:HB3	1:B:1028:TYR:CD1	2.47	0.50
1:A:1921:SER:O	1:A:1925:GLN:HG3	2.12	0.49
1:A:244:LEU:HD22	1:A:314:PRO:HG2	1.94	0.49
1:A:569:THR:HG23	1:A:572:GLY:H	1.77	0.49
1:A:1285:ILE:HG22	1:A:1335:GLN:O	2.12	0.49
1:A:1983:SER:HA	1:A:1986:THR:HG22	1.94	0.49
1:B:140:ILE:HG21	1:B:185:GLU:HA	1.93	0.49
1:B:1572:LEU:HG	1:B:1582:THR:HG21	1.92	0.49
1:B:164:ASP:HB3	1:B:167:ILE:HG12	1.94	0.49
1:A:1828:VAL:HA	1:A:1831:ILE:HG22	1.94	0.49
1:A:2038:ASN:OD1	1:A:2039:ASP:N	2.45	0.49
1:B:133:VAL:HG13	1:B:135:GLY:H	1.76	0.49
1:B:1835:LEU:HD21	1:B:2012:LEU:HD12	1.93	0.49
1:B:1522:GLY:HA2	1:B:1526:LYS:HB3	1.93	0.49
1:A:399:LEU:HD11	1:A:493:ILE:HG23	1.94	0.49
1:A:1608:ASN:HA	1:A:1611:VAL:HG12	1.93	0.49
1:A:1657:LEU:O	1:A:1661:THR:HG23	2.12	0.49
1:B:458:PHE:CZ	1:B:482:LYS:HG3	2.47	0.49
1:B:545:ARG:HD3	1:B:546:PRO:CD	2.42	0.49
1:B:1409:PHE:HE2	1:B:1425:ILE:HD13	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LYS:NZ	1:A:416:GLU:HG3	2.28	0.49
1:A:1390:ILE:HG13	1:A:1395:ILE:HD12	1.95	0.49
1:A:1599:ILE:O	1:A:1603:ILE:HG13	2.13	0.49
1:B:1828:VAL:HB	1:B:1855:PHE:CZ	2.47	0.49
1:B:2038:ASN:OD1	1:B:2039:ASP:N	2.45	0.49
1:A:45:PHE:O	1:A:49:PHE:HB3	2.12	0.49
1:A:1202:LYS:O	1:A:1978:ARG:NH2	2.44	0.49
1:B:223:GLN:HB2	1:B:226:GLU:HG3	1.94	0.49
1:B:1916:THR:O	1:B:1920:LYS:NZ	2.46	0.49
1:A:459:LEU:O	1:A:475:MSE:HA	2.13	0.48
1:A:1569:GLN:HB2	1:A:1776:LYS:HD2	1.95	0.48
1:B:1423:SER:O	1:B:1427:GLU:HB2	2.13	0.48
1:B:1053:GLN:NE2	1:B:1087:LEU:O	2.41	0.48
1:A:1026:LEU:HB3	1:A:1028:TYR:CD1	2.49	0.48
1:B:234:THR:HG21	1:B:329:GLU:OE1	2.13	0.48
1:B:1855:PHE:CZ	1:B:1859:VAL:HG21	2.48	0.48
1:B:1983:SER:HA	1:B:1986:THR:HG22	1.94	0.48
1:A:140:ILE:O	1:A:144:ILE:HG12	2.14	0.48
1:A:581:LEU:HD22	1:A:607:LEU:HD23	1.93	0.48
1:A:976:ILE:HG23	1:A:981:LYS:HB2	1.96	0.48
1:A:2051:THR:OG1	1:A:2053:GLU:OE2	2.31	0.48
1:B:806:ARG:HD2	1:B:1524:ASN:O	2.13	0.48
1:A:1653:VAL:HG12	1:A:1723:LEU:HD11	1.95	0.48
1:B:905:LEU:HD11	1:B:1094:ASN:HB3	1.94	0.48
1:B:1285:ILE:HD11	1:B:1348:ILE:CD1	2.42	0.48
1:A:806:ARG:HD2	1:A:1524:ASN:O	2.14	0.48
1:A:1543:GLY:HA2	1:A:1610:PHE:HD1	1.79	0.48
1:A:1855:PHE:CZ	1:A:1859:VAL:HG21	2.48	0.48
1:A:1154:MSE:HE1	1:A:1480:LEU:HD22	1.95	0.48
1:A:1430:ILE:HD13	1:A:1434:ILE:HD12	1.96	0.48
1:A:2087:PHE:HE1	1:A:2089:ASP:HB2	1.79	0.48
1:B:577:TRP:CZ3	1:B:672:ILE:HD11	2.48	0.48
1:B:628:ASN:OD1	1:B:1667:LYS:NZ	2.45	0.48
1:B:898:THR:HG23	1:B:899:TYR:HD1	1.79	0.48
1:B:1430:ILE:HG23	1:B:1435:LEU:HD23	1.96	0.48
1:B:1631:VAL:HG23	1:B:1729:PHE:HB3	1.96	0.48
1:A:895:VAL:O	1:A:898:THR:HG22	2.13	0.48
1:B:1761:LYS:HG3	1:B:2156:LEU:HD22	1.96	0.48
1:A:439:MSE:HA	1:A:455:MSE:HE3	1.95	0.47
1:A:647:LEU:HD21	1:A:859:VAL:HG23	1.96	0.47
1:A:1999:GLU:O	1:A:2002:PHE:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:ALA:O	1:B:582:LEU:HG	2.14	0.47
1:B:703:HIS:HB3	1:B:754:ILE:HD13	1.94	0.47
1:B:1867:PHE:CD2	1:B:1869:PRO:HD2	2.49	0.47
1:A:921:LEU:HD23	1:A:1074:VAL:HG21	1.96	0.47
1:A:148:VAL:HG21	1:A:178:GLU:HB2	1.96	0.47
1:A:1076:ASP:N	1:A:1080:ASP:O	2.40	0.47
1:B:447:VAL:HG12	1:B:450:ILE:HB	1.97	0.47
1:B:662:THR:HG21	1:B:1533:GLN:O	2.13	0.47
1:B:1348:ILE:HD13	1:B:1367:MSE:SE	2.63	0.47
1:B:1382:SER:HB3	1:B:1435:LEU:HD11	1.96	0.47
1:A:1876:MSE:HE1	1:A:1911:ASN:HB3	1.95	0.47
1:B:728:VAL:HG23	1:B:1068:ALA:O	2.15	0.47
1:B:961:THR:O	1:B:1060:VAL:HG11	2.15	0.47
1:A:1040:GLY:HA3	1:A:1253:ALA:HA	1.97	0.47
1:A:1819:LEU:HD12	1:A:1856:TYR:HD1	1.79	0.47
1:A:1915:ILE:HD13	1:A:1966:TYR:HE2	1.79	0.47
1:A:394:LEU:HD12	1:A:500:PRO:HG2	1.97	0.47
1:B:1736:LEU:O	1:B:1740:VAL:HG23	2.15	0.47
1:B:1828:VAL:HA	1:B:1831:ILE:HG22	1.96	0.47
1:A:585:GLU:OE2	1:A:606:ARG:NH2	2.46	0.47
1:A:944:SER:HB3	1:A:947:GLU:HB2	1.96	0.47
1:A:964:GLN:HE21	1:A:965:ALA:H	1.63	0.47
1:A:2148:ASP:OD1	1:A:2149:LYS:N	2.48	0.47
1:B:335:TYR:HE2	1:B:904:ASN:HB2	1.80	0.47
1:B:389:LEU:HD11	1:B:500:PRO:HB2	1.97	0.47
1:B:1159:ILE:HG12	1:B:1801:ASN:HB2	1.96	0.47
1:B:1471:ASN:HA	1:B:1475:GLN:OE1	2.14	0.47
1:B:1076:ASP:OD1	1:B:1077:GLU:N	2.43	0.47
1:A:1196:LEU:HB3	1:A:1212:ILE:HG21	1.96	0.47
1:B:141:GLN:HE22	1:B:182:ASP:HB3	1.79	0.47
1:B:323:ASP:OD1	1:B:324:GLU:N	2.48	0.47
1:B:1207:GLU:OE2	1:B:1217:TYR:OH	2.25	0.47
1:B:1407:HIS:HB2	1:B:1410:ASN:HB3	1.96	0.47
1:A:48:LYS:HB3	1:A:85:LEU:HD13	1.97	0.47
1:A:323:ASP:OD1	1:A:324:GLU:N	2.48	0.47
1:A:1316:LEU:HD12	1:A:1336:ILE:HB	1.97	0.46
1:B:424:ASP:N	1:B:424:ASP:OD1	2.48	0.46
1:B:1195:ASN:HB2	1:B:1929:TYR:CG	2.50	0.46
1:B:274:GLU:O	1:B:278:VAL:HG12	2.15	0.46
1:B:438:LEU:HA	1:B:441:VAL:HG12	1.96	0.46
1:A:134:GLU:OE2	1:A:196:LYS:HE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:PRO:HB2	1:A:471:ALA:HB2	1.97	0.46
1:A:909:LEU:N	1:A:913:ASP:OD2	2.41	0.46
1:A:1213:LYS:HG3	1:A:1214:ASP:N	2.30	0.46
1:B:409:LEU:O	1:B:413:THR:HG23	2.14	0.46
1:A:1072:ASN:HD22	1:A:1088:ASN:H	1.63	0.46
1:A:7:ASN:OD1	1:A:9:LYS:HG2	2.16	0.46
1:A:711:MSE:HE2	1:A:711:MSE:HB3	1.80	0.46
1:A:1285:ILE:HD11	1:A:1348:ILE:CD1	2.46	0.46
1:B:17:SER:OG	1:B:20:GLY:N	2.46	0.46
1:B:1514:PHE:HE1	1:B:1711:ILE:HG21	1.80	0.46
1:B:1312:ASP:HB2	1:B:1460:ASP:HA	1.96	0.46
1:A:545:ARG:HD3	1:A:546:PRO:CD	2.46	0.46
1:A:823:THR:HG23	1:A:850:GLN:NE2	2.31	0.46
1:A:1289:HIS:CE1	1:A:1291:GLN:HB3	2.50	0.46
1:A:1387:LYS:HA	1:A:1390:ILE:HG22	1.97	0.46
1:B:451:THR:HG23	1:B:454:ALA:H	1.81	0.46
1:B:1679:PHE:O	1:B:1683:VAL:HG13	2.15	0.46
1:A:875:THR:HA	1:A:879:THR:HB	1.98	0.46
1:A:1285:ILE:HD12	1:A:1334:LEU:HD13	1.97	0.46
1:A:1680:ASP:HA	1:A:1683:VAL:HG22	1.98	0.46
1:B:9:LYS:HD3	1:B:52:TRP:O	2.16	0.46
1:B:1805:PHE:O	1:B:1809:ILE:HG12	2.16	0.46
1:B:1999:GLU:O	1:B:2002:PHE:HB3	2.16	0.46
1:A:1354:ILE:HG22	1:A:1355:PRO:HD3	1.98	0.46
1:B:532:THR:HG22	1:B:541:TRP:CD1	2.51	0.46
1:A:478:GLN:CD	1:A:482:LYS:HE2	2.40	0.45
1:A:819:LEU:HB3	1:A:834:PHE:HE1	1.82	0.45
1:A:1303:ASP:N	1:A:1303:ASP:OD1	2.47	0.45
1:B:1361:ASP:OD1	1:B:1364:ILE:HB	2.16	0.45
1:B:1568:ASN:HA	1:B:1780:MSE:SE	2.66	0.45
1:B:1984:LYS:HD2	1:B:2101:PHE:CZ	2.51	0.45
1:B:2016:VAL:O	1:B:2062:VAL:HG23	2.16	0.45
1:B:152:LYS:HG3	1:B:171:LEU:HD12	1.98	0.45
1:B:303:LYS:HA	1:B:316:LEU:HD12	1.98	0.45
1:B:1586:LYS:HD3	1:B:1586:LYS:HA	1.79	0.45
1:B:2044:TYR:O	1:B:2057:PRO:HD3	2.17	0.45
1:A:1082:LEU:HB2	1:A:1085:ILE:HG12	1.99	0.45
1:B:585:GLU:HG3	1:B:593:VAL:HG22	1.98	0.45
1:B:1206:ILE:HA	1:B:1209:MSE:HE3	1.98	0.45
1:A:869:LEU:O	1:A:873:GLU:HG2	2.16	0.45
1:B:398:LYS:O	1:B:402:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:ASP:O	1:A:770:MSE:HG2	2.16	0.45
1:A:1303:ASP:OD1	1:A:1306:THR:OG1	2.22	0.45
1:B:266:ARG:HG3	1:B:267:SER:N	2.32	0.45
1:B:380:TYR:CE1	1:B:447:VAL:HG13	2.52	0.45
1:B:559:ASN:O	1:B:562:VAL:HG12	2.16	0.45
1:B:964:GLN:HE21	1:B:965:ALA:H	1.64	0.45
1:B:1828:VAL:HB	1:B:1855:PHE:CE2	2.51	0.45
1:A:412:LYS:HZ2	1:A:416:GLU:HG3	1.81	0.45
1:A:545:ARG:HD2	1:A:903:THR:HA	1.97	0.45
1:A:1207:GLU:OE1	1:A:1819:LEU:HD23	2.16	0.45
1:A:1540:TYR:CE1	1:A:1617:PRO:HG3	2.46	0.45
1:A:1631:VAL:HG11	1:A:1726:PHE:CE1	2.51	0.45
1:B:1207:GLU:HG3	1:B:1818:LEU:HB3	1.98	0.45
1:B:1319:ILE:HB	1:B:1370:MSE:HG2	1.99	0.45
1:B:1354:ILE:N	1:B:1355:PRO:HD2	2.32	0.45
1:A:894:ARG:HA	1:A:894:ARG:HD3	1.79	0.45
1:B:536:ASN:O	1:B:536:ASN:ND2	2.50	0.45
1:B:1514:PHE:CE2	1:B:1622:GLY:HA2	2.52	0.45
1:A:140:ILE:CG2	1:A:188:ILE:HD11	2.46	0.45
1:A:399:LEU:HD22	1:A:494:GLN:NE2	2.32	0.45
1:A:1041:THR:OG1	1:A:1245:GLY:O	2.22	0.45
1:A:1042:GLN:HB3	1:A:1081:ILE:HG12	1.99	0.45
1:B:428:TYR:O	1:B:432:GLU:HG3	2.16	0.45
1:A:763:ILE:HG22	1:A:764:THR:O	2.17	0.45
1:A:933:GLU:OE1	1:A:933:GLU:N	2.47	0.45
1:B:340:ASN:HA	1:B:367:SER:OG	2.17	0.45
1:B:1141:SER:O	1:B:1144:PHE:HB3	2.17	0.45
1:A:122:TYR:CD1	1:A:126:PHE:HB2	2.52	0.45
1:A:388:ILE:C	1:A:390:PRO:HD3	2.41	0.45
1:B:885:TYR:CD2	1:B:1066:VAL:HG11	2.51	0.45
1:A:2122:ASN:HA	1:A:2125:VAL:HG12	1.98	0.44
1:A:2038:ASN:N	1:A:2041:THR:OG1	2.49	0.44
1:B:1020:ASN:O	1:B:1020:ASN:ND2	2.50	0.44
1:A:1042:GLN:C	1:A:1081:ILE:HD11	2.43	0.44
1:A:1123:SER:HB2	1:A:1600:LYS:HD2	2.00	0.44
1:A:1410:ASN:HA	1:A:1414:ILE:HG23	1.98	0.44
1:A:1660:PHE:O	1:A:1664:TYR:HB2	2.16	0.44
1:A:1828:VAL:HB	1:A:1855:PHE:CZ	2.51	0.44
1:B:659:SER:HA	1:B:671:GLU:HG2	1.99	0.44
1:B:1122:TYR:HA	1:B:1125:LEU:HG	1.99	0.44
1:B:1289:HIS:CE1	1:B:1291:GLN:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1407:HIS:CE1	1:B:1411:ILE:HD11	2.52	0.44
1:A:961:THR:O	1:A:1060:VAL:HG11	2.17	0.44
1:B:1154:MSE:HE1	1:B:1480:LEU:HB2	2.00	0.44
1:A:291:VAL:HG11	1:A:914:HIS:CG	2.52	0.44
1:A:2067:TYR:HB3	1:A:2079:TYR:HB3	1.99	0.44
1:B:1387:LYS:HA	1:B:1390:ILE:HG22	2.00	0.44
1:A:452:PHE:O	1:A:455:MSE:HB2	2.18	0.44
1:A:2037:ILE:HD13	1:A:2054:GLU:OE1	2.18	0.44
1:A:2038:ASN:O	1:A:2042:LYS:HG3	2.18	0.44
1:A:29:ASP:HB3	1:A:32:ARG:HB3	1.99	0.44
1:A:409:LEU:O	1:A:413:THR:HG23	2.18	0.44
1:A:428:TYR:O	1:A:432:GLU:HG3	2.18	0.44
1:A:1861:LYS:HD3	1:A:1955:GLY:HA3	2.00	0.44
1:A:1875:PRO:HB3	1:A:1952:LEU:HD23	2.00	0.44
1:B:121:ILE:HD12	1:B:188:ILE:HD12	2.00	0.44
1:B:763:ILE:HG22	1:B:764:THR:O	2.17	0.44
1:A:1658:ALA:O	1:A:1661:THR:OG1	2.27	0.44
1:B:1133:ILE:HG22	1:B:1134:GLU:N	2.32	0.44
1:B:1631:VAL:HG11	1:B:1726:PHE:CE1	2.53	0.44
1:B:1786:TYR:HD1	1:B:1795:LEU:HD22	1.83	0.44
1:A:1984:LYS:HB2	1:A:1984:LYS:HE2	1.82	0.44
1:A:427:PHE:HB2	1:A:472:TYR:HD1	1.81	0.43
1:A:1831:ILE:HD13	1:A:1999:GLU:HG3	2.00	0.43
1:A:1862:TYR:CZ	1:A:1998:PHE:HB2	2.52	0.43
1:B:498:ILE:HG23	1:B:503:ILE:HG23	1.99	0.43
1:B:584:GLU:HB3	1:B:592:PHE:HE1	1.83	0.43
1:B:594:LEU:O	1:B:599:ARG:NH2	2.50	0.43
1:B:750:LYS:HG2	1:B:760:PHE:HE2	1.82	0.43
1:B:1509:GLU:HA	1:B:1512:ARG:HG2	2.00	0.43
1:A:1426:THR:O	1:A:1430:ILE:HG12	2.18	0.43
1:B:772:LYS:O	1:B:781:ILE:HG21	2.18	0.43
1:B:1801:ASN:HA	1:B:1805:PHE:HB2	2.00	0.43
1:A:1209:MSE:SE	1:A:1212:ILE:HD11	2.68	0.43
1:A:1357:LYS:HE3	1:A:1497:LEU:O	2.18	0.43
1:A:1568:ASN:HA	1:A:1780:MSE:SE	2.69	0.43
1:A:1827:LEU:HD22	1:A:1855:PHE:CE1	2.45	0.43
1:B:445:LEU:HD21	1:B:490:LEU:HD21	2.01	0.43
1:A:1020:ASN:O	1:A:1020:ASN:ND2	2.51	0.43
1:B:1661:THR:HG22	1:B:1678:SER:OG	2.19	0.43
1:B:1915:ILE:HD13	1:B:1966:TYR:HE2	1.83	0.43
1:A:458:PHE:CZ	1:A:482:LYS:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:GLN:HG2	1:A:1341:PRO:HG3	2.00	0.43
1:A:1560:SER:HB2	1:A:1563:ILE:HD11	2.00	0.43
1:A:1831:ILE:O	1:A:1835:LEU:HD13	2.19	0.43
1:B:1156:ASN:HA	1:B:1159:ILE:HG22	2.01	0.43
1:B:2000:GLU:HG3	1:B:2001:GLN:N	2.32	0.43
1:A:893:LYS:NZ	1:A:1615:LYS:O	2.51	0.43
1:A:1736:LEU:O	1:A:1740:VAL:HG23	2.17	0.43
1:A:1864:MSE:HE1	1:A:1981:ILE:HD11	2.01	0.43
1:B:195:LYS:HD2	1:B:238:LYS:HB3	2.00	0.43
1:B:1387:LYS:O	1:B:1390:ILE:HG22	2.18	0.43
1:B:1433:HIS:HD2	1:B:1439:SER:HB3	1.84	0.43
1:B:1703:SER:O	1:B:1707:LEU:HD13	2.19	0.43
1:A:753:HIS:ND1	1:A:754:ILE:HG13	2.34	0.43
1:A:1446:ASP:OD1	1:A:1447:PHE:N	2.52	0.43
1:A:1299:TYR:O	1:A:1307:LEU:HD11	2.18	0.43
1:B:928:SER:HB3	1:B:931:LEU:HD13	2.00	0.43
1:B:1038:VAL:O	1:B:1041:THR:HG22	2.19	0.43
1:A:266:ARG:HG3	1:A:526:GLU:OE2	2.19	0.43
1:A:702:ASP:HA	1:A:705:VAL:HG22	2.00	0.43
1:B:50:GLY:HA2	1:B:86:LYS:HE3	2.00	0.43
1:B:275:LEU:O	1:B:279:LEU:HB2	2.19	0.43
1:B:569:THR:HG23	1:B:572:GLY:H	1.83	0.43
1:B:2027:ILE:HG21	1:B:2032:VAL:HB	1.99	0.43
1:A:559:ASN:O	1:A:562:VAL:HG12	2.17	0.43
1:B:155:VAL:HG21	1:B:170:LEU:HD22	2.01	0.43
1:B:247:ILE:HG21	1:B:310:LYS:HB2	2.00	0.43
1:B:1553:MSE:HE3	1:B:1633:PHE:HB2	2.01	0.43
1:B:1920:LYS:HE3	1:B:1924:PHE:HE2	1.81	0.43
1:A:90:ARG:HD3	1:A:1978:ARG:NH2	2.34	0.42
1:A:274:GLU:O	1:A:278:VAL:HG22	2.19	0.42
1:A:1310:MSE:O	1:A:1458:LYS:HG3	2.18	0.42
1:A:1789:ASN:HB3	1:A:1791:LYS:NZ	2.34	0.42
1:B:1121:ILE:HG13	1:B:1487:VAL:HG11	2.00	0.42
1:A:1326:GLN:HB2	1:A:1501:ILE:HD11	2.01	0.42
1:B:234:THR:HG23	1:B:237:VAL:H	1.83	0.42
1:B:1042:GLN:C	1:B:1081:ILE:HD11	2.44	0.42
1:B:1176:LYS:HG3	1:B:1180:TYR:CE1	2.54	0.42
1:B:1553:MSE:HG3	1:B:1637:ARG:HD2	2.01	0.42
1:B:1831:ILE:O	1:B:1835:LEU:HD13	2.19	0.42
1:A:384:PHE:CE1	1:A:500:PRO:HB3	2.54	0.42
1:B:1329:SER:OG	1:B:1499:THR:O	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1385:LEU:HD12	1:B:1451:HIS:ND1	2.34	0.42
1:B:1911:ASN:ND2	1:B:2089:ASP:OD2	2.48	0.42
1:A:681:THR:OG1	1:A:862:ASP:OD1	2.34	0.42
1:B:1764:ILE:HD12	1:B:2160:LEU:HD21	2.00	0.42
1:B:2122:ASN:HA	1:B:2125:VAL:HG12	2.00	0.42
1:A:439:MSE:HG2	1:A:455:MSE:HG3	2.01	0.42
1:A:848:ASP:OD2	1:A:849:ILE:N	2.51	0.42
1:A:1129:ALA:HB2	1:A:1492:LYS:HG3	2.01	0.42
1:B:733:ASP:OD1	1:B:737:ASN:N	2.51	0.42
1:B:1921:SER:O	1:B:1925:GLN:HG3	2.19	0.42
1:A:682:ILE:HD12	1:A:685:PHE:CZ	2.54	0.42
1:A:799:ILE:O	1:A:803:LEU:HG	2.20	0.42
1:A:972:TRP:CE2	1:A:976:ILE:HD12	2.55	0.42
1:A:1305:LYS:HA	1:A:1305:LYS:HD3	1.75	0.42
1:A:1400:MSE:SE	1:A:1426:THR:HA	2.70	0.42
1:A:1567:PHE:CZ	1:A:1732:GLN:HB3	2.55	0.42
1:B:430:VAL:HG13	1:B:431:PHE:CD2	2.54	0.42
1:B:932:LYS:O	1:B:936:GLU:HG3	2.20	0.42
1:A:403:GLN:HG2	1:A:490:LEU:HB3	2.01	0.42
1:A:703:HIS:O	1:A:707:GLU:HG2	2.20	0.42
1:A:1495:GLY:O	1:A:1499:THR:HG23	2.19	0.42
1:B:1119:LYS:HD3	1:B:1746:ASP:OD2	2.20	0.42
1:A:620:GLU:HG3	1:A:1667:LYS:HD3	2.02	0.42
1:A:1382:SER:HB3	1:A:1435:LEU:HD21	2.02	0.42
1:A:1948:ILE:HG22	1:A:1952:LEU:HD13	2.02	0.42
1:B:1326:GLN:HG2	1:B:1607:LEU:HD22	2.02	0.42
1:B:460:LYS:CG	1:B:475:MSE:HE2	2.50	0.42
1:A:140:ILE:HD12	1:A:140:ILE:H	1.85	0.41
1:B:6:GLU:HA	1:B:16:GLU:HA	2.02	0.41
1:B:567:LEU:HD12	1:B:582:LEU:HD21	2.02	0.41
1:B:1736:LEU:HA	1:B:1779:MSE:HE3	2.02	0.41
1:B:1795:LEU:O	1:B:1799:VAL:HG12	2.20	0.41
1:A:1183:LEU:HD23	1:A:1216:LEU:HG	2.02	0.41
1:A:1344:MSE:HE3	1:A:1344:MSE:HB3	1.93	0.41
1:A:1827:LEU:CD1	1:A:1995:LEU:HB3	2.50	0.41
1:B:1133:ILE:HD11	1:B:1143:MSE:HE1	2.01	0.41
1:A:891:PHE:O	1:A:895:VAL:HG23	2.19	0.41
1:A:1786:TYR:CD1	1:A:1795:LEU:HD22	2.55	0.41
1:B:587:ASN:ND2	1:B:589:THR:HG22	2.35	0.41
1:B:941:SER:HB2	1:B:943:LEU:HD13	2.02	0.41
1:B:545:ARG:NH1	1:B:903:THR:OG1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:891:PHE:O	1:B:895:VAL:HG23	2.20	0.41
1:B:1812:ASN:C	1:B:1814:PRO:HD3	2.46	0.41
1:A:430:VAL:HG23	1:A:431:PHE:CD2	2.55	0.41
1:A:951:ILE:HD11	1:A:1499:THR:HG22	2.01	0.41
1:B:9:LYS:NZ	1:B:65:GLY:HA3	2.34	0.41
1:B:381:TYR:CE2	1:B:385:LYS:HD2	2.55	0.41
1:B:894:ARG:HA	1:B:894:ARG:HD3	1.80	0.41
1:A:155:VAL:HG21	1:A:170:LEU:HD22	2.01	0.41
1:A:331:VAL:O	1:A:335:TYR:N	2.54	0.41
1:A:1159:ILE:HG12	1:A:1801:ASN:HB2	2.03	0.41
1:A:1299:TYR:HE1	1:A:1342:GLU:OE2	2.04	0.41
1:A:1514:PHE:CE2	1:A:1622:GLY:HA2	2.56	0.41
1:B:83:PHE:HB2	1:B:91:PHE:HB3	2.03	0.41
1:B:140:ILE:HD12	1:B:188:ILE:HD11	2.01	0.41
1:B:696:ILE:HD13	1:B:865:LEU:HD13	2.01	0.41
1:B:1287:MSE:HE1	1:B:1371:LEU:HD21	2.02	0.41
1:B:1400:MSE:HG3	1:B:1429:PHE:CD1	2.55	0.41
1:A:1825:GLN:O	1:A:1828:VAL:HG12	2.21	0.41
1:B:759:SER:O	1:B:763:ILE:HG13	2.21	0.41
1:B:1143:MSE:SE	1:B:1483:LEU:HD22	2.70	0.41
1:B:1529:ASP:OD2	1:B:1531:LEU:HB2	2.21	0.41
1:A:380:TYR:CE1	1:A:447:VAL:HG13	2.56	0.41
1:A:1984:LYS:HD2	1:A:2101:PHE:CZ	2.56	0.41
1:B:461:GLN:HE21	1:B:478:GLN:HB2	1.86	0.41
1:B:1768:TYR:CD2	1:B:2159:ILE:HD12	2.56	0.41
1:A:153:ALA:HB3	1:A:154:PRO:HD3	2.03	0.41
1:A:623:LYS:HD3	1:A:623:LYS:HA	1.87	0.41
1:A:729:HIS:CD2	1:A:886:LYS:HA	2.55	0.41
1:A:1008:ALA:N	1:A:1343:ALA:O	2.52	0.41
1:A:1673:ASP:HB3	1:A:1676:LYS:HD2	2.03	0.41
1:A:1679:PHE:O	1:A:1683:VAL:HG13	2.21	0.41
1:B:580:HIS:CE1	1:B:606:ARG:HG2	2.56	0.41
1:B:918:VAL:HG22	1:B:1057:GLU:HB2	2.03	0.41
1:B:952:LEU:HD23	1:B:952:LEU:HA	1.91	0.41
1:B:1286:PHE:HB3	1:B:1340:LEU:HG	2.03	0.41
1:B:1386:ALA:HB1	1:B:1430:ILE:HG12	2.02	0.41
1:B:1543:GLY:HA2	1:B:1610:PHE:HD1	1.86	0.41
1:B:1859:VAL:O	1:B:1863:ILE:HG13	2.21	0.41
1:B:2118:LEU:HD23	1:B:2118:LEU:HA	1.94	0.41
1:A:545:ARG:HD3	1:A:546:PRO:HD3	2.03	0.41
1:A:2009:SER:HB3	1:A:2012:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2129:ILE:O	1:A:2135:TYR:HB2	2.20	0.41
1:B:373:ILE:HG21	1:B:515:ASN:HD22	1.86	0.41
1:B:545:ARG:HD3	1:B:546:PRO:HD3	2.02	0.41
1:B:555:THR:HG22	1:B:562:VAL:HG11	2.02	0.41
1:B:995:LYS:HB2	1:B:997:GLU:HG3	2.02	0.41
1:B:1121:ILE:HG21	1:B:1484:TYR:CE1	2.56	0.41
1:B:1180:TYR:OH	1:B:1204:LEU:O	2.33	0.41
1:B:1718:ILE:O	1:B:1722:VAL:HG13	2.20	0.41
1:A:247:ILE:HD13	1:A:310:LYS:HB2	2.03	0.40
1:A:336:LEU:HD23	1:A:545:ARG:HA	2.03	0.40
1:A:682:ILE:HD11	1:A:858:HIS:HA	2.03	0.40
1:A:730:TYR:CD1	1:A:748:ALA:HB2	2.56	0.40
1:A:787:VAL:HG13	1:A:792:LYS:HE3	2.02	0.40
1:B:1119:LYS:HE3	1:B:1555:VAL:CG2	2.49	0.40
1:A:279:LEU:HD23	1:A:298:MSE:SE	2.71	0.40
1:A:400:LYS:HG2	1:A:494:GLN:NE2	2.36	0.40
1:A:1361:ASP:H	1:A:1364:ILE:CD1	2.32	0.40
1:A:1822:LYS:CG	1:A:1823:PRO:HD3	2.51	0.40
1:B:1485:TRP:O	1:B:1489:THR:OG1	2.34	0.40
1:B:2009:SER:HB3	1:B:2012:LEU:HB2	2.02	0.40
1:A:1127:ASP:HA	1:A:1140:GLY:H	1.86	0.40
1:A:1241:LEU:HB3	1:A:1349:VAL:HG22	2.02	0.40
1:A:587:ASN:ND2	1:A:589:THR:HG22	2.34	0.40
1:A:905:LEU:HD23	1:A:1097:TRP:CE3	2.56	0.40
1:A:2056:LEU:HB3	1:A:2057:PRO:HD2	2.04	0.40
1:A:2073:ARG:HB2	1:A:2135:TYR:CD1	2.56	0.40
1:B:1038:VAL:HB	1:B:1044:GLN:HA	2.04	0.40
1:B:1818:LEU:HD13	1:B:1985:ASN:OD1	2.21	0.40
1:A:340:ASN:HD22	1:A:365:ASN:HD21	1.69	0.40
1:A:1509:GLU:HA	1:A:1512:ARG:HG2	2.03	0.40
1:B:612:LEU:HD23	1:B:613:SER:N	2.36	0.40
1:B:965:ALA:HB3	1:B:1028:TYR:HD2	1.87	0.40
1:B:1660:PHE:HE1	1:B:1681:ILE:HB	1.85	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	2164/2194 (99%)	2067 (96%)	97 (4%)	0	100	100
1	B	2164/2194 (99%)	2071 (96%)	93 (4%)	0	100	100
All	All	4328/4388 (99%)	4138 (96%)	190 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	1946/1934 (101%)	1946 (100%)	0	100	100
1	B	1946/1934 (101%)	1946 (100%)	0	100	100
All	All	3892/3868 (101%)	3892 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	160	ASN
1	A	383	ASN
1	A	403	GLN
1	A	440	GLN
1	A	494	GLN

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Mol	Chain	Res	Type
1	A	729	HIS
1	A	800	ASN
1	A	825	ASN
1	A	833	HIS
1	A	904	ASN
1	A	987	GLN
1	A	991	ASN
1	A	1030	GLN
1	A	1101	GLN
1	A	1145	GLN
1	A	1203	ASN
1	A	1326	GLN
1	A	1331	ASN
1	A	1445	ASN
1	A	1625	ASN
1	A	1741	GLN
1	A	1905	ASN
1	A	2108	ASN
1	A	2128	ASN
1	B	440	GLN
1	B	508	ASN
1	B	536	ASN
1	B	605	ASN
1	B	616	ASN
1	B	676	HIS
1	B	829	ASN
1	B	987	GLN
1	B	991	ASN
1	B	1118	GLN
1	B	1581	ASN
1	B	1608	ASN
1	B	1730	GLN
1	B	1737	ASN
1	B	1905	ASN
1	B	2006	ASN
1	B	2128	ASN
1	B	2133	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 27 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	2129/2194 (97%)	-0.13	8 (0%)	88 72	52, 88, 155, 319	0
1	B	2129/2194 (97%)	-0.14	15 (0%)	84 63	48, 82, 155, 452	0
All	All	4258/4388 (97%)	-0.14	23 (0%)	87 68	48, 85, 155, 452	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	PHE	4.5
1	B	1130	THR	3.6
1	A	27	PHE	3.2
1	B	1253	ALA	3.1
1	A	1130	THR	3.1
1	A	1397	VAL	3.0
1	B	369	ALA	2.9
1	B	1453	ILE	2.7
1	A	217	GLN	2.7
1	B	1954	ASN	2.6
1	B	1415	ALA	2.5
1	B	1133	ILE	2.4
1	A	483	LEU	2.4
1	A	466	LEU	2.4
1	B	26	ILE	2.4
1	B	1414	ILE	2.3
1	B	1132	THR	2.3
1	B	93	LEU	2.2
1	B	1660	PHE	2.2
1	B	1411	ILE	2.1
1	A	1662	GLN	2.1
1	B	376	LYS	2.0
1	A	1159	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](#)

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	NA	A	2212	1/1	0.75	0.35	68,68,68,68	0
3	NA	A	2215	1/1	0.80	0.47	91,91,91,91	0
2	CL	A	2211	1/1	0.81	0.23	106,106,106,106	0
2	CL	B	2204	1/1	0.82	0.09	74,74,74,74	0
3	NA	A	2213	1/1	0.84	0.14	54,54,54,54	0
2	CL	B	2210	1/1	0.87	0.18	81,81,81,81	0
3	NA	B	2211	1/1	0.88	0.36	70,70,70,70	0
2	CL	B	2203	1/1	0.89	0.09	73,73,73,73	0
3	NA	B	2212	1/1	0.89	0.37	64,64,64,64	0
2	CL	A	2206	1/1	0.90	0.10	79,79,79,79	0
2	CL	A	2210	1/1	0.91	0.06	94,94,94,94	0
2	CL	B	2205	1/1	0.91	0.07	76,76,76,76	0
2	CL	A	2204	1/1	0.91	0.14	83,83,83,83	0
2	CL	A	2202	1/1	0.91	0.36	96,96,96,96	0
2	CL	A	2209	1/1	0.92	0.11	78,78,78,78	0
2	CL	A	2203	1/1	0.92	0.11	72,72,72,72	0
2	CL	A	2207	1/1	0.92	0.07	80,80,80,80	0
2	CL	B	2202	1/1	0.93	0.16	73,73,73,73	0
2	CL	A	2201	1/1	0.93	0.07	67,67,67,67	0
2	CL	B	2208	1/1	0.93	0.06	80,80,80,80	0
2	CL	A	2205	1/1	0.95	0.13	95,95,95,95	0
2	CL	B	2201	1/1	0.96	0.08	65,65,65,65	0
2	CL	B	2209	1/1	0.96	0.08	81,81,81,81	0
2	CL	A	2208	1/1	0.97	0.05	80,80,80,80	0
2	CL	B	2207	1/1	0.97	0.35	94,94,94,94	0
3	NA	A	2214	1/1	0.98	0.23	49,49,49,49	0
2	CL	B	2206	1/1	0.98	0.04	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.