Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2020 – 02:27 PM BST

PDB ID	:	6VR4
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 following versions of software and data (see references ①) were used in the production of this report:

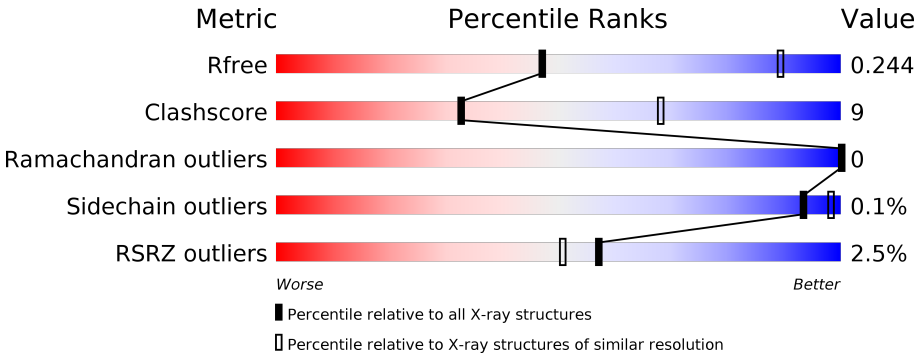
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 Overall quality at a glance (i)

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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on 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 <=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	2% 78% 21%
1	B	2194	3% 78% 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	A	2212	-	-	-	X
3	NA	B	2211	-	-	-	X

2 Entry composition (i)

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 (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

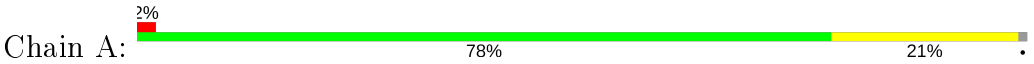
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Na 2 2	0	0
3	A	4	Total Na 4 4	0	0

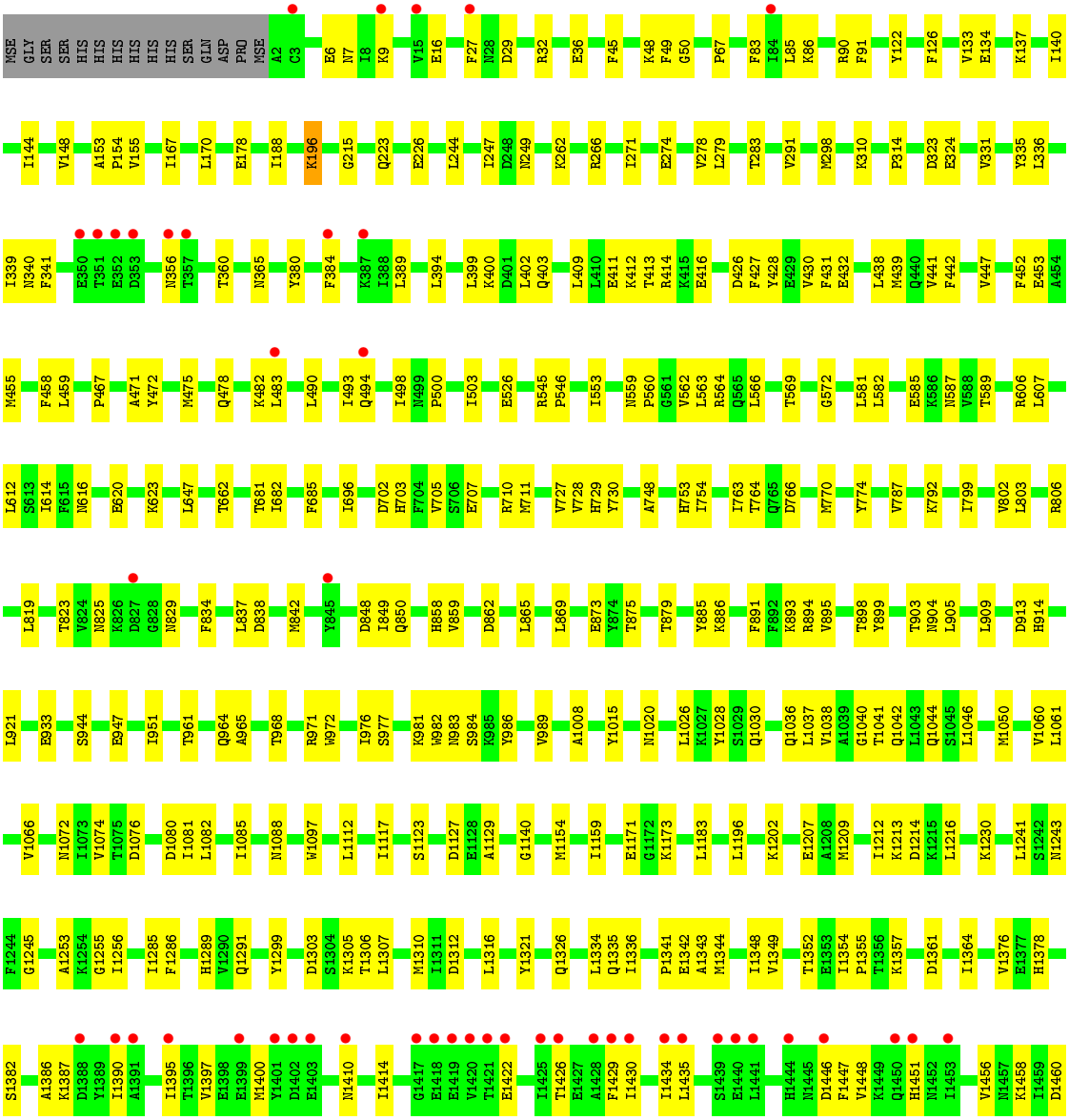
3 Residue-property plots (i)

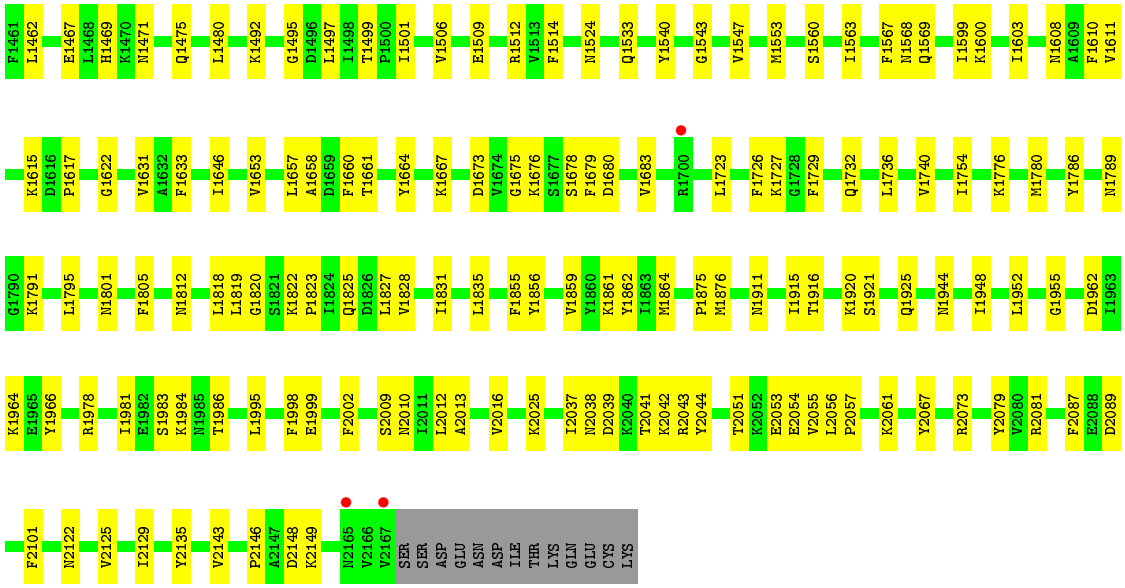
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: DNA-dependent RNA polymerase

Chain A:

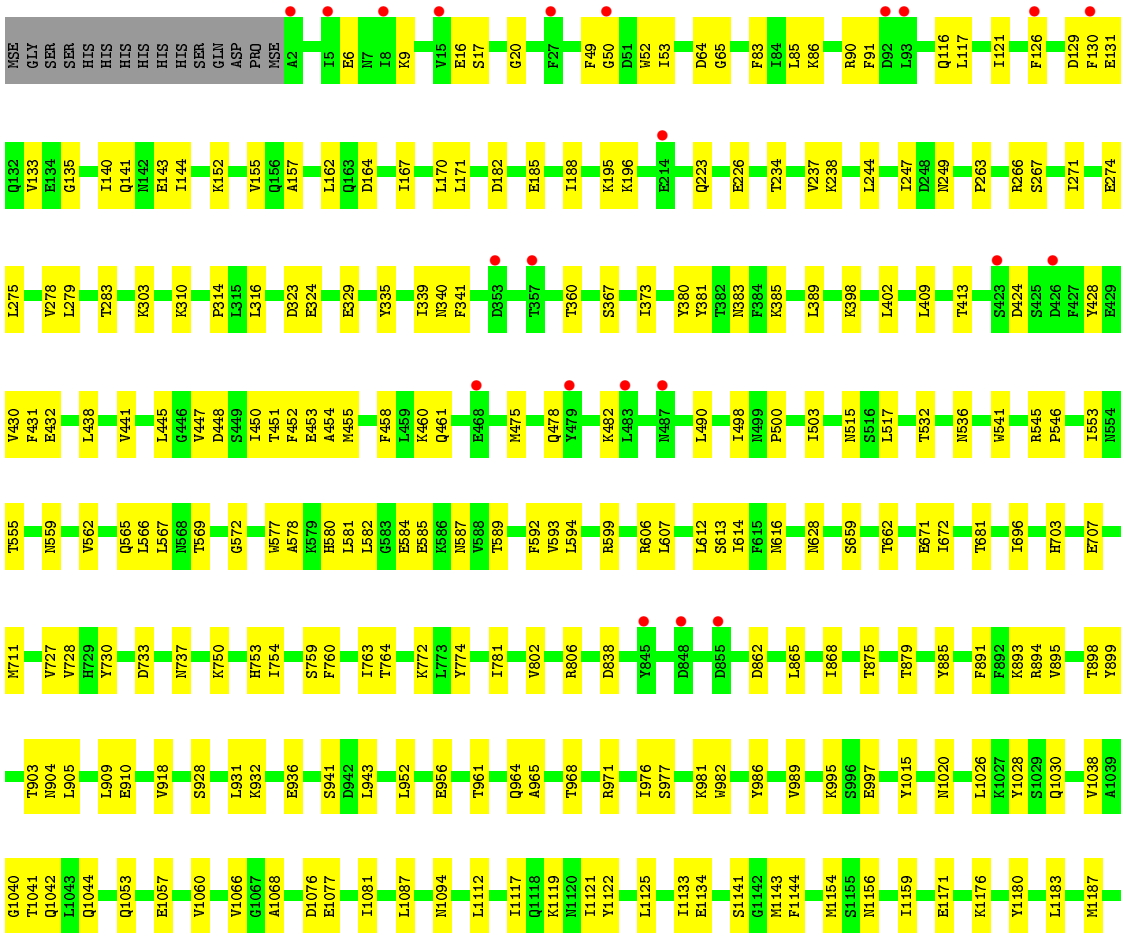


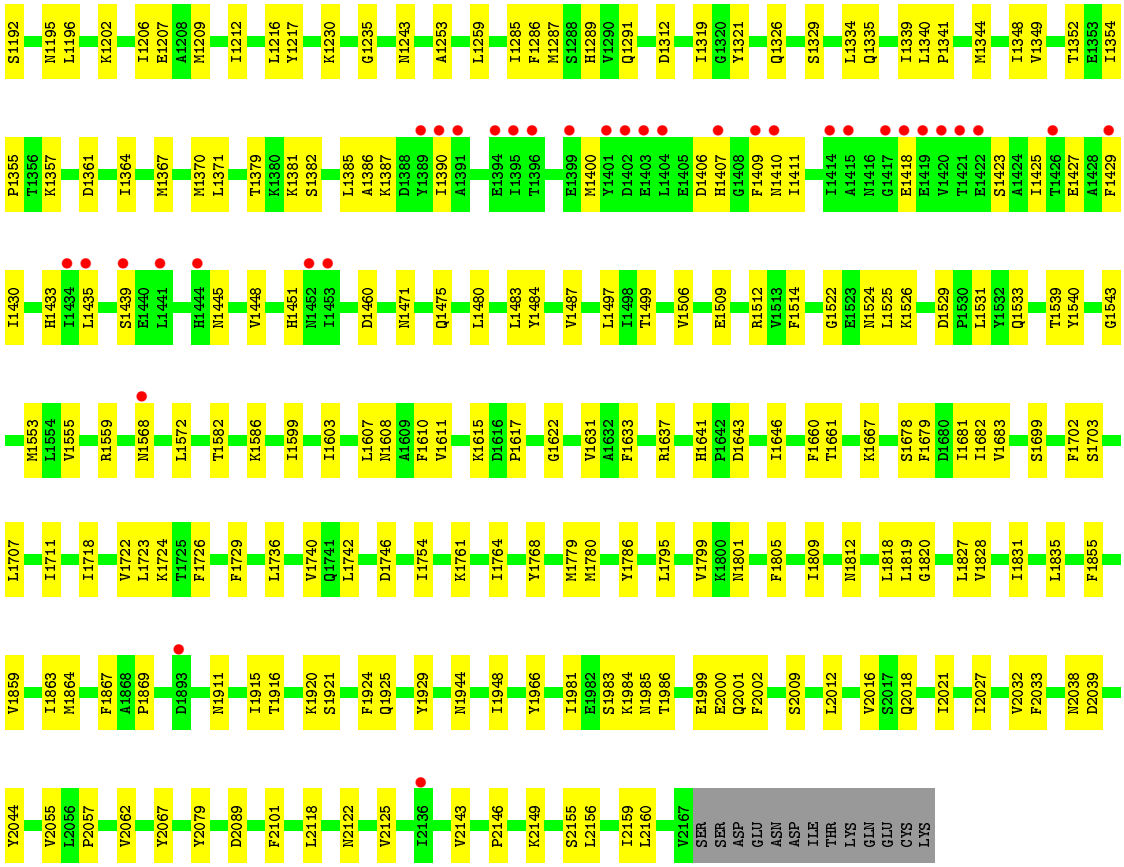




• Molecule 1: DNA-dependent RNA polymerase

Chain B:




S1192 N1195 L1196 K1202 I1206 E1207 A1208 M1209 I1212 L1216 Y1217 K1230 G1235 N1243 A1253 L1259 I1285 F1286 M1287 S1288 H1289 V1290 Q1291 D1312 I1319 G1320 Y1321 Q1326 S1329 L1334 Q1335 I1339 L1340 P1341 M1344 I1348 V1349 T1352 E1353 I1354
P1355 T1356 K1357 D1361 I1364 M1367 M1370 L1371 T1379 K1380 K1381 S1382 L1385 A1386 K1387 D1388 Y1389 I1390 A1391 E1394 I1395 T1396 E1399 M1400 Y1401 D1402 E1403 L1404 E1405 D1406 H1407 G1408 F1409 N1410 I1411 I1414 A1415 N1416 G1417 E1418 E1419 V1420 T1421 E1422 S1423 A1424 I1425 T1426 E1427 A1428 F1429
I1430 H1433 I1434 L1435 S1439 E1440 L1441 H1444 N1445 V1448 H1451 N1452 I1453 D1460 N1471 Q1475 L1480 L1483 Y1484 V1487 L1497 I1498 T1499 V1506 E1509 R1512 V1513 F1514 G1522 E1523 N1524 L1525 K1526 D1529 P1530 L1531 Y1532 Q1533 T1539 Y1540 G1543
M1553 L1554 V1555 R1559 N1568 L1572 T1582 K1586 I1599 I1603 L1607 N1608 A1609 F1610 V1611 K1615 D1616 P1617 G1622 V1631 A1632 F1633 R1637 H1641 P1642 D1643 I1646 F1660 T1661 K1667 S1678 F1679 D1680 I1681 I1682 V1683 S1699 F1702 S1703
L1707 I1711 I1718 V1722 L1723 K1724 T1725 F1726 F1729 L1736 V1740 Q1741 L1742 D1746 I1754 K1761 I1764 Y1768 M1779 M1780 Y1786 L1795 V1799 K1800 N1801 F1805 I1809 N1812 L1818 L1819 G1820 L1827 V1828 I1831 L1835 F1855
V1859 I1863 M1864 F1867 A1868 P1869 D1893 N1911 I1915 T1916 K1920 S1921 F1924 Q1925 Y1929 N1944 I1948 Y1966 I1981 E1982 S1983 K1984 N1985 T1986 E1999 E2000 Q2001 F2002 S2009 L2012 V2016 S2017 Q2018 I2021 I2027 V2032 F2033 N2038 D2039
Y2044 V2055 L2056 P2057 V2062 Y2067 Y2079 D2089 F2101 L2118 N2122 V2125 I2136 V2143 P2146 K2149 S2155 L2156 I2159 L2160 V2167 SER SER ASP GLU ASN ASP ILE THR LYS GLN GLU CYS LYS

4 Data and refinement statistics (i)

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 49.60 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (31.93-3.50) 99.7 (49.60-3.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.192 , 0.239 0.197 , 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)	0.32 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, CL

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	0.26	0/17630	0.44	0/23740
1	B	0.26	0/17630	0.45	0/23740
All	All	0.26	0/35260	0.45	0/47480

There are no bond length outliers.

There are no bond angle outliers.

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	301	0
1	B	17344	0	17141	298	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	597	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 (597) 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:1285:ILE:HD12	1:B:1334:LEU:HD13	1.76	0.67
1:B:553:ILE:HD12	1:B:612:LEU:HD12	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1117:ILE:HD12	1:A:1321:TYR:HB3	1.80	0.61
1:A:879:THR:HG21	1:A:891:PHE:HE1	1.65	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:1506:VAL:HG23	1:B:1646:ILE:HD11	1.83	0.60
1:B:9:LYS:HB2	1:B:53:ILE:HA	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:360:THR:HA	1:B:838:ASP:HB2	1.86	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:1329:SER:O	1:B:1357:LYS:NZ	2.38	0.56
1:B:283:THR:HA	1:B:335:TYR:HE1	1.69	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:B:126:PHE:CE2	1:B:133:VAL:HG11	2.41	0.56
1:A:167:ILE:HG12	1:B:162:LEU:HD22	1.87	0.56
1:A:879:THR:HG21	1:A:891:PHE:CE1	2.40	0.56
1:A:1256:ILE:HD12	1:A:1256:ILE:H	1.71	0.55
1:B:2062:VAL:HG12	1:B:2067:TYR:CE1	2.41	0.55
1:B:335:TYR:CE2	1:B:904:ASN:HB2	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
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:438:LEU:HD21	1:A:483:LEU:HD13	1.88	0.55
1:A:49:PHE:HB2	1:A:85:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:PHE:CZ	1:A:67:PRO:HB3	2.42	0.55
1:B:1682:ILE:HG22	1:B:1723:LEU:HD21	1.88	0.55
1:B:1683:VAL:HG12	1:B:1723:LEU:HD23	1.87	0.55
1:B:707:GLU:O	1:B:711:MSE:HG3	2.07	0.55
1:B:155:VAL:HG11	1:B:170:LEU:HD22	1.87	0.55
1:B:1196:LEU:HD12	1:B:1212:ILE:HG12	1.89	0.54
1:B:581:LEU:HD22	1:B:607:LEU:HD23	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:1183:LEU:HD23	1:B:1216:LEU:HG	1.88	0.54
1:B:562:VAL:O	1:B:565:GLN:HG2	2.08	0.54
1:A:1631:VAL:HG23	1:A:1729:PHE:HB3	1.90	0.54
1:A:696:ILE:HD13	1:A:865:LEU:HD13	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:1042:GLN:HB3	1:B:1081:ILE:HG12	1.90	0.54
1:B:566:LEU:O	1:B:569:THR:HG22	2.08	0.54
1:A:1171:GLU:HB3	1:A:1173:LYS:HE2	1.89	0.54
1:A:356:ASN:HB2	1:A:849:ILE:HD11	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:1864:MSE:HE1	1:B:1981:ILE:HD11	1.89	0.54
1:B:587:ASN:HD21	1:B:589:THR:HG22	1.73	0.54
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:566:LEU:O	1:A:569:THR:HG22	2.07	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:1707:LEU:O	1:B:1711:ILE:HG13	2.09	0.53
1:B:986:TYR:HA	1:B:989:VAL:HG12	1.91	0.53
1:B:1540:TYR:CE2	1:B:1617:PRO:HG3	2.44	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:HG11	1:A:170:LEU:HD22	1.90	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:1801:ASN:HA	1:A:1805:PHE:HB2	1.92	0.52
1:A:662:THR:HG21	1:A:1533:GLN:O	2.10	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:1243:ASN:HD21	1:A:1352:THR:HB	1.74	0.51
1:A:837:LEU:HD22	1:A:842:MSE:HB2	1.91	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: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: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: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: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:A:50:GLY:HA2	1:A:86:LYS:HE3	1.93	0.50
1:B:1509:GLU:OE2	1:B:1512:ARG:NH1	2.44	0.50
1:B:976:ILE:HG23	1:B:981:LYS:HB2	1.92	0.50
1:A:1036:GLN:O	1:A:1255:GLY:HA3	2.11	0.50
1:A:442:PHE:HD2	1:A:455:MSE:HE1	1.75	0.50
1:B:9:LYS:NZ	1:B:64:ASP:O	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:498:ILE:HG23	1:A:503:ILE:HG23	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:1235:GLY:HA2	1:B:1371:LEU:HD13	1.93	0.50
1:B:131:GLU:OE1	1:B:196:LYS:NZ	2.44	0.50
1:A:1471:ASN:HB3	1:A:1475:GLN:HB2	1.94	0.50
1:A:1827:LEU:HD12	1:A:1995:LEU:HB3	1.94	0.50
1:A:898:THR:HG23	1:A:899:TYR:HD1	1.77	0.50
1:A:1312:ASP:HB2	1:A:1460:ASP:HA	1.94	0.50
1:A:6:GLU:HA	1:A:16:GLU:HA	1.94	0.50
1:B:1026:LEU:HB3	1:B:1028:TYR:CD1	2.47	0.50
1:B:182:ASP:OD1	1:B:182:ASP:N	2.42	0.50
1:B:49:PHE:HB2	1:B:85:LEU:HD22	1.92	0.50
1:A:1921:SER:O	1:A:1925:GLN:HG3	2.12	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: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: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: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:A:399:LEU:HD11	1:A:493:ILE:HG23	1.94	0.49
1:B:1409:PHE:HE2	1:B:1425:ILE:HD13	1.78	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:A:1041:THR:OG1	1:A:1245:GLY:O	2.22	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:A:412:LYS:NZ	1:A:416:GLU:HG3	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1202:LYS:O	1:A:1978:ARG:NH2	2.44	0.49
1:A:45:PHE:O	1:A:49:PHE:HB3	2.12	0.49
1:B:223:GLN:HB2	1:B:226:GLU:HG3	1.94	0.49
1:A:1569:GLN:HB2	1:A:1776:LYS:HD2	1.95	0.48
1:A:459:LEU:O	1:A:475:MSE:HA	2.13	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: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:B:234:THR:HG21	1:B:329:GLU:OE1	2.13	0.48
1:A:140:ILE:O	1:A:144:ILE:HG12	2.14	0.48
1:A:2051:THR:OG1	1:A:2053:GLU:OE2	2.31	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: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:1285:ILE:HD11	1:B:1348:ILE:CD1	2.42	0.48
1:B:905:LEU:HD11	1:B:1094:ASN:HB3	1.94	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:806:ARG:HD2	1:A:1524:ASN:O	2.14	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: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: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: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:1999:GLU:O	1:A:2002:PHE:HB3	2.13	0.47
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:B:1867:PHE:CD2	1:B:1869:PRO:HD2	2.49	0.47
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:A:921:LEU:HD23	1:A:1074:VAL:HG21	1.96	0.47
1:A:1076:ASP:N	1:A:1080:ASP:O	2.40	0.47
1:A:148:VAL:HG21	1:A:178:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:964:GLN:HE21	1:A:965:ALA:H	1.63	0.47
1:B:1471:ASN:HA	1:B:1475:GLN:OE1	2.14	0.47
1:B:1159:ILE:HG12	1:B:1801:ASN:HB2	1.96	0.47
1:A:2148:ASP:OD1	1:A:2149:LYS:N	2.48	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:B:389:LEU:HD11	1:B:500:PRO:HB2	1.97	0.47
1:B:335:TYR:HE2	1:B:904:ASN:HB2	1.80	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:1407:HIS:HB2	1:B:1410:ASN:HB3	1.96	0.47
1:B:141:GLN:HE22	1:B:182:ASP:HB3	1.79	0.47
1:B:1916:THR:O	1:B:1920:LYS:NZ	2.46	0.47
1:B:323:ASP:OD1	1:B:324:GLU:N	2.48	0.47
1:A:323:ASP:OD1	1:A:324:GLU:N	2.48	0.47
1:A:48:LYS:HB3	1:A:85:LEU:HD13	1.97	0.47
1:A:1316:LEU:HD12	1:A:1336:ILE:HB	1.97	0.46
1:B:1195:ASN:HB2	1:B:1929:TYR:CG	2.50	0.46
1:B:424:ASP:OD1	1:B:424:ASP:N	2.48	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:1213:LYS:HG3	1:A:1214:ASP:N	2.30	0.46
1:A:134:GLU:OE2	1:A:196:LYS:HE2	2.15	0.46
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: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:1285:ILE:HD11	1:A:1348:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:MSE:HE2	1:A:711:MSE:HB3	1.80	0.46
1:A:7:ASN:OD1	1:A:9:LYS:HG2	2.16	0.46
1:B:1514:PHE:HE1	1:B:1711:ILE:HG21	1.80	0.46
1:B:17:SER:OG	1:B:20:GLY:N	2.46	0.46
1:B:1312:ASP:HB2	1:B:1460:ASP:HA	1.96	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: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:B:1679:PHE:O	1:B:1683:VAL:HG13	2.15	0.46
1:B:451:THR:HG23	1:B:454:ALA:H	1.81	0.46
1:A:1285:ILE:HD12	1:A:1334:LEU:HD13	1.97	0.46
1:A:875:THR:HA	1:A:879:THR:HB	1.98	0.46
1:A:1680:ASP:HA	1:A:1683:VAL:HG22	1.98	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:B:9:LYS:HD3	1:B:52:TRP:O	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:1303:ASP:N	1:A:1303:ASP:OD1	2.47	0.45
1:A:819:LEU:HB3	1:A:834:PHE:HE1	1.82	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:1586:LYS:HD3	1:B:1586:LYS:HA	1.79	0.45
1:B:152:LYS:HG3	1:B:171:LEU:HD12	1.98	0.45
1:B:2044:TYR:O	1:B:2057:PRO:HD3	2.17	0.45
1:B:303:LYS:HA	1:B:316:LEU:HD12	1.98	0.45
1:A:1082:LEU:HB2	1:A:1085:ILE:HG12	1.99	0.45
1:B:1206:ILE:HA	1:B:1209:MSE:HE3	1.98	0.45
1:B:1641:HIS:HD1	1:B:1643:ASP:H	1.63	0.45
1:B:585:GLU:HG3	1:B:593:VAL:HG22	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
1:A:1303:ASP:OD1	1:A:1306:THR:OG1	2.22	0.45
1:A:766:ASP:O	1:A:770:MSE:HG2	2.16	0.45
1:B:1828:VAL:HB	1:B:1855:PHE:CE2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:964:GLN:HE21	1:B:965:ALA:H	1.64	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:A:1207:GLU:OE1	1:A:1819:LEU:HD23	2.16	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: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:HD3	1:A:894:ARG:HA	1.79	0.45
1:B:1514:PHE:CE2	1:B:1622:GLY:HA2	2.52	0.45
1:B:536:ASN:O	1:B:536:ASN:ND2	2.50	0.45
1:A:1042:GLN:HB3	1:A:1081:ILE:HG12	1.99	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: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:N	1:A:933:GLU:OE1	2.47	0.45
1:B:1141:SER:O	1:B:1144:PHE:HB3	2.17	0.45
1:B:340:ASN:HA	1:B:367:SER:OG	2.17	0.45
1:A:122:TYR:CD1	1:A:126:PHE:HB2	2.52	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: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: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
1:B:1407:HIS:CE1	1:B:1411:ILE:HD11	2.52	0.44
1:B:659:SER:HA	1:B:671:GLU:HG2	1.99	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:2067:TYR:HB3	1:A:2079:TYR:HB3	1.99	0.44
1:A:291:VAL:HG11	1:A:914:HIS:CG	2.52	0.44
1:B:1387:LYS:HA	1:B:1390:ILE:HG22	2.00	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:452:PHE:O	1:A:455:MSE:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:HE2	1:A:1984:LYS:HB2	1.82	0.44
1:A:1862:TYR:CZ	1:A:1998:PHE:HB2	2.52	0.43
1:A:1831:ILE:HD13	1:A:1999:GLU:HG3	2.00	0.43
1:A:427:PHE:HB2	1:A:472:TYR:HD1	1.81	0.43
1:B:1509:GLU:HA	1:B:1512:ARG:HG2	2.00	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:A:1426:THR:O	1:A:1430:ILE:HG12	2.18	0.43
1:B:1801:ASN:HA	1:B:1805:PHE:HB2	2.00	0.43
1:B:772:LYS:O	1:B:781:ILE:HG21	2.18	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: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:A:458:PHE:CZ	1:A:482:LYS:HG3	2.53	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:1387:LYS:O	1:B:1390:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:195:LYS:HD2	1:B:238:LYS:HB3	2.00	0.43
1:A:1446:ASP:OD1	1:A:1447:PHE:N	2.52	0.43
1:A:753:HIS:ND1	1:A:754:ILE:HG13	2.34	0.43
1:A:1299:TYR:O	1:A:1307:LEU:HD11	2.18	0.43
1:B:1038:VAL:O	1:B:1041:THR:HG22	2.19	0.43
1:B:928:SER:HB3	1:B:931:LEU:HD13	2.00	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:2027:ILE:HG21	1:B:2032:VAL:HB	1.99	0.43
1:B:275:LEU:O	1:B:279:LEU:HB2	2.19	0.43
1:B:50:GLY:HA2	1:B:86:LYS:HE3	2.00	0.43
1:B:569:THR:HG23	1:B:572:GLY:H	1.83	0.43
1:A:559:ASN:O	1:A:562:VAL:HG12	2.17	0.43
1:B:1553:MSE:HE3	1:B:1633:PHE:HB2	2.01	0.43
1:B:155:VAL:HG21	1:B:170:LEU:HD22	2.01	0.43
1:B:1920:LYS:HE3	1:B:1924:PHE:HE2	1.81	0.43
1:B:247:ILE:HG21	1:B:310:LYS:HB2	2.00	0.43
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:A:274:GLU:O	1:A:278:VAL:HG22	2.19	0.42
1:A:90:ARG:HD3	1:A:1978:ARG:NH2	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: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:B:234:THR:HG23	1:B:237:VAL:H	1.83	0.42
1:A:2010:ASN:HA	1:A:2061:LYS:HZ1	1.85	0.42
1:A:384:PHE:CE1	1:A:500:PRO:HB3	2.54	0.42
1:B:1385:LEU:HD12	1:B:1451:HIS:ND1	2.34	0.42
1:B:1329:SER:OG	1:B:1499:THR:O	2.27	0.42
1:B:1911:ASN:ND2	1:B:2089:ASP:OD2	2.48	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:1129:ALA:HB2	1:A:1492:LYS:HG3	2.01	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:B:1921:SER:O	1:B:1925:GLN:HG3	2.19	0.42
1:B:733:ASP:OD1	1:B:737:ASN:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:ILE:HD12	1:A:685:PHE:CZ	2.54	0.42
1:A:1305:LYS:HD3	1:A:1305:LYS:HA	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: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: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:1495:GLY:O	1:A:1499:THR:HG23	2.19	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:B:1119:LYS:HD3	1:B:1746:ASP:OD2	2.20	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:A:620:GLU:HG3	1:A:1667:LYS:HD3	2.02	0.42
1:B:1326:GLN:HG2	1:B:1607:LEU:HD22	2.02	0.42
1:A:478:GLN:CD	1:A:482:LYS:HE2	2.40	0.42
1:B:460:LYS:CG	1:B:475:MSE:HE2	2.50	0.42
1:A:140:ILE:H	1:A:140:ILE:HD12	1.85	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:B:567:LEU:HD12	1:B:582:LEU:HD21	2.02	0.41
1:B:6:GLU:HA	1:B:16:GLU:HA	2.02	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:A:2013:ALA:O	1:A:2061:LYS:NZ	2.39	0.41
1:B:1133:ILE:HD11	1:B:1143:MSE:HE1	2.01	0.41
1:A:1786:TYR:CD1	1:A:1795:LEU:HD22	2.55	0.41
1:A:891:PHE:O	1:A:895:VAL:HG23	2.19	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:891:PHE:O	1:B:895:VAL:HG23	2.20	0.41
1:B:545:ARG:NH1	1:B:903:THR:OG1	2.53	0.41
1:A:951:ILE:HD11	1:A:1499:THR:HG22	2.01	0.41
1:A:430:VAL:HG23	1:A:431:PHE:CD2	2.55	0.41
1:B:381:TYR:CE2	1:B:385:LYS:HD2	2.55	0.41
1:B:9:LYS:NZ	1:B:65:GLY:HA3	2.34	0.41
1:B:894:ARG:HD3	1:B:894:ARG:HA	1.80	0.41
1:A:1299:TYR:HE1	1:A:1342:GLU:OE2	2.04	0.41
1:A:155:VAL:HG21	1:A:170:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1514:PHE:CE2	1:A:1622:GLY:HA2	2.56	0.41
1:A:1159:ILE:HG12	1:A:1801:ASN:HB2	2.03	0.41
1:A:331:VAL:O	1:A:335:TYR:N	2.54	0.41
1:B:1207:GLU:OE2	1:B:1217:TYR:OH	2.25	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:B:140:ILE:HD12	1:B:188:ILE:HD11	2.01	0.41
1:B:83:PHE:HB2	1:B:91:PHE:HB3	2.03	0.41
1:B:696:ILE:HD13	1:B:865:LEU:HD13	2.01	0.41
1:A:1825:GLN:O	1:A:1828:VAL:HG12	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:B:759:SER:O	1:B:763:ILE:HG13	2.21	0.41
1:A:1984:LYS:HD2	1:A:2101:PHE:CZ	2.56	0.41
1:A:380:TYR:CE1	1:A:447:VAL:HG13	2.56	0.41
1:B:1768:TYR:CD2	1:B:2159:ILE:HD12	2.56	0.41
1:B:461:GLN:HE21	1:B:478:GLN:HB2	1.86	0.41
1:A:153:ALA:HB3	1:A:154:PRO:HD3	2.03	0.41
1:A:1673:ASP:HB3	1:A:1676:LYS:HD2	2.03	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:1008:ALA:N	1:A:1343:ALA:O	2.52	0.41
1:A:1679:PHE:O	1:A:1683:VAL:HG13	2.21	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: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: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:HA	1:B:952:LEU:HD23	1.91	0.41
1:A:2009:SER:HB3	1:A:2012:LEU:HB2	2.02	0.41
1:A:2129:ILE:O	1:A:2135:TYR:HB2	2.20	0.41
1:A:545:ARG:HD3	1:A:546:PRO:HD3	2.03	0.41
1:B:1121:ILE:HG21	1:B:1484:TYR:CE1	2.56	0.41
1:B:1718:ILE:O	1:B:1722:VAL:HG13	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:A:247:ILE:HD13	1:A:310:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:A:587:ASN:ND2	1:A:589:THR:HG22	2.34	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:1509:GLU:HA	1:A:1512:ARG:HG2	2.03	0.40
1:A:340:ASN:HD22	1:A:365:ASN:HD21	1.69	0.40
1:B:1660:PHE:HE1	1:B:1681:ILE:HB	1.85	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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2164/2194 (99%)	2067 (96%)	97 (4%)	0	100	100
1	B	2164/2194 (99%)	2071 (96%)	93 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4328/4388 (99%)	4138 (96%)	190 (4%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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%)	1944 (100%)	2 (0%)	93 98
1	B	1946/1934 (101%)	1946 (100%)	0	100 100
All	All	3892/3868 (101%)	3890 (100%)	2 (0%)	93 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	LYS
1	A	2025	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	825	ASN
1	A	850	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.05	50 (2%)	60	54	52, 88, 155, 319	0
1	B	2129/2194 (97%)	-0.05	56 (2%)	56	49	48, 82, 155, 452	0
All	All	4258/4388 (97%)	-0.05	106 (2%)	57	51	48, 85, 155, 452	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1410	ASN	8.3
1	B	1419	GLU	7.7
1	B	1418	GLU	5.7
1	A	1421	THR	5.5
1	A	1418	GLU	5.3
1	A	1429	PHE	5.2
1	B	1414	ILE	5.0
1	B	1415	ALA	4.9
1	B	1409	PHE	4.4
1	A	1420	VAL	4.3
1	A	1425	ILE	4.3
1	A	1419	GLU	4.2
1	A	351	THR	4.1
1	B	1391	ALA	3.9
1	B	1394	GLU	3.8
1	B	1402	ASP	3.8
1	A	27	PHE	3.8
1	A	1453	ILE	3.7
1	B	487	ASN	3.6
1	A	1439	SER	3.6
1	A	1395	ILE	3.6
1	B	1417	GLY	3.5
1	B	1399	GLU	3.4
1	A	1450	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	1390	ILE	3.3
1	A	1444	HIS	3.2
1	B	1444	HIS	3.2
1	B	1420	VAL	3.2
1	B	126	PHE	3.2
1	B	2	ALA	3.1
1	A	1426	THR	3.1
1	A	3	CYS	3.0
1	B	479	TYR	3.0
1	A	1417	GLY	3.0
1	A	1435	LEU	2.9
1	B	353	ASP	2.9
1	B	1453	ILE	2.9
1	B	1422	GLU	2.9
1	A	352	GLU	2.8
1	A	357	THR	2.8
1	A	827	ASP	2.7
1	B	1426	THR	2.7
1	A	2165	ASN	2.7
1	B	1429	PHE	2.7
1	A	1402	ASP	2.7
1	B	1390	ILE	2.7
1	B	1404	LEU	2.7
1	B	93	LEU	2.7
1	A	15	VAL	2.7
1	B	1452	ASN	2.6
1	A	356	ASN	2.6
1	B	1407	HIS	2.6
1	B	15	VAL	2.6
1	B	1421	THR	2.5
1	B	483	LEU	2.5
1	B	1389	TYR	2.5
1	A	1700	ARG	2.5
1	B	8	ILE	2.5
1	B	1893	ASP	2.5
1	A	494	GLN	2.4
1	A	350	GLU	2.4
1	A	1440	GLU	2.4
1	A	1441	LEU	2.4
1	B	423	SER	2.4
1	A	1422	GLU	2.4
1	B	1403	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1434	ILE	2.4
1	B	5	ILE	2.4
1	A	1451	HIS	2.4
1	A	1388	ASP	2.4
1	A	353	ASP	2.4
1	A	9	LYS	2.3
1	B	468	GLU	2.3
1	A	1391	ALA	2.3
1	A	1428	ALA	2.3
1	B	2136	ILE	2.3
1	B	357	THR	2.3
1	B	426	ASP	2.3
1	A	384	PHE	2.3
1	B	1568	ASN	2.3
1	B	848	ASP	2.3
1	B	1401	TYR	2.3
1	B	130	PHE	2.2
1	A	1399	GLU	2.2
1	B	27	PHE	2.2
1	B	1395	ILE	2.2
1	B	1441	LEU	2.2
1	A	1401	TYR	2.2
1	B	50	GLY	2.2
1	A	2167	VAL	2.2
1	B	1434	ILE	2.1
1	A	1410	ASN	2.1
1	A	1403	GLU	2.1
1	A	483	LEU	2.1
1	A	1446	ASP	2.1
1	B	1435	LEU	2.1
1	B	214	GLU	2.1
1	B	1439	SER	2.0
1	A	387	LYS	2.0
1	A	1430	ILE	2.0
1	B	855	ASP	2.0
1	A	84	ILE	2.0
1	A	845	TYR	2.0
1	B	92	ASP	2.0
1	B	1396	THR	2.0
1	B	845	TYR	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 monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
3	NA	A	2212	1/1	0.71	0.89	68,68,68,68	0
2	CL	A	2204	1/1	0.71	0.35	83,83,83,83	0
3	NA	A	2213	1/1	0.73	0.22	54,54,54,54	0
2	CL	B	2201	1/1	0.77	0.33	65,65,65,65	0
3	NA	B	2211	1/1	0.77	0.71	70,70,70,70	0
2	CL	A	2205	1/1	0.78	0.23	95,95,95,95	0
2	CL	A	2207	1/1	0.81	0.34	80,80,80,80	0
2	CL	B	2209	1/1	0.82	0.33	81,81,81,81	0
2	CL	A	2211	1/1	0.83	0.88	106,106,106,106	0
2	CL	A	2210	1/1	0.83	0.13	94,94,94,94	0
3	NA	B	2212	1/1	0.84	0.15	64,64,64,64	0
2	CL	B	2204	1/1	0.85	0.24	74,74,74,74	0
2	CL	A	2206	1/1	0.87	0.13	79,79,79,79	0
2	CL	B	2203	1/1	0.87	0.21	73,73,73,73	0
2	CL	B	2202	1/1	0.87	0.30	73,73,73,73	0
2	CL	B	2206	1/1	0.88	0.17	59,59,59,59	0
2	CL	B	2207	1/1	0.89	0.49	94,94,94,94	0
2	CL	A	2208	1/1	0.89	0.33	80,80,80,80	0
3	NA	A	2215	1/1	0.89	0.60	91,91,91,91	0
2	CL	A	2209	1/1	0.89	0.40	78,78,78,78	0
2	CL	A	2201	1/1	0.91	0.17	67,67,67,67	0
2	CL	A	2203	1/1	0.91	0.35	72,72,72,72	0
2	CL	B	2208	1/1	0.92	0.18	80,80,80,80	0
2	CL	B	2210	1/1	0.92	0.55	81,81,81,81	0
2	CL	B	2205	1/1	0.93	0.35	76,76,76,76	0
3	NA	A	2214	1/1	0.93	0.32	49,49,49,49	0
2	CL	A	2202	1/1	0.94	0.41	96,96,96,96	0

6.5 Other polymers (i)

There are no such residues in this entry.