



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:23 pm BST

PDB ID : 5XA1
Title : Crystal structure of inositol 1,4,5-trisphosphate receptor cytosolic domain with inositol 1,4,5-trisphosphate
Authors : Hamada, K.; Miyatake, H.; Terauchi, A.; Mikoshiba, K.
Deposited on : 2017-03-10
Resolution : 6.20 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 ⓘ](#)) 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 : 2.11
buster-report : 1.1.7 (2018)
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) : 2.11

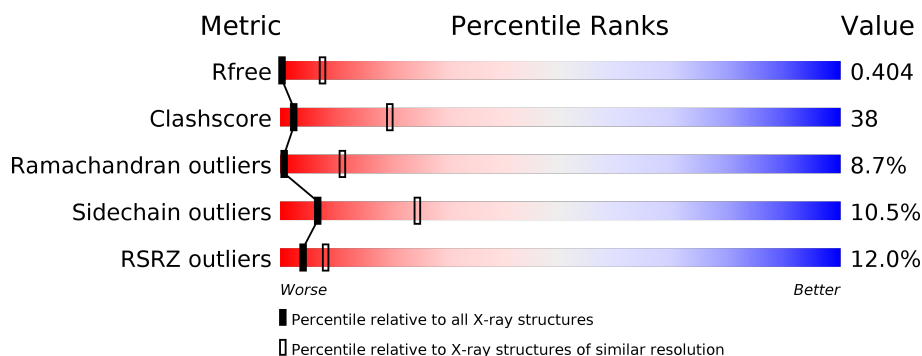
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.20 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	1007 (8.50-3.88)
Clashscore	141614	1056 (8.50-3.90)
Ramachandran outliers	138981	1004 (8.50-3.88)
Sidechain outliers	138945	1003 (8.50-3.84)
RSRZ outliers	127900	1017 (8.50-3.78)

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 $\leq 5\%$. 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	1581	<div> <div>10%</div> <div>40%</div> <div>33%</div> <div>6%</div> <div>20%</div> </div>
1	B	1581	<div> <div>9%</div> <div>42%</div> <div>32%</div> <div>6%</div> <div>20%</div> </div>

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
2	I3P	A	3000	-	-	-	X

2 Entry composition [i](#)

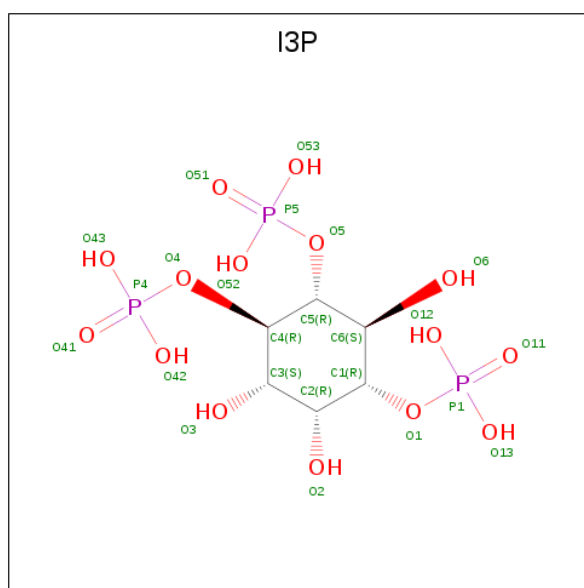
There are 2 unique types of molecules in this entry. The entry contains 25536 atoms, of which 10338 are hydrogens and 0 are deuteriums.

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 Inositol 1,4,5-trisphosphate receptor type 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1257	Total	C	H	N	O	S	0	0	0
			12735	4648	5160	1435	1475	17			
1	B	1257	Total	C	H	N	O	S	0	0	0
			12735	4648	5160	1435	1475	17			

- Molecule 2 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$).

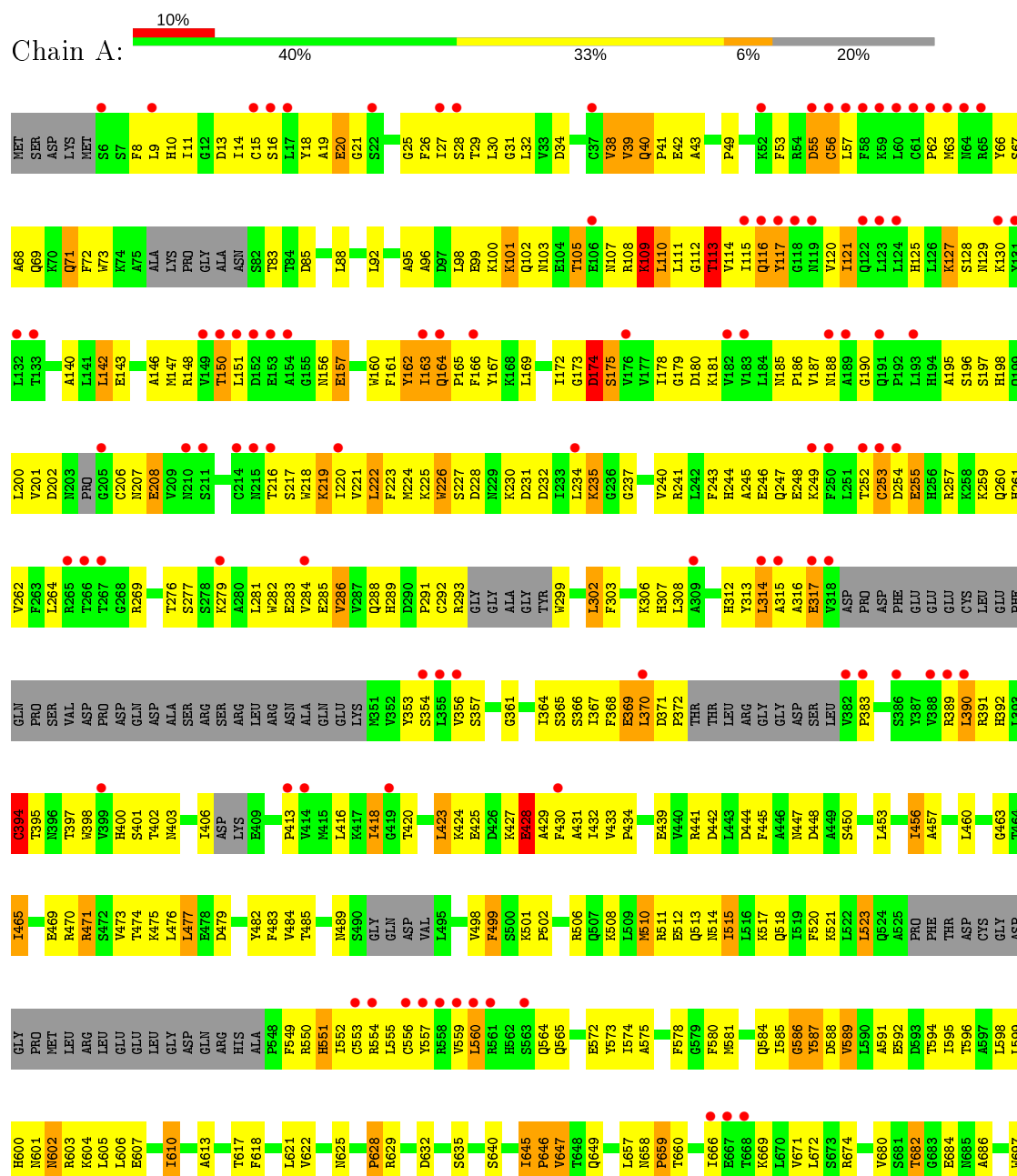


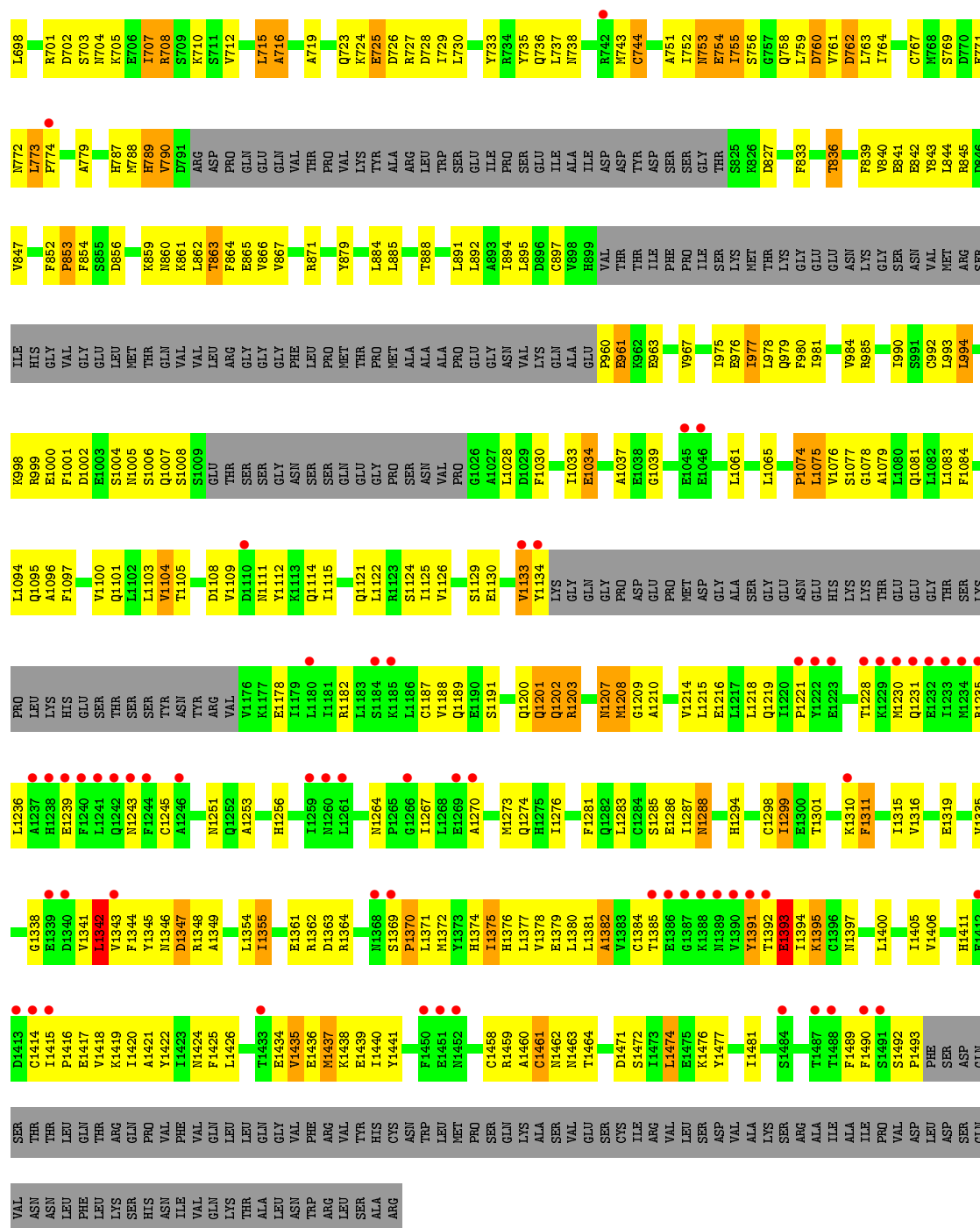
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			33	6	9	15	3		
2	B	1	Total	C	H	O	P	0	0
			33	6	9	15	3		

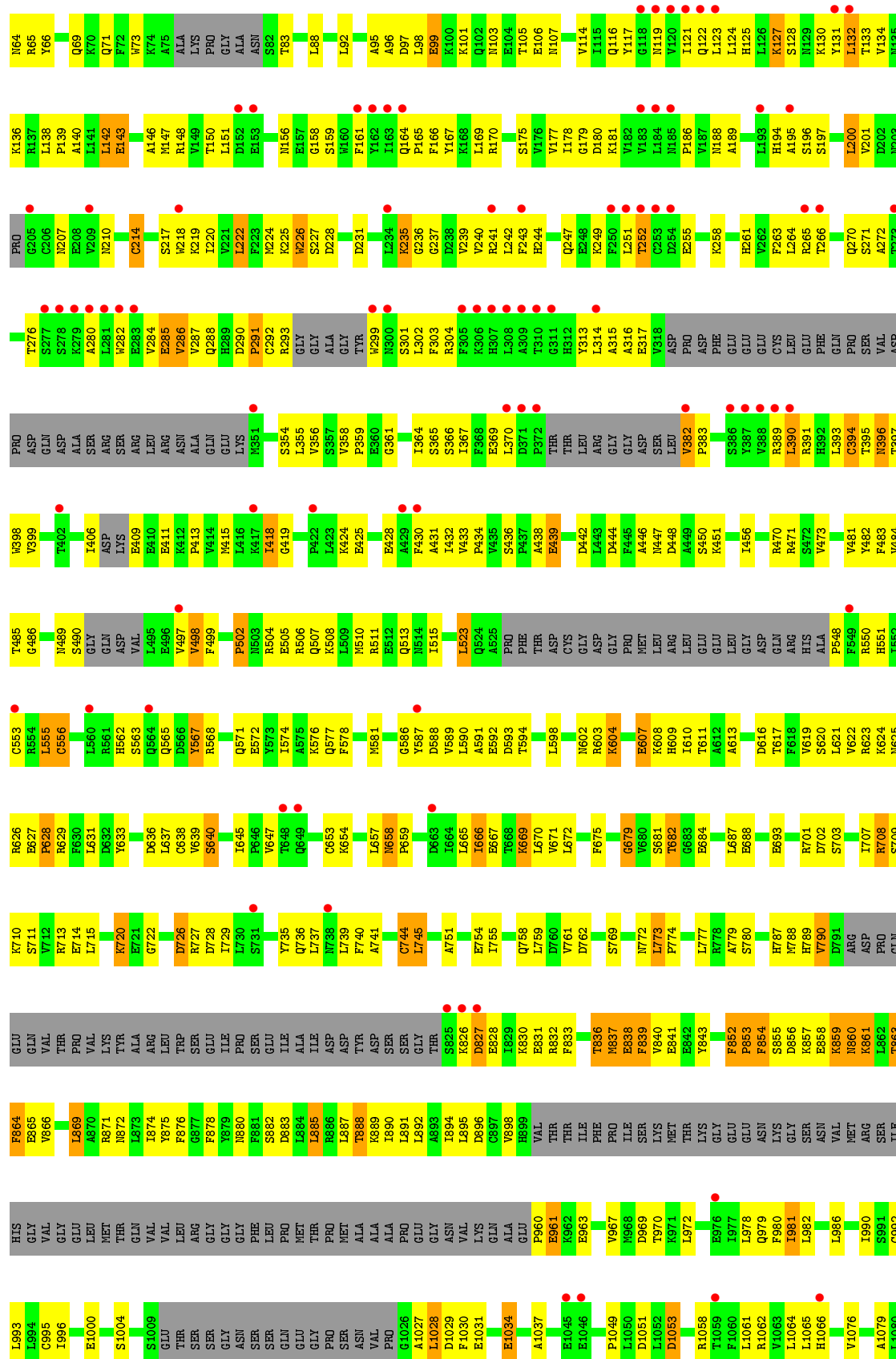
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Inositol 1,4,5-trisphosphate receptor type 1







ASN	ILE	VAL	GLN	LYS	THR	ALA	LEU	ASN	TRP	ARG	LEU	ARG	HIS	CYS	ASN	TRP	MET	PRO	SER	GLN	ALA	SER	VAL	GLU	SER	ASP	VAL	ALA	LYS	SER	ARG	ALA	ILE	ILE	PRO	VAL	ASP	LEU	ASP	SER	GLN	VAL	ASN	THR	LEU	PHE	LEU	THR	LYS	ARG	GLN	PRO	
C1414	I1415	P1416	E1417	K1419	I1420	A1421	Y1422	I1423	N1424	F1425	L1426	D1432	T1433	E1434	V1435	L1449	F1453	I1457	C1458	C1461	N1462	N1463	T1464	S1472	K1476	Y1477	V1478	T1479	F1480	I1481	V1482	M1483	S1484	I1485	S1491	S1492	F1493	PHE	SER	ASP	GLN	VAL	ASN	THR	LEU	PHE	LEU	THR	ARG	GLN	PRO		
VAL	PHE	VAL	GLN	LEU	LEU	GLN	GLY	VAL	PHE	ARG	VAL	TYR	HIS	CYS	ASN	TRP	LEU	MET	PRO	SER	GLN	ALA	SER	VAL	GLU	SER	ASP	VAL	ALA	LYS	SER	ARG	ALA	ILE	ILE	PRO	VAL	ASP	LEU	ASP	SER	GLN	VAL	ASN	THR	LEU	PHE	LEU	THR	LYS	ARG	GLN	PRO
V1335	G1338	V1341	L1342	V1343	F1344	Y1345	N1346	D1347	R1348	A1349	S1350	I1355	Q1356	M1357	M1358	R1359	D1363	D1366	P1370	L1371	M1372	Y1373	H1374	I1375	L1376	L1377	V1378	E1379	L1380	L1381	A1382	V1383	C1384	T1385	K1388	N1389	I1394	N1397	S1398	L1399	L1400	P1401	L1402	D1403	D1404	I1405	V1408						
C1245	A1246	G1247	N1251	L1255	H1256	K1257	N1264	L1267	A1270	M1273	Q1274	H1275	I1276	F1277	M1278	N1279	N1280	F1281	Q1282	L1283	C1284	S1285	E1286	I1287	N1288	E1289	R1290	V1291	V1292	Q1293	H1294	F1295	C1298	I1299	E1300	T1301	H1302	G1303	R1304	K1310	F1311	I1315	V1316	K1317	A1318	E1319	G1320	K1321	F1322	I1323			
Q1081	F1084	R1085	H1086	F1087	L1084	Q1095	Q1101	D1108	V1109	Y1112	K1116	Q1117	D1118	L1119	D1120	Q1121	E1122	L1125	V1126	S1129	E1130	V1133	Y1134	LYS	GLY	GLN	GLY	PRO	ASP	GLU	PRO	ASP	ASP	GLY	ALA	SER	GLY	GLU	ASN	GLU	HIS	LYS	LYS	THR	GLU	GLY	THR	SER	LYS				

4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	126.80Å 126.80Å 367.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.50 – 6.20 48.54 – 6.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.50-6.20) 99.6 (48.54-6.20)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 6.15Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.360 , 0.382 0.376 , 0.404	Depositor DCC
R_{free} test set	651 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	91.1	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 473.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.21$, $\langle L^2 \rangle = 0.07$	Xtriage
Estimated twinning fraction	0.377 for h,-k,-l	Xtriage
F_o, F_c correlation	0.63	EDS
Total number of atoms	25536	wwPDB-VP
Average B, all atoms (Å ²)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: I3P

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	0.91	19/7637 (0.2%)	1.01	27/10494 (0.3%)
1	B	0.80	10/7637 (0.1%)	0.91	8/10494 (0.1%)
All	All	0.86	29/15274 (0.2%)	0.96	35/20988 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
1	B	0	7
All	All	0	17

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	GLN	CB-CG	12.62	1.86	1.52
1	B	1491	SER	C-N	11.74	1.61	1.34
1	A	109	LYS	CB-CG	10.84	1.81	1.52
1	A	116	GLN	CG-CD	9.81	1.73	1.51
1	A	56	CYS	CB-SG	9.68	1.98	1.82
1	A	285	GLU	CA-CB	-8.99	1.34	1.53
1	A	109	LYS	CD-CE	8.79	1.73	1.51
1	B	285	GLU	CA-CB	8.60	1.72	1.53
1	A	428	GLU	CB-CG	-8.10	1.36	1.52
1	A	109	LYS	CG-CD	7.55	1.78	1.52
1	A	208	GLU	CG-CD	-7.24	1.41	1.51
1	A	55	ASP	CB-CG	-6.80	1.37	1.51
1	B	382	VAL	C-N	6.75	1.47	1.34
1	A	1393	GLU	N-CA	6.21	1.58	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	GLU	CB-CG	-6.02	1.40	1.52
1	A	303	PHE	CB-CG	5.97	1.61	1.51
1	B	42	GLU	CB-CG	5.93	1.63	1.52
1	A	283	GLU	CB-CG	5.85	1.63	1.52
1	B	20	GLU	CB-CG	-5.61	1.41	1.52
1	A	175	SER	N-CA	5.50	1.57	1.46
1	A	219	LYS	CB-CG	-5.43	1.37	1.52
1	B	439	GLU	CG-CD	-5.43	1.43	1.51
1	A	369	GLU	CG-CD	-5.39	1.43	1.51
1	B	99	GLU	CG-CD	-5.27	1.44	1.51
1	B	505	GLU	CG-CD	5.24	1.59	1.51
1	B	20	GLU	CG-CD	-5.22	1.44	1.51
1	A	157	GLU	CB-CG	5.18	1.61	1.52
1	A	279	LYS	CB-CG	5.05	1.66	1.52
1	B	119	ASN	CB-CG	5.00	1.62	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	CYS	CA-CB-SG	9.02	130.24	114.00
1	A	1393	GLU	C-N-CA	8.16	142.11	121.70
1	B	390	LEU	CA-CB-CG	7.72	133.07	115.30
1	A	1395	LYS	CB-CA-C	-7.40	95.59	110.40
1	A	116	GLN	CB-CA-C	7.34	125.08	110.40
1	A	116	GLN	CB-CG-CD	6.88	129.49	111.60
1	B	869	LEU	O-C-N	6.82	133.61	122.70
1	A	253	CYS	CA-CB-SG	6.78	126.20	114.00
1	B	132	LEU	CA-CB-CG	6.70	130.70	115.30
1	A	113	THR	CA-CB-CG2	-6.62	103.13	112.40
1	A	109	LYS	CB-CG-CD	6.62	128.80	111.60
1	A	175	SER	CA-CB-OG	6.32	128.27	111.20
1	B	214	CYS	CA-CB-SG	6.28	125.31	114.00
1	A	390	LEU	CA-CB-CG	6.28	129.74	115.30
1	A	1395	LYS	N-CA-CB	6.18	121.72	110.60
1	A	109	LYS	CG-CD-CE	6.17	130.40	111.90
1	A	477	LEU	CB-CG-CD1	-6.13	100.57	111.00
1	B	869	LEU	CA-C-O	-5.96	107.59	120.10
1	A	1287	ILE	C-N-CA	5.90	136.45	121.70
1	A	314	LEU	CA-CB-CG	5.88	128.81	115.30
1	A	1393	GLU	O-C-N	-5.87	113.31	122.70
1	A	109	LYS	CA-CB-CG	5.86	126.30	113.40
1	A	162	TYR	CA-CB-CG	5.73	124.29	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ASP	CA-C-N	5.58	129.48	117.20
1	A	394	CYS	CA-CB-SG	-5.58	103.95	114.00
1	A	1391	TYR	N-CA-CB	-5.51	100.68	110.60
1	A	370	LEU	C-N-CA	5.38	135.15	121.70
1	A	560	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	1393	GLU	CA-C-N	5.31	128.88	117.20
1	A	110	LEU	CB-CG-CD1	5.29	120.00	111.00
1	B	1491	SER	C-N-CA	5.25	134.83	121.70
1	A	116	GLN	N-CA-CB	-5.18	101.28	110.60
1	B	556	CYS	CA-CB-SG	5.13	123.23	114.00
1	B	56	CYS	CA-CB-SG	5.11	123.19	114.00
1	A	510	MET	CA-CB-CG	5.05	121.88	113.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1034	GLU	Peptide
1	A	1203	ARG	Peptide
1	A	1228	THR	Peptide
1	A	1342	LEU	Peptide
1	A	1375	ILE	Peptide
1	A	1382	ALA	Peptide
1	A	1393	GLU	Peptide
1	A	173	GLY	Peptide
1	A	174	ASP	Mainchain
1	A	707	ILE	Peptide
1	B	1034	GLU	Peptide
1	B	1375	ILE	Peptide
1	B	1380	LEU	Peptide
1	B	1461	CYS	Peptide
1	B	679	GLY	Peptide
1	B	708	ARG	Peptide
1	B	744	CYS	Peptide

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	7575	5160	5277	516	8
1	B	7575	5160	5277	457	0
2	A	24	9	9	0	0
2	B	24	9	9	0	0
All	All	15198	10338	10572	973	8

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 38.

All (973) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LYS:CG	1:A:109:LYS:CD	1.78	1.61
1:A:109:LYS:CG	1:A:109:LYS:CB	1.81	1.54
1:A:116:GLN:CG	1:A:116:GLN:CB	1.86	1.52
1:B:856:ASP:O	1:B:860:ASN:CB	1.89	1.20
1:A:1214:VAL:O	1:A:1218:LEU:CB	1.92	1.17
1:A:1281:PHE:O	1:A:1285:SER:CB	1.95	1.12
1:B:1116:LYS:O	1:B:1119:LEU:N	1.84	1.09
1:B:1281:PHE:O	1:B:1285:SER:CB	2.03	1.06
1:B:1371:LEU:O	1:B:1375:ILE:N	1.91	1.02
1:A:1371:LEU:O	1:A:1375:ILE:N	1.93	1.01
1:A:1125:ILE:O	1:A:1129:SER:CB	2.09	1.01
1:B:892:LEU:O	1:B:896:ASP:CB	2.10	1.00
1:B:1341:VAL:O	1:B:1345:TYR:N	1.95	0.99
1:A:1422:TYR:O	1:A:1426:LEU:CB	2.12	0.97
1:B:1377:LEU:O	1:B:1381:LEU:CB	2.12	0.97
1:A:705:LYS:HA	1:A:736:GLN:CB	1.94	0.97
1:A:1377:LEU:O	1:A:1381:LEU:CB	2.13	0.97
1:B:654:LYS:O	1:B:658:ASN:N	1.97	0.97
1:B:885:LEU:O	1:B:888:THR:N	1.97	0.96
1:A:1231:GLN:O	1:A:1235:ARG:CB	2.15	0.94
1:B:610:ILE:O	1:B:613:ALA:N	2.01	0.93
1:B:882:SER:O	1:B:885:LEU:N	2.00	0.93
1:B:1118:ASP:O	1:B:1120:ASP:N	2.03	0.91
1:B:840:VAL:O	1:B:843:TYR:N	2.04	0.90
1:A:755:ILE:O	1:A:758:GLN:N	2.03	0.90
1:B:653:CYS:O	1:B:657:LEU:N	2.04	0.90
1:A:885:LEU:O	1:A:888:THR:N	2.06	0.89
1:B:1472:SER:O	1:B:1476:LYS:CB	2.19	0.89
1:B:978:LEU:O	1:B:981:ILE:N	2.05	0.89
1:B:888:THR:O	1:B:891:LEU:N	2.06	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1126:VAL:O	1:A:1130:GLU:CB	2.21	0.88
1:A:1421:ALA:O	1:A:1425:PHE:CB	2.21	0.87
1:B:777:LEU:O	1:B:780:SER:N	2.07	0.87
1:A:1381:LEU:HA	1:A:1384:CYS:CB	2.05	0.87
1:A:1459:ARG:O	1:A:1461:CYS:N	2.08	0.86
1:B:1270:ALA:HB2	1:B:1319:GLU:CB	2.05	0.86
1:A:603:ARG:O	1:A:605:LEU:N	2.08	0.85
1:A:1191:SER:CB	1:A:1236:LEU:O	2.25	0.84
1:A:574:ILE:O	1:A:578:PHE:N	2.09	0.84
1:B:285:GLU:O	1:B:287:VAL:N	2.11	0.84
1:B:140:ALA:N	1:B:146:ALA:O	2.09	0.84
1:B:18:TYR:OH	1:B:45:ASP:OD1	1.95	0.83
1:A:1111:ASN:O	1:A:1114:GLN:N	2.12	0.83
1:B:963:GLU:O	1:B:967:VAL:CB	2.27	0.83
1:A:277:SER:OG	1:A:512:GLU:OE1	1.96	0.82
1:B:276:THR:O	1:B:508:LYS:NZ	2.13	0.82
1:B:622:VAL:HA	1:B:631:LEU:CB	2.09	0.82
1:A:703:SER:CB	1:A:710:LYS:CB	2.57	0.82
1:B:624:LYS:O	1:B:626:ARG:N	2.12	0.82
1:B:865:GLU:O	1:B:869:LEU:CB	2.29	0.81
1:B:598:LEU:O	1:B:602:ASN:N	2.13	0.81
1:B:1231:GLN:O	1:B:1235:ARG:CB	2.29	0.81
1:B:1421:ALA:O	1:B:1425:PHE:CB	2.28	0.80
1:B:237:GLY:N	1:B:284:VAL:O	2.15	0.80
1:A:20:GLU:N	1:A:217:SER:O	2.14	0.80
1:A:618:PHE:O	1:A:622:VAL:N	2.15	0.80
1:A:586:GLY:O	1:A:588:ASP:N	2.16	0.79
1:A:49:PRO:HG2	1:A:291:PRO:HG2	1.64	0.79
1:A:595:ILE:O	1:A:598:LEU:CB	2.32	0.79
1:B:1125:ILE:O	1:B:1129:SER:CB	2.30	0.79
1:A:859:LYS:O	1:A:863:THR:CB	2.31	0.78
1:A:15:CYS:SG	1:A:222:LEU:HA	2.23	0.78
1:B:838:GLU:O	1:B:841:GLU:N	2.16	0.78
1:A:140:ALA:N	1:A:146:ALA:O	2.17	0.78
1:A:200:LEU:HD21	1:A:208:GLU:HB2	1.67	0.77
1:B:1049:PRO:O	1:B:1053:ASP:N	2.18	0.77
1:B:1287:ILE:HA	1:B:1344:PHE:CB	2.14	0.77
1:A:1417:GLU:O	1:A:1419:LYS:N	2.17	0.77
1:B:669:LYS:O	1:B:671:VAL:N	2.18	0.77
1:A:1294:HIS:O	1:A:1298:CYS:N	2.17	0.76
1:A:755:ILE:O	1:A:759:LEU:N	2.17	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:PRO:HG2	1:B:291:PRO:HG2	1.67	0.76
1:A:595:ILE:O	1:A:599:LEU:N	2.19	0.76
1:A:1121:GLN:O	1:A:1124:SER:N	2.19	0.75
1:A:863:THR:O	1:A:866:VAL:N	2.18	0.75
1:A:20:GLU:O	1:A:217:SER:OG	2.05	0.75
1:B:47:ASN:O	1:B:49:PRO:HD3	1.86	0.75
1:B:885:LEU:O	1:B:888:THR:CB	2.35	0.74
1:B:607:GLU:O	1:B:611:THR:HA	1.87	0.74
1:A:1376:HIS:O	1:A:1380:LEU:CB	2.35	0.74
1:A:707:ILE:CB	1:A:737:LEU:N	2.51	0.73
1:B:1335:VAL:O	1:B:1384:CYS:CB	2.36	0.73
1:B:32:LEU:HD21	1:B:128:SER:HA	1.71	0.73
1:A:1437:MET:O	1:A:1440:ILE:N	2.17	0.73
1:A:1341:VAL:O	1:A:1345:TYR:N	2.19	0.73
1:B:969:ASP:O	1:B:972:LEU:N	2.20	0.73
1:B:1207:ASN:O	1:B:1209:GLY:N	2.22	0.72
1:A:724:LYS:O	1:A:726:ASP:N	2.22	0.72
1:A:601:ASN:O	1:A:603:ARG:N	2.22	0.72
1:A:16:SER:N	1:A:221:VAL:O	2.19	0.72
1:B:29:THR:HG22	1:B:151:LEU:HD11	1.72	0.72
1:A:1134:TYR:O	1:A:1230:MET:N	2.21	0.72
1:A:224:MET:SD	1:A:228:ASP:HB3	2.30	0.72
1:A:581:MET:HA	1:A:591:ALA:HB1	1.72	0.71
1:A:963:GLU:O	1:A:967:VAL:CB	2.36	0.71
1:B:18:TYR:OH	1:B:24:ASN:HB3	1.89	0.71
1:B:857:LYS:O	1:B:861:LYS:CB	2.39	0.70
1:B:874:ILE:O	1:B:878:PHE:CB	2.39	0.70
1:B:1291:VAL:O	1:B:1293:GLN:N	2.24	0.70
1:A:316:ALA:HB3	1:A:392:HIS:ND1	2.06	0.70
1:A:1435:VAL:CB	1:A:1492:SER:CB	2.70	0.70
1:B:1420:ILE:O	1:B:1424:ASN:CB	2.39	0.70
1:A:871:ARG:HA	1:A:980:PHE:CB	2.21	0.70
1:B:885:LEU:O	1:B:888:THR:CA	2.40	0.70
1:A:523:LEU:HD12	1:A:553:CYS:SG	2.32	0.70
1:B:485:THR:HG21	1:B:562:HIS:CE1	2.26	0.70
1:B:128:SER:HB2	1:B:130:LYS:HE3	1.74	0.70
1:A:1270:ALA:HB2	1:A:1319:GLU:CB	2.22	0.70
1:A:230:LYS:HA	1:A:232:ASP:N	2.06	0.69
1:B:860:ASN:O	1:B:863:THR:N	2.25	0.69
1:A:450:SER:OG	1:A:513:GLN:O	2.09	0.69
1:A:981:ILE:O	1:A:985:ARG:CB	2.40	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1291:VAL:O	1:B:1294:HIS:N	2.26	0.69
1:B:1381:LEU:HA	1:B:1384:CYS:CB	2.22	0.69
1:A:756:SER:O	1:A:760:ASP:N	2.26	0.69
1:A:264:LEU:HG	1:A:418:ILE:HD11	1.73	0.69
1:B:301:SER:O	1:B:303:PHE:CE1	2.46	0.69
1:A:1215:LEU:O	1:A:1219:GLN:N	2.23	0.68
1:B:290:ASP:O	1:B:292:CYS:N	2.25	0.68
1:B:483:PHE:O	1:B:506:ARG:NH1	2.26	0.68
1:B:755:ILE:O	1:B:758:GLN:N	2.26	0.68
1:A:162:TYR:HB3	1:A:164:GLN:NE2	2.08	0.68
1:B:367:ILE:O	1:B:367:ILE:HG23	1.91	0.68
1:A:72:PHE:O	1:A:72:PHE:CG	2.47	0.68
1:B:15:CYS:SG	1:B:222:LEU:HA	2.34	0.68
1:A:1096:ALA:O	1:A:1100:VAL:N	2.27	0.68
1:B:29:THR:HG22	1:B:151:LEU:CD1	2.24	0.68
1:B:194:HIS:CE1	1:B:214:CYS:SG	2.87	0.68
1:B:1203:ARG:CB	1:B:1207:ASN:CB	2.72	0.67
1:A:842:GLU:O	1:A:845:ARG:N	2.27	0.67
1:A:960:PRO:O	1:A:961:GLU:CB	2.41	0.67
1:B:1338:GLY:O	1:B:1342:LEU:CB	2.42	0.67
1:B:1449:LEU:O	1:B:1453:PHE:CB	2.42	0.67
1:B:855:SER:O	1:B:859:LYS:CB	2.43	0.67
1:A:55:ASP:OD1	1:A:127:LYS:HD3	1.94	0.67
1:A:610:ILE:O	1:A:613:ALA:HB3	1.95	0.67
1:B:863:THR:O	1:B:866:VAL:N	2.28	0.67
1:B:39:VAL:HG21	1:B:195:ALA:HB1	1.77	0.66
1:B:1380:LEU:O	1:B:1384:CYS:CB	2.43	0.66
1:B:236:GLY:HA2	1:B:286:VAL:H	1.59	0.66
1:A:1472:SER:O	1:A:1476:LYS:CB	2.43	0.66
1:A:469:GLU:O	1:A:473:VAL:HG23	1.96	0.66
1:A:1285:SER:O	1:A:1341:VAL:CB	2.44	0.66
1:A:243:PHE:O	1:A:430:PHE:HA	1.94	0.66
1:B:313:TYR:CD2	1:B:361:GLY:HA3	2.30	0.66
1:A:29:THR:HG22	1:A:151:LEU:CD1	2.26	0.66
1:A:1251:ASN:CB	1:A:1283:LEU:O	2.44	0.66
1:B:510:MET:HA	1:B:515:ILE:HG13	1.78	0.65
1:B:138:LEU:O	1:B:147:MET:HA	1.97	0.65
1:A:703:SER:O	1:A:733:TYR:HA	1.97	0.65
1:A:477:LEU:O	1:A:555:LEU:HD21	1.97	0.65
1:A:1187:CYS:O	1:A:1191:SER:CB	2.45	0.65
1:A:117:TYR:CZ	1:A:165:PRO:HB3	2.32	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD21	1:A:128:SER:HA	1.79	0.64
1:A:581:MET:CA	1:A:591:ALA:HB1	2.26	0.64
1:B:31:GLY:HA3	1:B:448:ASP:OD2	1.96	0.64
1:B:726:ASP:O	1:B:729:ILE:N	2.30	0.64
1:A:196:SER:HB2	1:A:208:GLU:O	1.96	0.64
1:A:885:LEU:O	1:A:888:THR:CB	2.46	0.64
1:A:584:GLN:O	1:A:588:ASP:O	2.15	0.64
1:B:769:SER:CB	1:B:779:ALA:HA	2.28	0.64
1:A:117:TYR:O	1:A:172:ILE:HG12	1.97	0.64
1:B:439:GLU:HA	1:B:442:ASP:OD2	1.96	0.64
1:B:891:LEU:O	1:B:895:LEU:CB	2.46	0.64
1:A:162:TYR:CE2	1:A:187:VAL:HA	2.33	0.64
1:A:20:GLU:HB2	1:A:217:SER:O	1.97	0.64
1:A:1417:GLU:O	1:A:1420:ILE:N	2.31	0.64
1:A:871:ARG:CB	1:A:980:PHE:CA	2.75	0.64
1:B:252:THR:OG1	1:B:265:ARG:HB2	1.98	0.63
1:B:65:ARG:N	1:B:103:ASN:OD1	2.31	0.63
1:B:130:LYS:HD2	1:B:151:LEU:HB3	1.81	0.63
1:B:224:MET:SD	1:B:228:ASP:HB3	2.39	0.63
1:B:617:THR:O	1:B:621:LEU:CB	2.46	0.63
1:A:1178:GLU:O	1:A:1182:ARG:CB	2.47	0.63
1:B:852:PHE:O	1:B:856:ASP:N	2.26	0.63
1:A:1245:CYS:CB	1:A:1285:SER:O	2.46	0.63
1:A:261:HIS:ND1	1:A:406:ILE:HD13	2.14	0.63
1:A:240:VAL:HG12	1:A:434:PRO:HA	1.79	0.63
1:B:32:LEU:CD2	1:B:128:SER:HA	2.28	0.63
1:B:1315:ILE:O	1:B:1319:GLU:CB	2.47	0.63
1:A:397:THR:HB	1:A:420:THR:OG1	1.99	0.63
1:A:744:CYS:HA	1:A:1077:SER:CB	2.28	0.63
1:B:1126:VAL:O	1:B:1130:GLU:CB	2.46	0.63
1:B:241:ARG:HG2	1:B:280:ALA:O	1.99	0.63
1:B:364:ILE:HG22	1:B:394:CYS:SG	2.39	0.62
1:A:1335:VAL:O	1:A:1384:CYS:CB	2.47	0.62
1:A:671:VAL:O	1:A:674:ARG:N	2.32	0.62
1:A:1459:ARG:C	1:A:1461:CYS:H	2.01	0.62
1:B:1210:ALA:O	1:B:1214:VAL:CB	2.46	0.62
1:A:1344:PHE:O	1:A:1347:ASP:N	2.31	0.62
1:B:313:TYR:CG	1:B:361:GLY:HA3	2.34	0.62
1:A:1381:LEU:O	1:A:1385:THR:CB	2.47	0.62
1:A:230:LYS:HA	1:A:232:ASP:H	1.63	0.62
1:A:701:ARG:CB	1:A:729:ILE:CB	2.78	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLN:NE2	1:A:73:TRP:HZ2	1.98	0.62
1:B:1345:TYR:O	1:B:1350:SER:CB	2.47	0.62
1:A:871:ARG:CB	1:A:980:PHE:HA	2.30	0.62
1:A:705:LYS:C	1:A:707:ILE:H	2.03	0.62
1:B:1085:ARG:C	1:B:1087:PHE:H	2.02	0.62
1:A:244:HIS:CE1	1:A:428:GLU:HA	2.35	0.62
1:A:398:TRP:CZ2	1:A:424:LYS:HD2	2.35	0.61
1:B:367:ILE:O	1:B:367:ILE:CG2	2.49	0.61
1:B:755:ILE:O	1:B:759:LEU:N	2.32	0.61
1:A:253:CYS:HB2	1:A:307:HIS:CE1	2.36	0.61
1:B:1118:ASP:O	1:B:1121:GLN:N	2.34	0.61
1:B:116:GLN:HA	1:B:175:SER:HA	1.81	0.61
1:B:240:VAL:HG12	1:B:434:PRO:HA	1.81	0.61
1:A:701:ARG:O	1:A:703:SER:N	2.33	0.61
1:A:769:SER:CB	1:A:779:ALA:HA	2.30	0.61
1:A:863:THR:O	1:A:864:PHE:C	2.37	0.61
1:B:313:TYR:CE2	1:B:361:GLY:HA3	2.35	0.61
1:A:761:VAL:O	1:A:764:ILE:N	2.27	0.61
1:B:1118:ASP:O	1:B:1119:LEU:C	2.39	0.61
1:B:134:VAL:HG21	1:B:186:PRO:HG3	1.81	0.61
1:A:1273:MET:O	1:A:1276:ILE:N	2.33	0.61
1:A:243:PHE:HB3	1:A:431:ALA:HB3	1.82	0.61
1:A:761:VAL:O	1:A:763:LEU:N	2.34	0.61
1:B:982:LEU:O	1:B:986:LEU:CB	2.49	0.61
1:A:581:MET:O	1:A:585:ILE:N	2.34	0.60
1:B:117:TYR:OH	1:B:180:ASP:OD2	2.13	0.60
1:A:245:ALA:N	1:A:429:ALA:O	2.34	0.60
1:A:755:ILE:O	1:A:758:GLN:CA	2.49	0.60
1:B:1374:HIS:HA	1:B:1377:LEU:CB	2.32	0.60
1:B:369:GLU:HG2	1:B:370:LEU:N	2.17	0.60
1:B:751:ALA:O	1:B:754:GLU:N	2.34	0.60
1:A:1471:ASP:O	1:A:1474:LEU:N	2.34	0.60
1:A:281:LEU:O	1:A:308:LEU:CB	2.49	0.60
1:A:20:GLU:OE1	1:A:181:LYS:HD3	2.01	0.60
1:B:568:ARG:NH1	1:B:572:GLU:OE1	2.35	0.60
1:B:594:THR:O	1:B:598:LEU:N	2.34	0.60
1:A:196:SER:CB	1:A:208:GLU:O	2.50	0.60
1:A:224:MET:HA	1:A:293:ARG:CB	2.32	0.60
1:A:470:ARG:HD2	1:A:471:ARG:HH21	1.65	0.60
1:A:841:GLU:O	1:A:844:LEU:N	2.34	0.60
1:B:36:ARG:NH1	1:B:200:LEU:HD13	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:VAL:O	1:B:640:SER:CB	2.49	0.60
1:B:1215:LEU:O	1:B:1217:LEU:N	2.35	0.60
1:A:728:ASP:CB	1:A:865:GLU:O	2.50	0.59
1:A:15:CYS:CB	1:A:222:LEU:HA	2.32	0.59
1:A:249:LYS:O	1:A:264:LEU:HD22	2.02	0.59
1:A:16:SER:O	1:A:221:VAL:N	2.23	0.59
1:B:134:VAL:N	1:B:158:GLY:O	2.35	0.59
1:A:1203:ARG:CB	1:A:1207:ASN:CB	2.80	0.59
1:B:243:PHE:HB3	1:B:431:ALA:HB3	1.84	0.59
1:A:31:GLY:HA3	1:A:448:ASP:OD2	2.02	0.59
1:B:1405:ILE:O	1:B:1408:VAL:N	2.36	0.59
1:A:1310:LYS:O	1:A:1311:PHE:CB	2.50	0.59
1:A:423:LEU:HD22	1:A:425:GLU:OE1	2.02	0.59
1:B:264:LEU:HG	1:B:418:ILE:HD11	1.85	0.59
1:A:11:ILE:O	1:A:112:GLY:N	2.35	0.59
1:A:456:ILE:HG12	1:A:473:VAL:HG21	1.84	0.59
1:A:313:TYR:CD2	1:A:361:GLY:HA3	2.37	0.59
1:A:439:GLU:HA	1:A:442:ASP:OD2	2.03	0.59
1:B:1317:LYS:HA	1:B:1323:ILE:CB	2.33	0.59
1:A:477:LEU:HB3	1:A:555:LEU:HD22	1.84	0.58
1:A:1061:LEU:HA	1:A:1101:GLN:CB	2.33	0.58
1:A:1438:LYS:O	1:A:1441:TYR:N	2.36	0.58
1:A:20:GLU:OE2	1:A:181:LYS:NZ	2.34	0.58
1:A:313:TYR:CG	1:A:361:GLY:HA3	2.38	0.58
1:A:836:THR:O	1:A:839:PHE:N	2.36	0.58
1:B:1000:GLU:CB	1:B:1004:SER:O	2.51	0.58
1:B:54:ARG:CZ	1:B:127:LYS:HG3	2.32	0.58
1:A:1200:GLN:O	1:A:1201:GLN:C	2.41	0.58
1:A:839:PHE:O	1:A:842:GLU:CB	2.51	0.58
1:B:852:PHE:O	1:B:853:PRO:O	2.22	0.58
1:B:1200:GLN:O	1:B:1202:GLN:N	2.36	0.58
1:B:592:GLU:O	1:B:594:THR:N	2.36	0.58
1:A:1203:ARG:O	1:A:1207:ASN:CB	2.51	0.58
1:A:1203:ARG:O	1:A:1207:ASN:N	2.37	0.58
1:A:398:TRP:CD2	1:A:424:LYS:HG3	2.38	0.58
1:B:313:TYR:CD1	1:B:361:GLY:HA3	2.38	0.58
1:A:220:ILE:HG23	1:A:220:ILE:O	2.03	0.58
1:B:225:LYS:C	1:B:227:SER:H	2.06	0.58
1:A:600:HIS:O	1:A:603:ARG:CB	2.52	0.58
1:A:282:TRP:CH2	1:A:314:LEU:HD22	2.39	0.58
1:B:1298:CYS:O	1:B:1299:ILE:CB	2.51	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:GLN:O	1:B:574:ILE:N	2.36	0.58
1:A:142:LEU:HB2	1:A:208:GLU:CD	2.24	0.57
1:B:1379:GLU:HA	1:B:1382:ALA:HB3	1.86	0.57
1:B:286:VAL:O	1:B:288:GLN:HG2	2.04	0.57
1:A:489:ASN:OD1	1:A:499:PHE:O	2.23	0.57
1:A:1074:PRO:C	1:A:1076:VAL:H	2.07	0.57
1:A:1210:ALA:O	1:A:1214:VAL:CB	2.53	0.57
1:A:1188:VAL:HA	1:A:1236:LEU:CB	2.34	0.57
1:B:450:SER:OG	1:B:513:GLN:O	2.22	0.57
1:A:364:ILE:O	1:A:394:CYS:SG	2.63	0.57
1:A:1375:ILE:HA	1:A:1378:VAL:CB	2.35	0.57
1:A:555:LEU:HD23	1:A:555:LEU:O	2.05	0.57
1:A:246:GLU:HB2	1:A:427:LYS:HB3	1.86	0.57
1:B:1273:MET:O	1:B:1276:ILE:N	2.38	0.57
1:A:761:VAL:O	1:A:762:ASP:C	2.44	0.57
1:B:863:THR:O	1:B:864:PHE:C	2.42	0.57
1:B:1122:LEU:O	1:B:1125:ILE:N	2.38	0.56
1:B:313:TYR:CZ	1:B:361:GLY:HA3	2.40	0.56
1:A:1294:HIS:O	1:A:1298:CYS:CB	2.54	0.56
1:A:264:LEU:HG	1:A:418:ILE:CD1	2.35	0.56
1:A:71:GLN:HB3	1:A:92:LEU:CD2	2.35	0.56
1:B:55:ASP:OD1	1:B:127:LYS:HD3	2.06	0.56
1:A:744:CYS:O	1:A:1077:SER:CB	2.53	0.56
1:A:39:VAL:O	1:A:41:PRO:HD3	2.04	0.56
1:A:400:HIS:HA	1:A:428:GLU:HG2	1.87	0.56
1:B:1108:ASP:O	1:B:1112:TYR:CB	2.53	0.56
1:B:1435:VAL:CB	1:B:1492:SER:CB	2.83	0.56
1:A:767:CYS:O	1:A:771:GLU:CB	2.54	0.56
1:B:616:ASP:O	1:B:620:SER:CB	2.54	0.56
1:A:1207:ASN:O	1:A:1210:ALA:N	2.37	0.56
1:B:20:GLU:OE2	1:B:181:LYS:NZ	2.36	0.56
1:B:64:ASN:HB2	1:B:66:TYR:CE2	2.40	0.56
1:A:1215:LEU:O	1:A:1218:LEU:N	2.39	0.56
1:B:871:ARG:CB	1:B:980:PHE:HA	2.36	0.56
1:B:194:HIS:CD2	1:B:214:CYS:HB2	2.41	0.56
1:B:165:PRO:HB2	1:B:170:ARG:O	2.06	0.56
1:B:20:GLU:HB2	1:B:217:SER:O	2.06	0.56
1:A:19:ALA:HB2	1:A:218:TRP:CZ3	2.41	0.56
1:A:368:PHE:CD1	1:A:392:HIS:HA	2.41	0.56
1:A:975:ILE:O	1:A:979:GLN:CB	2.54	0.56
1:B:1203:ARG:O	1:B:1207:ASN:CB	2.54	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:ARG:CA	1:A:980:PHE:CB	2.83	0.55
1:B:1434:GLU:O	1:B:1492:SER:CB	2.55	0.55
1:B:170:ARG:NH2	1:B:180:ASP:OD1	2.38	0.55
1:B:769:SER:O	1:B:773:LEU:CB	2.54	0.55
1:A:708:ARG:O	1:A:712:VAL:N	2.39	0.55
1:A:1434:GLU:O	1:A:1492:SER:CB	2.54	0.55
1:A:610:ILE:O	1:A:613:ALA:CB	2.53	0.55
1:B:142:LEU:HD21	1:B:200:LEU:HA	1.88	0.55
1:B:30:LEU:HD12	1:B:36:ARG:NH2	2.20	0.55
1:A:1361:GLU:O	1:A:1364:ARG:CB	2.54	0.55
1:B:1245:CYS:CB	1:B:1341:VAL:H	2.20	0.55
1:B:1284:CYS:CB	1:B:1295:PHE:CB	2.85	0.55
1:B:20:GLU:N	1:B:217:SER:O	2.38	0.55
1:B:633:TYR:O	1:B:636:ASP:N	2.40	0.55
1:B:860:ASN:O	1:B:861:LYS:C	2.45	0.55
1:A:312:HIS:CB	1:A:357:SER:OG	2.54	0.55
1:A:364:ILE:O	1:A:367:ILE:HG22	2.07	0.55
1:A:66:TYR:O	1:A:157:GLU:OE2	2.23	0.55
1:A:1200:GLN:C	1:A:1202:GLN:N	2.56	0.55
1:B:1245:CYS:CB	1:B:1285:SER:O	2.55	0.55
1:B:726:ASP:O	1:B:728:ASP:N	2.40	0.55
1:A:181:LYS:HA	1:A:218:TRP:O	2.07	0.55
1:A:142:LEU:HB2	1:A:208:GLU:OE2	2.06	0.55
1:A:671:VAL:O	1:A:674:ARG:CB	2.55	0.55
1:B:1422:TYR:O	1:B:1426:LEU:CB	2.55	0.55
1:B:1245:CYS:CB	1:B:1285:SER:CB	2.84	0.55
1:B:1285:SER:HA	1:B:1341:VAL:CB	2.37	0.55
1:B:136:LYS:HB3	1:B:189:ALA:HA	1.89	0.55
1:A:861:LYS:O	1:A:864:PHE:N	2.40	0.54
1:A:885:LEU:O	1:A:888:THR:CA	2.55	0.54
1:A:844:LEU:HA	1:A:847:VAL:CB	2.38	0.54
1:B:13:ASP:OD1	1:B:226:TRP:N	2.40	0.54
1:B:511:ARG:O	1:B:511:ARG:HG2	2.07	0.54
1:A:244:HIS:CD2	1:A:264:LEU:HD11	2.43	0.54
1:A:788:MET:O	1:A:790:VAL:N	2.41	0.54
1:B:1234:MET:O	1:B:1237:ALA:HB3	2.08	0.54
1:B:389:ARG:CZ	1:B:425:GLU:O	2.55	0.54
1:A:999:ARG:HA	1:A:1007:GLN:HA	1.88	0.54
1:A:223:PHE:CD1	1:A:292:CYS:HA	2.43	0.54
1:B:270:GLN:NE2	1:B:1257:LYS:HA	2.22	0.54
1:B:34:ASP:OD2	1:B:36:ARG:HB2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1315:ILE:O	1:A:1319:GLU:CB	2.56	0.54
1:B:18:TYR:HA	1:B:25:GLY:O	2.08	0.54
1:B:65:ARG:H	1:B:103:ASN:CG	2.11	0.54
1:A:142:LEU:HD21	1:A:200:LEU:HA	1.88	0.54
1:A:142:LEU:HD23	1:A:200:LEU:HD23	1.90	0.54
1:A:20:GLU:OE1	1:A:219:LYS:HB2	2.08	0.54
1:A:39:VAL:HG21	1:A:195:ALA:HB1	1.89	0.54
1:A:477:LEU:O	1:A:555:LEU:CD2	2.56	0.54
1:A:756:SER:HA	1:A:759:LEU:CB	2.37	0.54
1:A:789:HIS:O	1:A:790:VAL:CB	2.56	0.54
1:B:744:CYS:CB	1:B:1081:GLN:O	2.56	0.54
1:B:130:LYS:HB2	1:B:151:LEU:HD22	1.90	0.54
1:A:879:TYR:H	1:A:884:LEU:CB	2.21	0.54
1:B:270:GLN:HE22	1:B:1257:LYS:HA	1.73	0.54
1:B:225:LYS:O	1:B:227:SER:N	2.38	0.54
1:B:836:THR:O	1:B:838:GLU:N	2.41	0.54
1:A:108:ARG:O	1:A:111:LEU:HB2	2.08	0.53
1:A:29:THR:HG22	1:A:151:LEU:HD11	1.90	0.53
1:A:1251:ASN:CB	1:A:1283:LEU:HA	2.39	0.53
1:A:257:ARG:O	1:A:259:LYS:HG3	2.08	0.53
1:A:316:ALA:HA	1:A:354:SER:O	2.09	0.53
1:B:19:ALA:O	1:B:24:ASN:HA	2.08	0.53
1:B:14:ILE:HG22	1:B:57:LEU:HD22	1.91	0.53
1:B:313:TYR:CE1	1:B:361:GLY:HA3	2.43	0.53
1:A:10:HIS:HA	1:A:113:THR:O	2.09	0.53
1:A:115:ILE:CG2	1:A:116:GLN:N	2.71	0.53
1:A:196:SER:OG	1:A:197:SER:N	2.41	0.53
1:A:371:ASP:HB3	1:A:389:ARG:O	2.09	0.53
1:A:1207:ASN:O	1:A:1209:GLY:N	2.41	0.53
1:A:707:ILE:CB	1:A:733:TYR:O	2.57	0.53
1:A:871:ARG:HA	1:A:980:PHE:HA	1.89	0.53
1:B:186:PRO:HB2	1:B:189:ALA:HB3	1.91	0.53
1:B:1191:SER:CB	1:B:1236:LEU:O	2.57	0.53
1:B:772:ASN:O	1:B:773:LEU:C	2.46	0.53
1:B:856:ASP:HA	1:B:859:LYS:CB	2.39	0.53
1:B:882:SER:O	1:B:885:LEU:CA	2.56	0.53
1:A:40:GLN:CB	1:A:43:ALA:CB	2.87	0.53
1:A:63:MET:SD	1:A:120:VAL:HG21	2.48	0.53
1:A:867:VAL:CB	1:A:976:GLU:CB	2.87	0.53
1:B:194:HIS:CD2	1:B:214:CYS:CB	2.92	0.53
1:A:38:VAL:HG11	1:A:200:LEU:HD11	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:LEU:HD12	1:B:553:CYS:SG	2.49	0.53
1:A:1201:GLN:O	1:A:1202:GLN:C	2.47	0.52
1:A:353:TYR:O	1:A:420:THR:HG22	2.08	0.52
1:B:484:VAL:HG11	1:B:562:HIS:HB3	1.91	0.52
1:A:142:LEU:HD12	1:A:198:HIS:HB3	1.91	0.52
1:A:225:LYS:O	1:A:227:SER:N	2.39	0.52
1:A:657:LEU:O	1:A:659:PRO:N	2.41	0.52
1:B:669:LYS:C	1:B:671:VAL:N	2.62	0.52
1:A:1438:LYS:HA	1:A:1441:TYR:CB	2.39	0.52
1:A:772:ASN:O	1:A:773:LEU:C	2.48	0.52
1:B:1200:GLN:C	1:B:1202:GLN:N	2.62	0.52
1:A:113:THR:O	1:A:114:VAL:C	2.44	0.52
1:A:369:GLU:OE2	1:A:391:ARG:NH2	2.33	0.52
1:A:581:MET:O	1:A:585:ILE:CB	2.57	0.52
1:B:1476:LYS:O	1:B:1479:THR:N	2.42	0.52
1:B:701:ARG:O	1:B:703:SER:N	2.43	0.52
1:B:1207:ASN:O	1:B:1210:ALA:N	2.43	0.52
1:B:1245:CYS:CB	1:B:1341:VAL:N	2.72	0.52
1:A:15:CYS:HA	1:A:223:PHE:N	2.25	0.52
1:A:299:TRP:CZ2	1:A:372:PRO:HD3	2.45	0.52
1:A:511:ARG:O	1:A:511:ARG:HG2	2.10	0.52
1:A:871:ARG:CB	1:A:980:PHE:N	2.72	0.52
1:B:1116:LYS:O	1:B:1117:GLN:C	2.48	0.52
1:B:124:LEU:HD13	1:B:131:TYR:CE1	2.45	0.52
1:B:69:GLN:HG2	1:B:73:TRP:CZ2	2.45	0.52
1:A:117:TYR:CE2	1:A:165:PRO:HB3	2.43	0.52
1:A:1379:GLU:HA	1:A:1382:ALA:HB3	1.92	0.52
1:A:753:ASN:O	1:A:754:GLU:C	2.48	0.52
1:B:194:HIS:CG	1:B:214:CYS:HG	2.28	0.52
1:B:830:LYS:O	1:B:833:PHE:CB	2.58	0.52
1:A:447:ASN:O	1:A:448:ASP:C	2.45	0.52
1:A:514:ASN:ND2	1:A:517:LYS:HD3	2.25	0.52
1:B:134:VAL:HG23	1:B:161:PHE:CZ	2.45	0.52
1:B:470:ARG:NH2	1:B:548:PRO:HA	2.25	0.52
1:B:992:CYS:O	1:B:995:CYS:N	2.43	0.52
1:A:772:ASN:O	1:A:774:PRO:N	2.43	0.52
1:B:1064:LEU:CB	1:B:1101:GLN:CB	2.87	0.52
1:B:627:GLU:O	1:B:629:ARG:N	2.43	0.51
1:B:669:LYS:C	1:B:671:VAL:H	2.13	0.51
1:A:727:ARG:O	1:A:730:LEU:N	2.43	0.51
1:B:485:THR:CG2	1:B:562:HIS:ND1	2.73	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1338:GLY:O	1:A:1342:LEU:CB	2.59	0.51
1:A:861:LYS:O	1:A:862:LEU:C	2.47	0.51
1:B:1200:GLN:C	1:B:1202:GLN:H	2.14	0.51
1:B:859:LYS:O	1:B:860:ASN:C	2.49	0.51
1:A:1346:ASN:O	1:A:1348:ARG:N	2.44	0.51
1:A:15:CYS:SG	1:A:222:LEU:HG	2.51	0.51
1:A:148:ARG:HG2	1:A:150:THR:HG22	1.93	0.51
1:A:1436:GLU:CB	1:A:1493:PRO:C	2.79	0.51
1:A:14:ILE:O	1:A:222:LEU:HD23	2.10	0.51
1:B:288:GLN:HG3	1:B:292:CYS:O	2.11	0.51
1:B:669:LYS:O	1:B:672:LEU:N	2.43	0.51
1:B:860:ASN:O	1:B:863:THR:CB	2.59	0.51
1:B:888:THR:O	1:B:889:LYS:C	2.49	0.51
1:B:967:VAL:HA	1:B:970:THR:CB	2.40	0.51
1:A:20:GLU:OE2	1:A:181:LYS:CE	2.58	0.51
1:A:460:LEU:HD13	1:A:465:ILE:HG23	1.93	0.51
1:A:843:TYR:O	1:A:847:VAL:CB	2.59	0.51
1:A:998:LYS:CB	1:A:1008:SER:CB	2.89	0.51
1:B:1251:ASN:O	1:B:1255:LEU:CB	2.58	0.51
1:A:140:ALA:HB2	1:A:147:MET:O	2.11	0.51
1:A:697:TRP:CB	1:A:726:ASP:CB	2.89	0.51
1:A:66:TYR:CD1	1:A:69:GLN:OE1	2.64	0.51
1:B:1084:PHE:O	1:B:1087:PHE:CB	2.59	0.51
1:B:196:SER:OG	1:B:197:SER:N	2.44	0.51
1:A:11:ILE:HG21	1:A:62:PRO:HG3	1.93	0.50
1:A:241:ARG:NH2	1:A:439:GLU:OE1	2.42	0.50
1:B:122:GLN:HG2	1:B:159:SER:O	2.10	0.50
1:B:665:LEU:O	1:B:666:ILE:CB	2.59	0.50
1:A:1034:GLU:HA	1:A:1037:ALA:HB3	1.93	0.50
1:A:21:GLY:HA3	1:A:216:THR:HA	1.94	0.50
1:A:398:TRP:CH2	1:A:424:LYS:HE3	2.46	0.50
1:A:473:VAL:O	1:A:476:LEU:N	2.44	0.50
1:A:708:ARG:O	1:A:712:VAL:CB	2.58	0.50
1:A:999:ARG:HA	1:A:1007:GLN:CA	2.40	0.50
1:B:1215:LEU:O	1:B:1218:LEU:N	2.45	0.50
1:A:8:PHE:O	1:A:10:HIS:CE1	2.64	0.50
1:A:255:GLU:HA	1:A:259:LYS:O	2.11	0.50
1:B:1207:ASN:O	1:B:1208:MET:C	2.49	0.50
1:B:609:HIS:O	1:B:610:ILE:C	2.50	0.50
1:A:224:MET:SD	1:A:228:ASP:CB	2.99	0.50
1:A:502:PRO:HG3	1:A:565:GLN:HG2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:HIS:CD2	1:B:214:CYS:SG	3.05	0.50
1:B:38:VAL:HG11	1:B:200:LEU:HD11	1.93	0.50
1:A:306:LYS:HB2	1:A:313:TYR:CZ	2.47	0.50
1:A:852:PHE:O	1:A:856:ASP:CB	2.60	0.50
1:A:856:ASP:O	1:A:860:ASN:CB	2.60	0.50
1:B:1061:LEU:O	1:B:1065:LEU:N	2.31	0.50
1:B:711:SER:CB	1:B:737:LEU:CB	2.89	0.50
1:A:1375:ILE:C	1:A:1378:VAL:H	2.15	0.50
1:A:475:LYS:NZ	1:A:479:ASP:OD1	2.42	0.50
1:A:581:MET:HA	1:A:591:ALA:CB	2.39	0.50
1:A:645:ILE:O	1:A:646:PRO:C	2.50	0.50
1:A:730:LEU:O	1:A:733:TYR:N	2.45	0.50
1:B:891:LEU:HA	1:B:894:ILE:H	1.77	0.50
1:A:245:ALA:HB2	1:A:429:ALA:O	2.11	0.50
1:A:353:TYR:HB2	1:A:420:THR:CG2	2.42	0.50
1:A:871:ARG:CA	1:A:980:PHE:HA	2.42	0.50
1:A:9:LEU:HD13	1:A:178:ILE:CD1	2.42	0.50
1:B:1371:LEU:O	1:B:1375:ILE:CA	2.60	0.50
1:B:1375:ILE:HA	1:B:1378:VAL:CB	2.42	0.50
1:B:194:HIS:CG	1:B:214:CYS:SG	3.05	0.50
1:B:36:ARG:HH12	1:B:200:LEU:HD13	1.76	0.50
1:B:313:TYR:CG	1:B:361:GLY:CA	2.94	0.50
1:B:1215:LEU:O	1:B:1216:GLU:C	2.50	0.50
1:B:1357:MET:O	1:B:1359:ARG:N	2.44	0.50
1:B:39:VAL:HG23	1:B:207:ASN:HB2	1.94	0.50
1:B:263:PHE:CE2	1:B:415:MET:HG2	2.46	0.50
1:B:48:ASN:O	1:B:49:PRO:C	2.49	0.50
1:B:127:LYS:O	1:B:127:LYS:HG2	2.12	0.49
1:B:140:ALA:HB3	1:B:143:GLU:O	2.12	0.49
1:B:502:PRO:HG3	1:B:565:GLN:HG2	1.93	0.49
1:B:978:LEU:O	1:B:981:ILE:CA	2.60	0.49
1:A:40:GLN:CB	1:A:43:ALA:HB2	2.42	0.49
1:B:608:LYS:O	1:B:611:THR:CB	2.60	0.49
1:A:554:ARG:CB	1:A:557:TYR:CB	2.91	0.49
1:B:1134:TYR:O	1:B:1230:MET:CB	2.61	0.49
1:B:1382:ALA:HA	1:B:1385:THR:CB	2.42	0.49
1:B:456:ILE:HG12	1:B:473:VAL:HG21	1.94	0.49
1:B:523:LEU:CD1	1:B:553:CYS:SG	3.01	0.49
1:A:632:ASP:O	1:A:635:SER:N	2.45	0.49
1:B:1027:ALA:O	1:B:1029:ASP:N	2.38	0.49
1:B:235:LYS:O	1:B:236:GLY:C	2.51	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:LYS:HZ2	1:B:266:THR:HA	1.78	0.49
1:A:103:ASN:O	1:A:107:ASN:ND2	2.46	0.49
1:A:162:TYR:HB3	1:A:164:GLN:CD	2.33	0.49
1:A:753:ASN:O	1:A:755:ILE:N	2.46	0.49
1:B:1310:LYS:O	1:B:1311:PHE:CB	2.61	0.49
1:B:603:ARG:O	1:B:604:LYS:CB	2.61	0.49
1:B:720:LYS:O	1:B:722:GLY:N	2.44	0.49
1:A:125:HIS:O	1:A:129:ASN:HA	2.12	0.49
1:A:977:ILE:C	1:A:979:GLN:H	2.16	0.49
1:B:1085:ARG:C	1:B:1087:PHE:N	2.66	0.49
1:B:354:SER:HA	1:B:419:GLY:HA2	1.95	0.49
1:B:576:LYS:O	1:B:578:PHE:N	2.45	0.49
1:B:836:THR:O	1:B:839:PHE:N	2.46	0.49
1:A:1096:ALA:O	1:A:1097:PHE:C	2.50	0.49
1:A:428:GLU:CA	1:A:428:GLU:OE2	2.58	0.49
1:A:125:HIS:CE1	1:A:127:LYS:HB3	2.48	0.49
1:A:514:ASN:O	1:A:518:GLN:HG2	2.12	0.49
1:A:549:PHE:O	1:A:552:ILE:N	2.45	0.49
1:A:992:CYS:C	1:A:994:LEU:N	2.65	0.49
1:B:140:ALA:HB2	1:B:147:MET:O	2.13	0.49
1:A:841:GLU:O	1:A:844:LEU:CB	2.60	0.48
1:A:96:ALA:O	1:A:100:LYS:HB2	2.13	0.48
1:B:18:TYR:CE1	1:B:25:GLY:CA	2.96	0.48
1:B:242:LEU:HD23	1:B:432:ILE:HD13	1.94	0.48
1:B:391:ARG:HD2	1:B:396:ASN:OD1	2.13	0.48
1:B:654:LYS:O	1:B:657:LEU:C	2.50	0.48
1:A:125:HIS:HE1	1:A:127:LYS:HB3	1.79	0.48
1:A:1416:PRO:O	1:A:1417:GLU:C	2.50	0.48
1:A:735:TYR:O	1:A:738:ASN:O	2.32	0.48
1:B:236:GLY:CA	1:B:286:VAL:H	2.25	0.48
1:A:20:GLU:OE1	1:A:181:LYS:CD	2.61	0.48
1:A:20:GLU:OE2	1:A:181:LYS:HE2	2.12	0.48
1:B:1207:ASN:C	1:B:1209:GLY:N	2.64	0.48
1:B:285:GLU:C	1:B:287:VAL:N	2.66	0.48
1:B:888:THR:O	1:B:890:ILE:N	2.46	0.48
1:A:725:GLU:CB	1:A:865:GLU:CB	2.91	0.48
1:B:188:ASN:OD1	1:B:189:ALA:N	2.46	0.48
1:B:47:ASN:O	1:B:49:PRO:CD	2.58	0.48
1:B:504:ARG:HD2	1:B:567:TYR:CZ	2.49	0.48
1:B:739:LEU:O	1:B:740:PHE:C	2.49	0.48
1:A:254:ASP:O	1:A:260:GLN:HA	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:LEU:CB	1:A:779:ALA:N	2.77	0.48
1:B:20:GLU:OE1	1:B:219:LYS:HB2	2.13	0.48
1:B:863:THR:O	1:B:865:GLU:N	2.46	0.48
1:B:484:VAL:CG1	1:B:562:HIS:HB3	2.43	0.48
1:A:1076:VAL:O	1:A:1079:ALA:HB3	2.14	0.48
1:A:755:ILE:O	1:A:756:SER:C	2.50	0.48
1:A:759:LEU:O	1:A:760:ASP:O	2.32	0.48
1:B:236:GLY:H	1:B:286:VAL:CB	2.26	0.48
1:B:165:PRO:CB	1:B:170:ARG:O	2.62	0.48
1:B:666:ILE:N	1:B:667:GLU:HA	2.29	0.48
1:A:1189:GLN:C	1:A:1191:SER:H	2.18	0.48
1:A:992:CYS:O	1:A:993:LEU:C	2.51	0.48
1:B:32:LEU:HD22	1:B:128:SER:HB2	1.96	0.48
1:B:166:PHE:HE1	1:B:167:TYR:CE1	2.32	0.48
1:B:18:TYR:CE1	1:B:25:GLY:N	2.82	0.48
1:A:235:LYS:HD3	1:A:235:LYS:HA	1.64	0.47
1:A:703:SER:O	1:A:733:TYR:CA	2.60	0.47
1:B:744:CYS:C	1:B:745:LEU:O	2.51	0.47
1:A:1420:ILE:O	1:A:1424:ASN:CB	2.62	0.47
1:A:179:GLY:H	1:A:220:ILE:HG23	1.79	0.47
1:A:30:LEU:HB2	1:A:34:ASP:OD2	2.14	0.47
1:B:1076:VAL:O	1:B:1079:ALA:HB3	2.14	0.47
1:B:853:PRO:O	1:B:854:PHE:C	2.51	0.47
1:A:20:GLU:HB2	1:A:217:SER:OG	2.14	0.47
1:A:551:HIS:C	1:A:552:ILE:HG13	2.34	0.47
1:A:704:ASN:O	1:A:736:GLN:CB	2.62	0.47
1:A:891:LEU:O	1:A:894:ILE:N	2.45	0.47
1:B:166:PHE:CE1	1:B:167:TYR:CE1	3.02	0.47
1:A:1298:CYS:O	1:A:1299:ILE:CB	2.63	0.47
1:A:39:VAL:HG23	1:A:207:ASN:HB2	1.96	0.47
1:A:671:VAL:O	1:A:672:LEU:C	2.52	0.47
1:A:69:GLN:CD	1:A:73:TRP:HZ2	2.18	0.47
1:B:1417:GLU:O	1:B:1420:ILE:N	2.44	0.47
1:B:1481:ILE:O	1:B:1485:ILE:CB	2.62	0.47
1:A:162:TYR:HB3	1:A:164:GLN:HE22	1.78	0.47
1:A:705:LYS:C	1:A:707:ILE:N	2.67	0.47
1:B:482:TYR:HD1	1:B:489:ASN:O	1.98	0.47
1:A:98:LEU:HD23	1:A:101:LYS:HE2	1.97	0.47
1:A:115:ILE:CG2	1:A:116:GLN:H	2.27	0.47
1:B:883:ASP:O	1:B:887:LEU:CB	2.63	0.47
1:A:286:VAL:O	1:A:288:GLN:HG2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ILE:CB	1:A:736:GLN:CB	2.92	0.47
1:A:847:VAL:CB	1:A:897:CYS:O	2.63	0.47
1:B:409:GLU:HG3	1:B:409:GLU:O	2.14	0.47
1:B:64:ASN:CB	1:B:66:TYR:CE2	2.98	0.47
1:A:891:LEU:O	1:A:892:LEU:C	2.53	0.47
1:B:1289:GLU:C	1:B:1291:VAL:H	2.18	0.47
1:A:1078:GLY:O	1:A:1081:GLN:CB	2.63	0.47
1:A:115:ILE:HG22	1:A:116:GLN:N	2.30	0.47
1:B:1061:LEU:O	1:B:1064:LEU:CB	2.62	0.47
1:A:113:THR:O	1:A:115:ILE:N	2.47	0.46
1:A:510:MET:SD	1:A:515:ILE:HG21	2.55	0.46
1:B:1363:ASP:O	1:B:1366:ASP:CB	2.63	0.46
1:A:20:GLU:CB	1:A:217:SER:OG	2.64	0.46
1:A:680:VAL:C	1:A:682:THR:N	2.68	0.46
1:A:871:ARG:HA	1:A:980:PHE:CA	2.45	0.46
1:A:69:GLN:HA	1:A:96:ALA:HB2	1.97	0.46
1:B:470:ARG:HH22	1:B:548:PRO:HA	1.79	0.46
1:B:49:PRO:O	1:B:50:PRO:O	2.34	0.46
1:B:872:ASN:O	1:B:875:TYR:CB	2.63	0.46
1:A:160:TRP:O	1:A:186:PRO:HA	2.16	0.46
1:B:510:MET:SD	1:B:515:ILE:HG21	2.55	0.46
1:B:980:PHE:O	1:B:981:ILE:C	2.53	0.46
1:A:1477:TYR:O	1:A:1481:ILE:CB	2.63	0.46
1:A:596:THR:C	1:A:598:LEU:N	2.66	0.46
1:A:769:SER:O	1:A:773:LEU:CB	2.64	0.46
1:A:162:TYR:HB2	1:A:185:ASN:O	2.15	0.46
1:A:68:ALA:HA	1:A:71:GLN:HB2	1.98	0.46
1:B:1094:LEU:O	1:B:1095:GLN:C	2.54	0.46
1:B:60:LEU:HD13	1:B:123:LEU:HD23	1.96	0.46
1:B:389:ARG:NH2	1:B:425:GLU:H	2.14	0.46
1:B:891:LEU:HA	1:B:894:ILE:CB	2.45	0.46
1:A:40:GLN:CB	1:A:43:ALA:HB3	2.46	0.46
1:A:479:ASP:O	1:A:482:TYR:HB3	2.16	0.46
1:A:72:PHE:O	1:A:72:PHE:CD1	2.69	0.46
1:A:1065:LEU:HA	1:A:1104:VAL:CB	2.46	0.46
1:B:1028:LEU:O	1:B:1031:GLU:N	2.48	0.46
1:B:1034:GLU:HA	1:B:1037:ALA:HB3	1.98	0.46
1:B:32:LEU:CD2	1:B:128:SER:HB2	2.46	0.46
1:B:231:ASP:OD2	1:B:434:PRO:HG3	2.16	0.46
1:B:993:LEU:HA	1:B:996:ILE:CB	2.46	0.46
1:A:581:MET:O	1:A:591:ALA:CB	2.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:LEU:O	1:A:716:ALA:C	2.54	0.46
1:B:1238:HIS:O	1:B:1240:PHE:N	2.49	0.46
1:B:707:ILE:CB	1:B:736:GLN:CB	2.94	0.46
1:A:1378:VAL:O	1:A:1382:ALA:HB2	2.16	0.45
1:B:139:PRO:O	1:B:148:ARG:HB2	2.16	0.45
1:B:194:HIS:NE2	1:B:214:CYS:SG	2.89	0.45
1:B:18:TYR:CD1	1:B:25:GLY:C	2.90	0.45
1:B:498:VAL:HB	1:B:499:PHE:CD1	2.51	0.45
1:A:1001:PHE:O	1:A:1002:ASP:CB	2.63	0.45
1:B:622:VAL:CA	1:B:631:LEU:CB	2.89	0.45
1:B:65:ARG:HH22	1:B:106:GLU:HG2	1.81	0.45
1:B:315:ALA:HB1	1:B:365:SER:OG	2.16	0.45
1:B:220:ILE:HG23	1:B:220:ILE:O	2.17	0.45
1:B:836:THR:O	1:B:837:MET:C	2.55	0.45
1:A:485:THR:HB	1:A:501:LYS:O	2.17	0.45
1:A:477:LEU:HD11	1:A:556:CYS:SG	2.57	0.45
1:A:751:ALA:O	1:A:752:ILE:C	2.55	0.45
1:A:833:PHE:O	1:A:836:THR:CB	2.65	0.45
1:B:58:PHE:CZ	1:B:125:HIS:CD2	3.05	0.45
1:B:853:PRO:C	1:B:855:SER:N	2.69	0.45
1:A:121:ILE:HD13	1:A:161:PHE:O	2.16	0.45
1:A:32:LEU:CD2	1:A:128:SER:HA	2.46	0.45
1:A:39:VAL:O	1:A:41:PRO:CD	2.65	0.45
1:B:316:ALA:HA	1:B:354:SER:O	2.16	0.45
1:A:769:SER:HA	1:A:773:LEU:CB	2.47	0.45
1:A:85:ASP:HB2	1:A:88:LEU:HB3	1.99	0.45
1:B:1085:ARG:O	1:B:1087:PHE:N	2.50	0.45
1:B:1201:GLN:O	1:B:1203:ARG:N	2.50	0.45
1:B:1457:ILE:O	1:B:1458:CYS:O	2.34	0.45
1:B:395:THR:O	1:B:396:ASN:C	2.55	0.45
1:B:860:ASN:O	1:B:863:THR:CA	2.65	0.45
1:B:889:LYS:O	1:B:892:LEU:CB	2.65	0.45
1:A:998:LYS:C	1:A:1007:GLN:HA	2.37	0.45
1:A:245:ALA:CB	1:A:429:ALA:O	2.65	0.45
1:A:977:ILE:O	1:A:979:GLN:N	2.50	0.45
1:B:124:LEU:CD1	1:B:131:TYR:CE1	3.00	0.45
1:B:1355:ILE:C	1:B:1357:MET:H	2.20	0.45
1:A:67:SER:O	1:A:71:GLN:OE1	2.34	0.45
1:B:315:ALA:CB	1:B:365:SER:O	2.64	0.45
1:A:196:SER:OG	1:A:198:HIS:N	2.39	0.45
1:A:222:LEU:HD21	1:A:224:MET:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:TYR:CZ	1:A:395:THR:HG22	2.52	0.45
1:B:1251:ASN:CB	1:B:1283:LEU:HA	2.47	0.45
1:B:1371:LEU:O	1:B:1372:MET:C	2.55	0.45
1:B:961:GLU:CB	1:B:963:GLU:H	2.30	0.45
1:A:224:MET:HG3	1:A:293:ARG:CB	2.47	0.44
1:B:1201:GLN:O	1:B:1202:GLN:C	2.55	0.44
1:B:143:GLU:HB2	1:B:210:ASN:HD21	1.82	0.44
1:B:143:GLU:HB2	1:B:210:ASN:ND2	2.32	0.44
1:A:589:VAL:O	1:A:592:GLU:CB	2.65	0.44
1:A:596:THR:HA	1:A:599:LEU:CB	2.47	0.44
1:B:1374:HIS:CA	1:B:1377:LEU:CB	2.95	0.44
1:A:1037:ALA:C	1:A:1039:GLY:N	2.70	0.44
1:A:1094:LEU:O	1:A:1095:GLN:C	2.56	0.44
1:A:1381:LEU:C	1:A:1385:THR:H	2.20	0.44
1:A:601:ASN:C	1:A:603:ARG:N	2.70	0.44
1:A:840:VAL:O	1:A:841:GLU:C	2.52	0.44
1:B:1242:GLN:O	1:B:1243:ASN:CB	2.65	0.44
1:B:304:ARG:CB	1:B:366:SER:O	2.65	0.44
1:B:243:PHE:O	1:B:430:PHE:HA	2.18	0.44
1:B:709:SER:O	1:B:713:ARG:CB	2.65	0.44
1:A:1215:LEU:O	1:A:1216:GLU:C	2.56	0.44
1:A:1253:ALA:HA	1:A:1256:HIS:CB	2.48	0.44
1:A:1371:LEU:O	1:A:1372:MET:C	2.56	0.44
1:A:179:GLY:O	1:A:180:ASP:C	2.55	0.44
1:A:453:LEU:O	1:A:457:ALA:HB3	2.17	0.44
1:B:1200:GLN:O	1:B:1201:GLN:C	2.56	0.44
1:B:18:TYR:CZ	1:B:24:ASN:HB3	2.52	0.44
1:B:735:TYR:C	1:B:737:LEU:H	2.21	0.44
1:B:769:SER:HA	1:B:773:LEU:CB	2.48	0.44
1:B:788:MET:O	1:B:790:VAL:N	2.50	0.44
1:A:249:LYS:HB2	1:A:264:LEU:HD13	1.99	0.44
1:A:313:TYR:CD1	1:A:313:TYR:N	2.84	0.44
1:A:457:ALA:HB1	1:A:521:LYS:O	2.17	0.44
1:B:1116:LYS:O	1:B:1119:LEU:CA	2.63	0.44
1:B:484:VAL:HG13	1:B:485:THR:HG23	2.00	0.44
1:B:523:LEU:HD11	1:B:556:CYS:SG	2.58	0.44
1:B:761:VAL:O	1:B:762:ASP:C	2.55	0.44
1:B:831:GLU:O	1:B:832:ARG:C	2.55	0.44
1:B:1371:LEU:O	1:B:1375:ILE:CB	2.65	0.44
1:B:701:ARG:CB	1:B:729:ILE:CB	2.95	0.44
1:A:225:LYS:C	1:A:227:SER:H	2.19	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:O	1:A:249:LYS:HG3	2.17	0.44
1:A:598:LEU:O	1:A:599:LEU:C	2.56	0.44
1:B:299:TRP:HB2	1:B:382:VAL:CB	2.48	0.44
1:B:54:ARG:O	1:B:54:ARG:HG2	2.18	0.44
1:B:588:ASP:C	1:B:590:LEU:H	2.21	0.44
1:B:741:ALA:CB	1:B:876:PHE:HA	2.47	0.44
1:A:1245:CYS:CB	1:A:1341:VAL:H	2.30	0.44
1:A:21:GLY:CA	1:A:216:THR:HA	2.47	0.44
1:A:353:TYR:HB2	1:A:420:THR:HG21	1.99	0.44
1:A:484:VAL:HG13	1:A:485:THR:HG23	2.00	0.44
1:B:555:LEU:HD23	1:B:555:LEU:O	2.17	0.44
1:B:507:GLN:HG2	1:B:563:SER:HA	2.00	0.44
1:B:99:GLU:O	1:B:103:ASN:ND2	2.51	0.44
1:A:264:LEU:CG	1:A:418:ILE:HD11	2.46	0.44
1:A:69:GLN:HG2	1:A:73:TRP:NE1	2.32	0.44
1:A:773:LEU:CB	1:A:779:ALA:H	2.31	0.44
1:B:364:ILE:O	1:B:394:CYS:SG	2.76	0.44
1:A:224:MET:HE2	1:A:293:ARG:O	2.17	0.43
1:A:166:PHE:CD1	1:A:167:TYR:CE2	3.06	0.43
1:A:237:GLY:N	1:A:284:VAL:O	2.48	0.43
1:A:306:LYS:HD2	1:A:313:TYR:OH	2.17	0.43
1:A:317:GLU:N	1:A:354:SER:O	2.51	0.43
1:A:364:ILE:HG22	1:A:394:CYS:SG	2.59	0.43
1:A:581:MET:CB	1:A:591:ALA:HB1	2.47	0.43
1:A:602:ASN:O	1:A:606:LEU:CB	2.66	0.43
1:B:1284:CYS:O	1:B:1292:VAL:CB	2.66	0.43
1:B:451:LYS:HE2	1:B:451:LYS:HA	2.00	0.43
1:A:1362:ARG:O	1:A:1363:ASP:C	2.55	0.43
1:A:142:LEU:CD2	1:A:200:LEU:HD23	2.48	0.43
1:A:57:LEU:HD21	1:A:223:PHE:HB2	2.00	0.43
1:A:498:VAL:HG12	1:A:499:PHE:HD1	1.82	0.43
1:A:707:ILE:CB	1:A:737:LEU:H	2.26	0.43
1:B:32:LEU:CD2	1:B:128:SER:CB	2.96	0.43
1:B:681:SER:O	1:B:682:THR:C	2.57	0.43
1:B:69:GLN:O	1:B:73:TRP:CE2	2.71	0.43
1:A:20:GLU:C	1:A:217:SER:H	2.22	0.43
1:A:621:LEU:O	1:A:625:ASN:CB	2.66	0.43
1:A:682:THR:O	1:A:686:ALA:HB3	2.19	0.43
1:B:1292:VAL:HA	1:B:1295:PHE:CB	2.49	0.43
1:B:271:SER:O	1:B:272:ALA:C	2.56	0.43
1:B:313:TYR:CD1	1:B:361:GLY:CA	3.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ALA:HB2	1:B:355:LEU:HD12	2.00	0.43
1:B:627:GLU:O	1:B:628:PRO:C	2.57	0.43
1:A:549:PHE:O	1:A:551:HIS:N	2.52	0.43
1:B:177:VAL:HG12	1:B:178:ILE:N	2.33	0.43
1:B:484:VAL:O	1:B:484:VAL:HG22	2.19	0.43
1:B:49:PRO:O	1:B:50:PRO:C	2.55	0.43
1:B:826:LYS:O	1:B:828:GLU:N	2.51	0.43
1:B:960:PRO:O	1:B:961:GLU:CB	2.66	0.43
1:A:114:VAL:CG1	1:A:175:SER:HB3	2.49	0.43
1:A:196:SER:HB3	1:A:208:GLU:O	2.18	0.43
1:A:479:ASP:O	1:A:482:TYR:N	2.52	0.43
1:A:483:PHE:O	1:A:506:ARG:NH1	2.48	0.43
1:A:680:VAL:C	1:A:682:THR:H	2.20	0.43
1:A:73:TRP:N	1:A:73:TRP:CD1	2.87	0.43
1:B:1293:GLN:CB	1:B:1345:TYR:O	2.67	0.43
1:B:18:TYR:CE1	1:B:25:GLY:HA2	2.53	0.43
1:B:586:GLY:O	1:B:588:ASP:N	2.52	0.43
1:A:231:ASP:OD2	1:A:434:PRO:HG3	2.19	0.43
1:A:586:GLY:O	1:A:587:TYR:C	2.54	0.43
1:B:133:THR:HG21	1:B:156:ASN:HD21	1.84	0.43
1:B:224:MET:SD	1:B:228:ASP:CB	3.06	0.43
1:B:485:THR:HG21	1:B:562:HIS:ND1	2.33	0.43
1:B:960:PRO:O	1:B:963:GLU:CB	2.67	0.43
1:A:315:ALA:HB1	1:A:365:SER:OG	2.18	0.43
1:A:95:ALA:O	1:A:99:GLU:HB2	2.18	0.43
1:B:38:VAL:CG1	1:B:200:LEU:HD11	2.49	0.43
1:A:701:ARG:O	1:A:703:SER:O	2.36	0.43
1:B:10:HIS:CE1	1:B:114:VAL:HG22	2.53	0.43
1:B:1291:VAL:C	1:B:1293:GLN:N	2.72	0.43
1:B:134:VAL:HB	1:B:189:ALA:CB	2.49	0.43
1:A:18:TYR:HA	1:A:25:GLY:O	2.19	0.43
1:A:15:CYS:HA	1:A:223:PHE:H	1.84	0.43
1:A:402:THR:O	1:A:403:ASN:OD1	2.37	0.43
1:A:69:GLN:O	1:A:73:TRP:CD1	2.71	0.43
1:A:853:PRO:O	1:A:856:ASP:N	2.51	0.43
1:B:978:LEU:O	1:B:979:GLN:C	2.55	0.43
1:A:1000:GLU:CB	1:A:1005:ASN:HA	2.49	0.42
1:A:1103:LEU:O	1:A:1105:THR:N	2.52	0.42
1:A:1369:SER:O	1:A:1370:PRO:C	2.56	0.42
1:A:744:CYS:CB	1:A:1075:LEU:HA	2.48	0.42
1:A:753:ASN:C	1:A:755:ILE:N	2.70	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1285:SER:O	1:B:1341:VAL:CB	2.67	0.42
1:B:1357:MET:O	1:B:1358:MET:C	2.57	0.42
1:A:361:GLY:O	1:A:366:SER:OG	2.36	0.42
1:B:95:ALA:O	1:B:96:ALA:C	2.55	0.42
1:A:316:ALA:HB3	1:A:392:HIS:CE1	2.54	0.42
1:A:499:PHE:HB2	1:A:501:LYS:HZ3	1.84	0.42
1:B:1062:ARG:O	1:B:1066:HIS:N	2.50	0.42
1:B:1134:TYR:C	1:B:1230:MET:CB	2.87	0.42
1:B:1215:LEU:C	1:B:1217:LEU:N	2.73	0.42
1:B:288:GLN:CD	1:B:293:ARG:C	2.78	0.42
1:B:626:ARG:C	1:B:628:PRO:N	2.71	0.42
1:A:1133:VAL:O	1:A:1134:TYR:CB	2.66	0.42
1:A:755:ILE:O	1:A:758:GLN:CB	2.68	0.42
1:B:62:PRO:HB2	1:B:107:ASN:OD1	2.19	0.42
1:A:1122:LEU:HA	1:A:1125:ILE:CB	2.50	0.42
1:A:163:ILE:O	1:A:164:GLN:OE1	2.38	0.42
1:A:188:ASN:O	1:A:190:GLY:N	2.52	0.42
1:A:253:CYS:SG	1:A:262:VAL:HG22	2.60	0.42
1:A:473:VAL:O	1:A:474:THR:C	2.57	0.42
1:A:73:TRP:CZ3	1:A:156:ASN:HB3	2.55	0.42
1:B:143:GLU:CB	1:B:210:ASN:ND2	2.83	0.42
1:B:389:ARG:NE	1:B:425:GLU:O	2.53	0.42
1:A:1344:PHE:C	1:A:1347:ASP:H	2.23	0.42
1:A:520:PHE:CE2	1:A:560:LEU:HD21	2.53	0.42
1:A:863:THR:O	1:A:866:VAL:CB	2.67	0.42
1:B:1378:VAL:O	1:B:1382:ALA:HB2	2.20	0.42
1:B:167:TYR:HE2	1:B:181:LYS:HD2	1.85	0.42
1:B:447:ASN:O	1:B:448:ASP:C	2.57	0.42
1:A:398:TRP:CE2	1:A:424:LYS:HD2	2.54	0.42
1:A:595:ILE:C	1:A:598:LEU:CB	2.88	0.42
1:A:69:GLN:CD	1:A:73:TRP:CZ2	2.92	0.42
1:B:179:GLY:H	1:B:220:ILE:HG23	1.84	0.42
1:A:1273:MET:O	1:A:1274:GLN:C	2.58	0.42
1:A:128:SER:HB2	1:A:130:LYS:HE3	2.00	0.42
1:A:1415:ILE:O	1:A:1416:PRO:C	2.58	0.42
1:A:15:CYS:HA	1:A:222:LEU:HA	2.01	0.42
1:B:1224:LYS:CB	1:B:1319:GLU:O	2.68	0.42
1:B:1415:ILE:O	1:B:1416:PRO:C	2.57	0.42
1:B:398:TRP:CD2	1:B:424:LYS:HG3	2.54	0.42
1:B:438:ALA:O	1:B:442:ASP:OD1	2.37	0.42
1:A:38:VAL:CG1	1:A:200:LEU:HD11	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:VAL:HA	1:B:282:TRP:O	2.20	0.42
1:B:391:ARG:HH22	1:B:393:LEU:HD12	1.85	0.42
1:B:261:HIS:CD2	1:B:406:ILE:HD13	2.55	0.42
1:B:58:PHE:CE2	1:B:125:HIS:HB2	2.54	0.42
1:A:200:LEU:HG	1:A:206:CYS:O	2.20	0.42
1:A:580:PHE:O	1:A:581:MET:C	2.57	0.42
1:A:724:LYS:C	1:A:726:ASP:H	2.23	0.42
1:B:270:GLN:OE1	1:B:1257:LYS:HA	2.20	0.42
1:B:1321:LYS:O	1:B:1323:ILE:N	2.43	0.42
1:B:286:VAL:HA	1:B:303:PHE:CD2	2.55	0.42
1:B:314:LEU:O	1:B:315:ALA:HB2	2.20	0.42
1:A:1200:GLN:O	1:A:1202:GLN:N	2.53	0.41
1:A:1354:LEU:O	1:A:1355:ILE:C	2.58	0.41
1:A:594:THR:O	1:A:598:LEU:N	2.50	0.41
1:A:69:GLN:HA	1:A:96:ALA:CB	2.50	0.41
1:B:316:ALA:HA	1:B:355:LEU:HA	2.02	0.41
1:A:1361:GLU:O	1:A:1364:ARG:N	2.52	0.41
1:A:26:PHE:HB3	1:A:56:CYS:SG	2.60	0.41
1:A:460:LEU:O	1:A:460:LEU:HG	2.20	0.41
1:B:485:THR:O	1:B:486:GLY:C	2.57	0.41
1:B:607:GLU:O	1:B:611:THR:CA	2.62	0.41
1:B:687:LEU:O	1:B:688:GLU:C	2.59	0.41
1:B:755:ILE:O	1:B:758:GLN:CA	2.68	0.41
1:A:1253:ALA:O	1:A:1256:HIS:CB	2.69	0.41
1:A:1437:MET:O	1:A:1438:LYS:C	2.57	0.41
1:A:441:ARG:HA	1:A:444:ASP:OD2	2.20	0.41
1:A:460:LEU:HD12	1:A:463:GLY:O	2.21	0.41
1:A:842:GLU:C	1:A:844:LEU:N	2.73	0.41
1:B:571:GLN:C	1:B:574:ILE:H	2.21	0.41
1:B:826:LYS:O	1:B:827:ASP:C	2.58	0.41
1:B:88:LEU:CD2	1:B:92:LEU:HD12	2.51	0.41
1:A:1030:PHE:O	1:A:1033:ILE:N	2.52	0.41
1:A:1083:LEU:O	1:A:1084:PHE:C	2.59	0.41
1:A:15:CYS:O	1:A:57:LEU:CD2	2.69	0.41
1:A:222:LEU:CD2	1:A:224:MET:O	2.68	0.41
1:A:302:LEU:N	1:A:302:LEU:CD1	2.83	0.41
1:B:236:GLY:HA2	1:B:284:VAL:HG12	2.02	0.41
1:B:244:HIS:CD2	1:B:264:LEU:HD11	2.56	0.41
1:B:446:ALA:HB1	1:B:515:ILE:HD11	2.02	0.41
1:B:666:ILE:CB	1:B:669:LYS:N	2.83	0.41
1:A:13:ASP:OD1	1:A:226:TRP:N	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:THR:O	1:A:621:LEU:CB	2.68	0.41
1:A:727:ARG:O	1:A:728:ASP:C	2.57	0.41
1:B:27:ILE:HG12	1:B:218:TRP:CZ3	2.56	0.41
1:B:484:VAL:HG11	1:B:562:HIS:CB	2.50	0.41
1:B:49:PRO:C	1:B:50:PRO:O	2.57	0.41
1:B:637:LEU:O	1:B:639:VAL:N	2.53	0.41
1:A:10:HIS:HB3	1:A:112:GLY:O	2.21	0.41
1:A:234:LEU:HD13	1:A:432:ILE:HG21	2.02	0.41
1:A:523:LEU:CD1	1:A:553:CYS:SG	3.07	0.41
1:A:756:SER:O	1:A:759:LEU:N	2.54	0.41
1:A:842:GLU:O	1:A:844:LEU:N	2.54	0.41
1:B:1381:LEU:O	1:B:1385:THR:CB	2.69	0.41
1:B:235:LYS:HD3	1:B:235:LYS:HA	1.83	0.41
1:B:675:PHE:O	1:B:679:GLY:N	2.54	0.41
1:B:772:ASN:O	1:B:774:PRO:N	2.53	0.41
1:B:777:LEU:C	1:B:780:SER:H	2.14	0.41
1:A:166:PHE:CE1	1:A:167:TYR:CZ	3.09	0.41
1:A:313:TYR:HD1	1:A:313:TYR:N	2.18	0.41
1:A:841:GLU:O	1:A:844:LEU:CA	2.67	0.41
1:B:136:LYS:O	1:B:147:MET:HG2	2.21	0.41
1:B:619:VAL:O	1:B:623:ARG:CB	2.69	0.41
1:A:1251:ASN:CB	1:A:1283:LEU:CA	2.99	0.41
1:A:1459:ARG:C	1:A:1461:CYS:N	2.66	0.41
1:A:226:TRP:O	1:A:226:TRP:CE3	2.73	0.41
1:A:276:THR:O	1:A:508:LYS:NZ	2.34	0.41
1:B:576:LYS:C	1:B:578:PHE:N	2.74	0.41
1:A:398:TRP:CZ3	1:A:424:LYS:HE3	2.56	0.41
1:A:555:LEU:O	1:A:559:VAL:HG23	2.20	0.41
1:A:560:LEU:O	1:A:564:GLN:HG2	2.21	0.41
1:A:723:GLN:O	1:A:862:LEU:CB	2.68	0.41
1:B:369:GLU:HG2	1:B:370:LEU:H	1.84	0.41
1:B:95:ALA:O	1:B:98:LEU:N	2.53	0.41
1:A:1374:HIS:O	1:A:1377:LEU:CB	2.69	0.41
1:A:647:VAL:O	1:A:649:GLN:N	2.54	0.41
1:A:863:THR:O	1:A:866:VAL:CA	2.69	0.41
1:B:28:SER:O	1:B:37:CYS:HA	2.21	0.41
1:B:444:ASP:C	1:B:446:ALA:H	2.25	0.41
1:B:852:PHE:O	1:B:856:ASP:CB	2.69	0.41
1:A:19:ALA:HB2	1:A:218:TRP:CH2	2.56	0.41
1:A:401:SER:OG	1:A:428:GLU:OE1	2.34	0.41
1:A:853:PRO:O	1:A:854:PHE:C	2.59	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:GLN:NE2	1:B:73:TRP:HZ2	2.18	0.41
1:B:707:ILE:HA	1:B:710:LYS:CB	2.50	0.41
1:A:1079:ALA:O	1:A:1081:GLN:N	2.54	0.40
1:A:1436:GLU:O	1:A:1439:GLU:CB	2.69	0.40
1:A:1489:PHE:O	1:A:1490:PHE:C	2.60	0.40
1:A:369:GLU:HG2	1:A:370:LEU:N	2.35	0.40
1:A:510:MET:CE	1:A:515:ILE:HG13	2.51	0.40
1:A:999:ARG:O	1:A:1006:SER:O	2.39	0.40
1:B:1303:GLY:O	1:B:1304:ARG:C	2.59	0.40
1:B:358:VAL:HA	1:B:359:PRO:HD3	1.91	0.40
1:A:1112:TYR:HA	1:A:1115:ILE:CB	2.51	0.40
1:A:1207:ASN:C	1:A:1209:GLY:N	2.73	0.40
1:A:1405:ILE:O	1:A:1406:VAL:C	2.58	0.40
1:A:143:GLU:HG3	1:A:198:HIS:HE1	1.87	0.40
1:A:367:ILE:O	1:A:367:ILE:HG23	2.21	0.40
1:A:403:ASN:HA	1:A:416:LEU:HD22	2.04	0.40
1:B:196:SER:C	1:B:207:ASN:HD22	2.21	0.40
1:B:838:GLU:O	1:B:840:VAL:N	2.53	0.40
1:B:88:LEU:C	1:B:88:LEU:HD23	2.42	0.40
1:A:142:LEU:HD23	1:A:200:LEU:CD2	2.50	0.40
1:A:166:PHE:HD1	1:A:167:TYR:CD2	2.40	0.40
1:B:194:HIS:ND1	1:B:214:CYS:SG	2.93	0.40
1:B:251:LEU:HD13	1:B:418:ILE:HD12	2.02	0.40
1:B:18:TYR:HD1	1:B:26:PHE:CD1	2.39	0.40
1:B:969:ASP:O	1:B:972:LEU:CB	2.68	0.40
1:A:1074:PRO:C	1:A:1076:VAL:N	2.74	0.40
1:A:1316:VAL:HA	1:A:1319:GLU:CB	2.51	0.40
1:A:628:PRO:O	1:A:629:ARG:C	2.59	0.40
1:A:701:ARG:HA	1:A:730:LEU:HA	2.03	0.40
1:A:71:GLN:HB3	1:A:92:LEU:HD22	2.03	0.40
1:B:166:PHE:HD1	1:B:167:TYR:CD2	2.39	0.40
1:B:481:VAL:HB	1:B:490:SER:O	2.21	0.40
1:A:1207:ASN:O	1:A:1208:MET:C	2.59	0.40
1:A:1437:MET:C	1:A:1439:GLU:N	2.75	0.40
1:A:66:TYR:HD1	1:A:69:GLN:OE1	2.03	0.40
1:B:1028:LEU:O	1:B:1030:PHE:N	2.54	0.40
1:B:148:ARG:HG2	1:B:150:THR:HG22	2.03	0.40
1:B:29:THR:HG23	1:B:125:HIS:CD2	2.56	0.40
1:B:315:ALA:O	1:B:355:LEU:HA	2.22	0.40
1:B:840:VAL:O	1:B:841:GLU:C	2.59	0.40
1:B:88:LEU:O	1:B:92:LEU:HD12	2.21	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASP:O	1:A:1393:GLU:N[2_655]	1.65	0.55
1:A:116:GLN:NE2	1:A:1391:TYR:O[2_655]	1.85	0.35
1:A:117:TYR:H	1:A:1392:THR:O[2_655]	1.45	0.15
1:A:175:SER:H	1:A:1395:LYS:N[2_655]	1.51	0.09
1:A:174:ASP:O	1:A:1392:THR:C[2_655]	2.11	0.09
1:A:117:TYR:N	1:A:1392:THR:O[2_655]	2.14	0.06
1:A:116:GLN:HE21	1:A:1391:TYR:O[2_655]	1.55	0.05
1:A:109:LYS:N	1:A:1288:ASN:O[2_655]	2.18	0.02

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	1231/1581 (78%)	891 (72%)	234 (19%)	106 (9%)	1	11
1	B	1231/1581 (78%)	894 (73%)	228 (18%)	109 (9%)	1	11
All	All	2462/3162 (78%)	1785 (72%)	462 (19%)	215 (9%)	1	11

All (215) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	383	PRO
1	A	587	TYR
1	A	602	ASN
1	A	604	LYS
1	A	628	PRO
1	A	645	ILE
1	A	658	ASN
1	A	666	ILE
1	A	702	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	708	ARG
1	A	744	CYS
1	A	762	ASP
1	A	789	HIS
1	A	863	THR
1	A	961	GLU
1	A	977	ILE
1	A	990	ILE
1	A	994	LEU
1	A	1133	VAL
1	A	1239	GLU
1	A	1243	ASN
1	A	1264	ASN
1	A	1286	GLU
1	A	1288	ASN
1	A	1299	ILE
1	A	1343	VAL
1	A	1347	ASP
1	A	1370	PRO
1	A	1394	ILE
1	A	1400	LEU
1	A	1418	VAL
1	A	1435	VAL
1	A	1437	MET
1	A	1458	CYS
1	A	1460	ALA
1	A	1461	CYS
1	B	48	ASN
1	B	200	LEU
1	B	286	VAL
1	B	383	PRO
1	B	587	TYR
1	B	625	ASN
1	B	628	PRO
1	B	640	SER
1	B	658	ASN
1	B	659	PRO
1	B	666	ILE
1	B	669	LYS
1	B	715	LEU
1	B	836	THR
1	B	838	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	853	PRO
1	B	859	LYS
1	B	860	ASN
1	B	863	THR
1	B	898	VAL
1	B	961	GLU
1	B	990	ILE
1	B	1119	LEU
1	B	1201	GLN
1	B	1202	GLN
1	B	1221	PRO
1	B	1264	ASN
1	B	1267	ILE
1	B	1288	ASN
1	B	1299	ILE
1	B	1346	ASN
1	B	1370	PRO
1	B	1394	ILE
1	B	1400	LEU
1	B	1418	VAL
1	B	1458	CYS
1	B	1461	CYS
1	B	1464	THR
1	A	105	THR
1	A	226	TRP
1	A	550	ARG
1	A	640	SER
1	A	647	VAL
1	A	669	LYS
1	A	684	GLU
1	A	755	ILE
1	A	760	ASP
1	A	787	HIS
1	A	790	VAL
1	A	836	THR
1	A	853	PRO
1	A	895	LEU
1	A	1108	ASP
1	A	1109	VAL
1	A	1208	MET
1	A	1267	ILE
1	A	1301	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1311	PHE
1	A	1349	ALA
1	A	1464	THR
1	B	226	TRP
1	B	396	ASN
1	B	550	ARG
1	B	638	CYS
1	B	670	LEU
1	B	708	ARG
1	B	839	PHE
1	B	861	LYS
1	B	864	PHE
1	B	888	THR
1	B	1028	LEU
1	B	1051	ASP
1	B	1053	ASP
1	B	1058	ARG
1	B	1109	VAL
1	B	1117	GLN
1	B	1208	MET
1	B	1216	GLU
1	B	1239	GLU
1	B	1292	VAL
1	B	1311	PHE
1	B	1347	ASP
1	B	1463	ASN
1	A	428	GLU
1	A	575	ALA
1	A	610	ILE
1	A	660	THR
1	A	682	THR
1	A	716	ALA
1	A	719	ALA
1	A	725	GLU
1	A	827	ASP
1	A	1028	LEU
1	A	1207	ASN
1	A	1414	CYS
1	A	1463	ASN
1	A	1474	LEU
1	B	50	PRO
1	B	291	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	399	VAL
1	B	577	GLN
1	B	581	MET
1	B	589	VAL
1	B	591	ALA
1	B	604	LYS
1	B	693	GLU
1	B	714	GLU
1	B	726	ASP
1	B	727	ARG
1	B	787	HIS
1	B	789	HIS
1	B	790	VAL
1	B	827	ASP
1	B	837	MET
1	B	1133	VAL
1	B	1207	ASN
1	B	1301	THR
1	B	1322	PHE
1	B	1358	MET
1	B	1414	CYS
1	A	53	PHE
1	A	445	PHE
1	A	572	GLU
1	A	607	GLU
1	A	659	PRO
1	A	698	LEU
1	A	715	LEU
1	A	773	LEU
1	A	978	LEU
1	A	1004	SER
1	A	1075	LEU
1	A	1104	VAL
1	A	1355	ILE
1	A	1462	ASN
1	B	47	ASN
1	B	413	PRO
1	B	607	GLU
1	B	682	THR
1	B	720	LYS
1	B	858	GLU
1	B	981	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1081	GLN
1	B	1349	ALA
1	B	1356	GLN
1	B	1416	PRO
1	A	110	LEU
1	A	269	ARG
1	A	573	TYR
1	A	753	ASN
1	A	754	GLU
1	A	1074	PRO
1	A	1201	GLN
1	A	1202	GLN
1	A	1342	LEU
1	A	1397	ASN
1	A	1411	HIS
1	B	702	ASP
1	B	880	ASN
1	B	885	LEU
1	A	413	PRO
1	A	586	GLY
1	A	589	VAL
1	A	743	MET
1	B	593	ASP
1	B	645	ILE
1	B	684	GLU
1	B	745	LEU
1	B	773	LEU
1	B	852	PHE
1	B	854	PHE
1	A	286	VAL
1	B	647	VAL
1	B	1220	ILE
1	A	1221	PRO
1	B	497	VAL
1	A	646	PRO
1	B	498	VAL
1	A	984	VAL

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	400/1427 (28%)	356 (89%)	44 (11%)	6	23
1	B	400/1427 (28%)	360 (90%)	40 (10%)	7	26
All	All	800/2854 (28%)	716 (90%)	84 (10%)	7	24

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	28	SER
1	A	38	VAL
1	A	39	VAL
1	A	42	GLU
1	A	71	GLN
1	A	83	THR
1	A	101	LYS
1	A	102	GLN
1	A	105	THR
1	A	109	LYS
1	A	113	THR
1	A	117	TYR
1	A	121	ILE
1	A	127	LYS
1	A	142	LEU
1	A	150	THR
1	A	163	ILE
1	A	164	GLN
1	A	169	LEU
1	A	201	VAL
1	A	202	ASP
1	A	222	LEU
1	A	235	LYS
1	A	247	GLN
1	A	252	THR
1	A	255	GLU
1	A	289	HIS
1	A	302	LEU
1	A	317	GLU
1	A	356	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	390	LEU
1	A	394	CYS
1	A	418	ILE
1	A	423	LEU
1	A	428	GLU
1	A	433	VAL
1	A	456	ILE
1	A	465	ILE
1	A	471	ARG
1	A	499	PHE
1	A	515	ILE
1	A	523	LEU
1	A	551	HIS
1	B	27	ILE
1	B	38	VAL
1	B	39	VAL
1	B	42	GLU
1	B	71	GLN
1	B	83	THR
1	B	97	ASP
1	B	101	LYS
1	B	105	THR
1	B	121	ILE
1	B	127	LYS
1	B	132	LEU
1	B	142	LEU
1	B	143	GLU
1	B	164	GLN
1	B	169	LEU
1	B	201	VAL
1	B	222	LEU
1	B	235	LYS
1	B	247	GLN
1	B	252	THR
1	B	255	GLU
1	B	258	LYS
1	B	302	LEU
1	B	317	GLU
1	B	356	VAL
1	B	390	LEU
1	B	394	CYS
1	B	397	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	411	GLU
1	B	418	ILE
1	B	428	GLU
1	B	433	VAL
1	B	436	SER
1	B	471	ARG
1	B	502	PRO
1	B	523	LEU
1	B	551	HIS
1	B	555	LEU
1	B	567	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	122	GLN
1	A	194	HIS
1	A	198	HIS
1	A	513	GLN
1	B	10	HIS
1	B	69	GLN
1	B	194	HIS
1	B	198	HIS
1	B	207	ASN
1	B	244	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	I3P	B	3000	-	24,24,24	1.13	1 (4%)	36,39,39	1.09	3 (8%)
2	I3P	A	3000	-	24,24,24	1.17	3 (12%)	36,39,39	1.08	4 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	I3P	B	3000	-	-	0/15/39/39	0/1/1/1
2	I3P	A	3000	-	-	0/15/39/39	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3000	I3P	P5-O53	-2.21	1.46	1.54
2	A	3000	I3P	P4-O42	-2.21	1.46	1.54
2	A	3000	I3P	P1-O13	-2.17	1.46	1.54
2	B	3000	I3P	P1-O13	-2.15	1.46	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3000	I3P	O13-P1-O12	2.53	117.31	107.64
2	A	3000	I3P	O5-P5-O51	-2.41	100.10	109.39
2	B	3000	I3P	O43-P4-O42	2.38	116.74	107.64
2	B	3000	I3P	O53-P5-O52	2.31	116.45	107.64
2	A	3000	I3P	O1-C1-C2	2.10	113.55	108.66
2	B	3000	I3P	O1-C1-C2	2.09	113.53	108.66
2	A	3000	I3P	O53-P5-O52	2.02	115.34	107.64

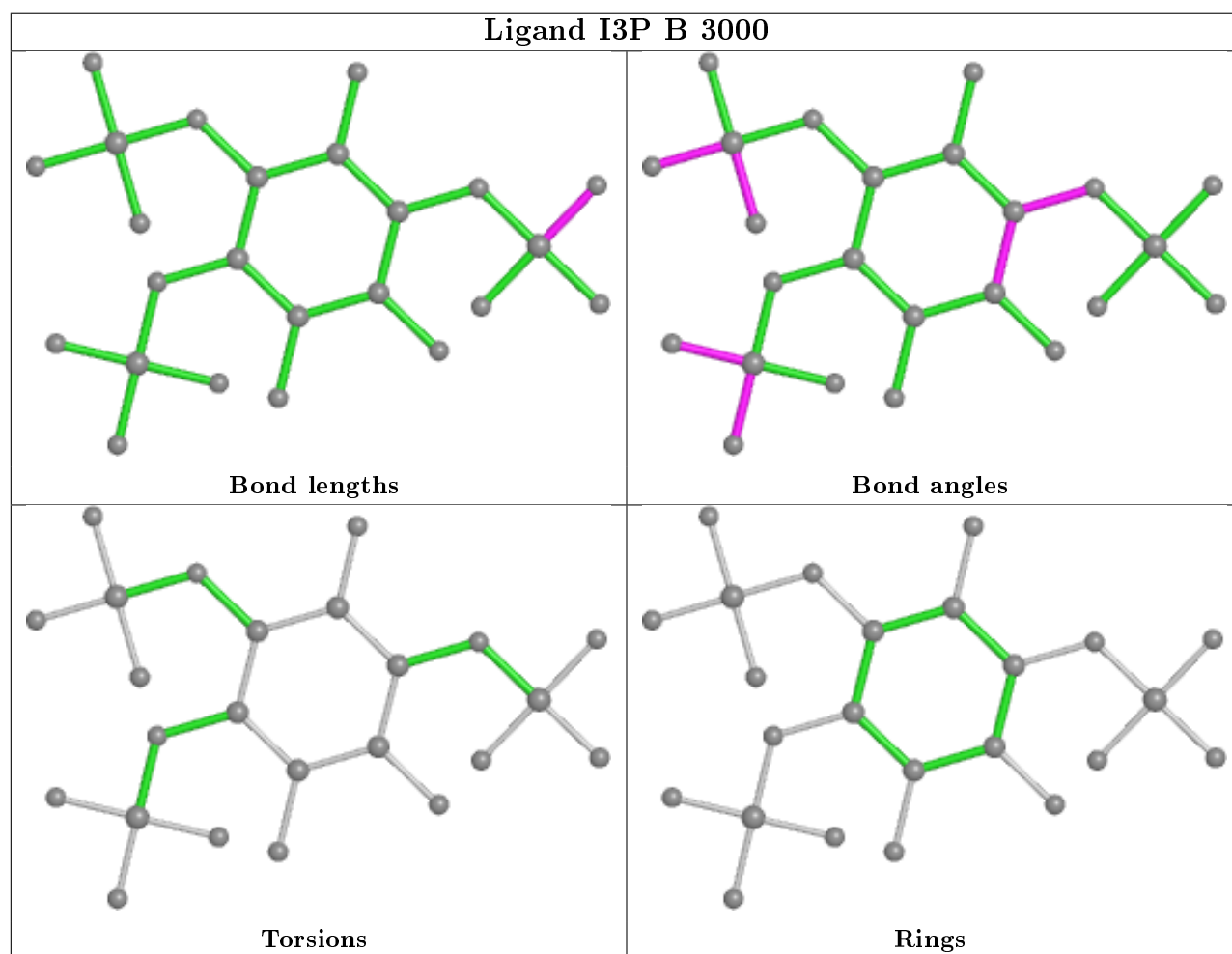
There are no chirality outliers.

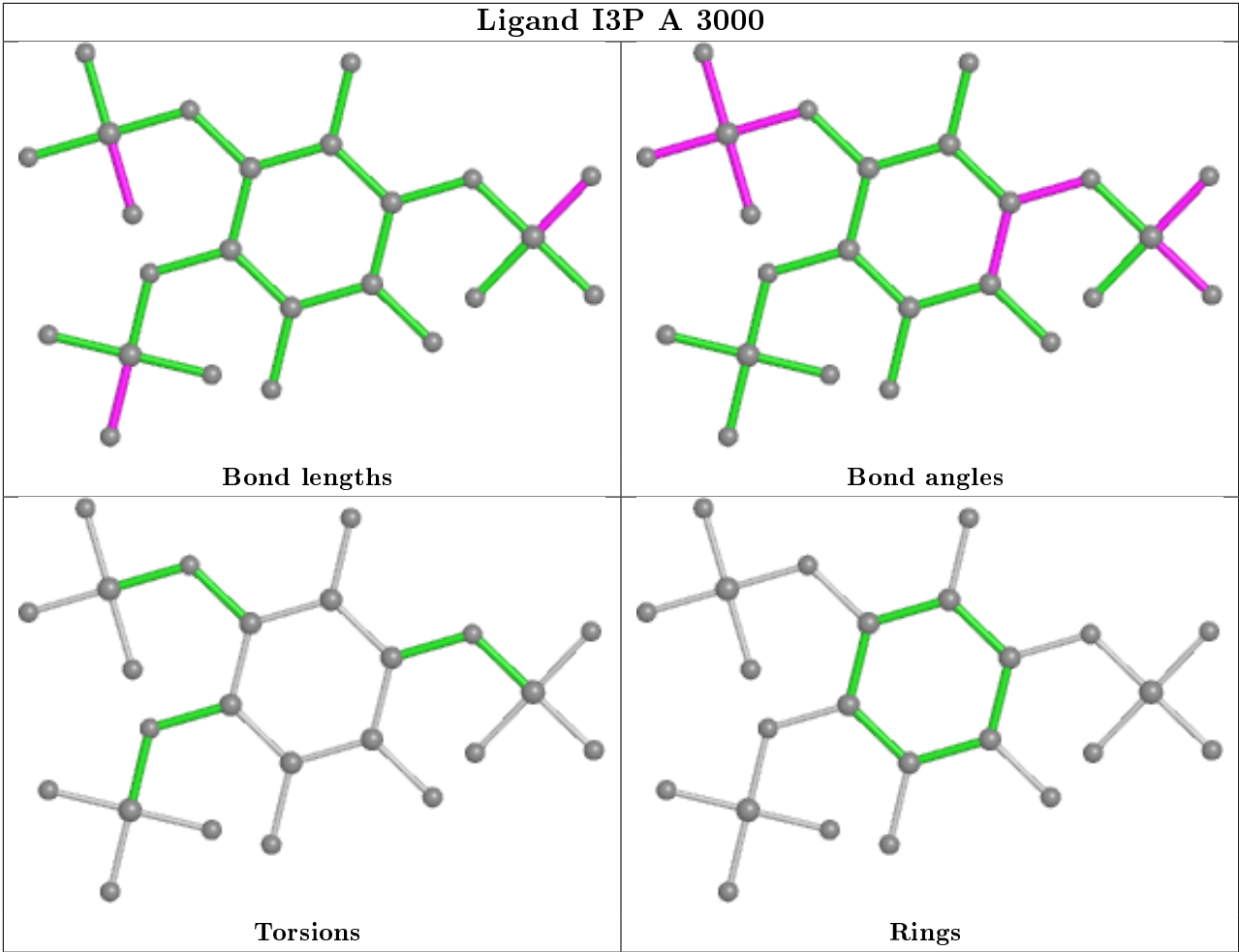
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1491:SER	C	1492:SER	N	1.61

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	1257/1581 (79%)	0.48	163 (12%) 3 7	165, 174, 178, 180	0
1	B	1257/1581 (79%)	0.38	138 (10%) 5 9	165, 174, 178, 180	0
All	All	2514/3162 (79%)	0.43	301 (11%) 4 8	165, 174, 178, 180	0

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	THR	8.7
1	A	1389	ASN	8.4
1	B	253	CYS	8.0
1	B	279	LYS	7.9
1	B	388	VAL	7.6
1	A	58	PHE	7.4
1	A	265	ARG	7.3
1	B	184	LEU	7.0
1	A	1260	ASN	6.9
1	B	387	TYR	6.8
1	A	1391	TYR	6.7
1	A	1243	ASN	6.6
1	B	252	THR	6.3
1	B	280	ALA	6.3
1	A	118	GLY	6.2
1	A	211	SER	6.0
1	A	16	SER	5.9
1	A	1388	LYS	5.8
1	A	317	GLU	5.8
1	A	1414	CYS	5.7
1	A	119	ASN	5.7
1	A	318	VAL	5.7
1	A	1390	VAL	5.6
1	A	355	LEU	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	388	VAL	5.5
1	A	27	ILE	5.5
1	B	132	LEU	5.4
1	A	1240	PHE	5.3
1	B	282	TRP	5.3
1	B	27	ILE	5.3
1	B	56	CYS	5.2
1	A	390	LEU	5.2
1	A	60	LEU	5.1
1	B	307	HIS	5.1
1	A	1234	MET	5.1
1	B	1401	PRO	5.1
1	A	1244	PHE	5.0
1	A	59	LYS	5.0
1	B	205	GLY	5.0
1	A	1238	HIS	4.9
1	A	1242	GLN	4.9
1	A	215	ASN	4.9
1	B	123	LEU	4.9
1	B	390	LEU	4.8
1	A	1392	THR	4.7
1	B	278	SER	4.7
1	A	1233	ILE	4.7
1	B	121	ILE	4.7
1	A	132	LEU	4.7
1	B	119	ASN	4.6
1	A	1387	GLY	4.5
1	A	1239	GLU	4.5
1	A	131	TYR	4.5
1	B	1402	LEU	4.4
1	B	185	ASN	4.4
1	B	162	TYR	4.4
1	A	28	SER	4.4
1	B	52	LYS	4.4
1	A	1413	ASP	4.4
1	B	825	SER	4.4
1	A	64	ASN	4.4
1	A	234	LEU	4.4
1	A	554	ARG	4.4
1	A	56	CYS	4.4
1	B	122	GLN	4.4
1	B	309	ALA	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1134	TYR	4.3
1	B	53	PHE	4.3
1	B	250	PHE	4.3
1	A	17	LEU	4.3
1	B	1403	ASP	4.2
1	A	205	GLY	4.2
1	B	372	PRO	4.2
1	A	1450	PHE	4.2
1	B	310	THR	4.1
1	B	1189	GLN	4.1
1	A	399	VAL	4.1
1	A	182	VAL	4.1
1	A	6	SER	4.1
1	A	63	MET	4.1
1	B	251	LEU	4.0
1	A	556	CYS	4.0
1	A	253	CYS	4.0
1	A	116	GLN	4.0
1	B	277	SER	3.9
1	A	123	LEU	3.9
1	A	153	GLU	3.9
1	B	370	LEU	3.9
1	A	279	LYS	3.9
1	B	305	PHE	3.9
1	A	267	THR	3.9
1	A	354	SER	3.9
1	A	414	VAL	3.9
1	A	254	ASP	3.9
1	B	1404	ASP	3.9
1	B	265	ARG	3.8
1	B	553	CYS	3.8
1	A	557	TYR	3.8
1	B	1279	ASN	3.8
1	A	1221	PRO	3.7
1	A	166	PHE	3.7
1	B	1190	GLU	3.7
1	B	161	PHE	3.7
1	B	183	VAL	3.7
1	A	419	GLY	3.7
1	A	188	ASN	3.7
1	A	1451	GLU	3.6
1	B	62	PRO	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1241	LEU	3.6
1	A	249	LYS	3.6
1	A	1310	LYS	3.6
1	A	1222	TYR	3.6
1	B	193	LEU	3.6
1	B	153	GLU	3.6
1	A	1046	GLU	3.5
1	B	382	VAL	3.5
1	A	1237	ALA	3.5
1	A	1184	SER	3.5
1	B	1397	ASN	3.5
1	A	183	VAL	3.5
1	B	54	ARG	3.4
1	B	1478	VAL	3.5
1	A	1368	ASN	3.4
1	A	370	LEU	3.4
1	B	1400	LEU	3.4
1	B	234	LEU	3.4
1	A	667	GLU	3.4
1	A	560	LEU	3.4
1	B	826	LYS	3.4
1	B	1247	GLY	3.4
1	A	1488	THR	3.4
1	A	1232	GLU	3.4
1	B	1187	CYS	3.3
1	A	389	ARG	3.3
1	B	22	SER	3.3
1	A	152	ASP	3.3
1	B	283	GLU	3.3
1	A	252	THR	3.3
1	A	1230	MET	3.3
1	A	124	LEU	3.2
1	B	1481	ILE	3.2
1	A	356	VAL	3.2
1	B	163	ILE	3.2
1	B	649	GLN	3.2
1	A	553	CYS	3.2
1	A	1259	ILE	3.1
1	B	281	LEU	3.1
1	B	1185	LYS	3.1
1	A	15	CYS	3.1
1	B	120	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1244	PHE	3.1
1	A	191	GLN	3.1
1	B	1188	VAL	3.1
1	B	299	TRP	3.1
1	B	1191	SER	3.1
1	A	62	PRO	3.1
1	B	430	PHE	3.1
1	B	1238	HIS	3.0
1	B	1246	ALA	3.0
1	B	1479	THR	3.0
1	A	561	ARG	3.0
1	B	61	CYS	3.0
1	B	429	ALA	3.0
1	B	564	GLN	3.0
1	A	1133	VAL	3.0
1	A	1223	GLU	3.0
1	B	402	THR	2.9
1	B	1480	GLU	2.9
1	B	1389	ASN	2.9
1	A	151	LEU	2.9
1	A	382	VAL	2.9
1	A	668	THR	2.9
1	B	266	THR	2.9
1	A	1412	GLU	2.8
1	A	559	VAL	2.8
1	B	1282	GLN	2.8
1	A	1229	LYS	2.8
1	A	55	ASP	2.8
1	B	1108	ASP	2.8
1	A	164	GLN	2.8
1	A	1491	SER	2.8
1	A	284	VAL	2.8
1	B	351	MET	2.8
1	A	1235	ARG	2.8
1	B	1482	VAL	2.7
1	B	1237	ALA	2.7
1	B	9	LEU	2.7
1	B	118	GLY	2.7
1	A	216	THR	2.7
1	B	587	TYR	2.7
1	A	115	ILE	2.7
1	B	40	GLN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	195	ALA	2.6
1	B	386	SER	2.6
1	B	422	PRO	2.6
1	A	1246	ALA	2.6
1	A	1415	ILE	2.6
1	A	57	LEU	2.6
1	A	1369	SER	2.6
1	A	309	ALA	2.6
1	B	738	ASN	2.6
1	A	1266	GLY	2.6
1	B	131	TYR	2.6
1	A	117	TYR	2.6
1	A	193	LEU	2.5
1	A	250	PHE	2.5
1	A	22	SER	2.5
1	A	1386	GLU	2.5
1	A	210	ASN	2.5
1	A	1180	LEU	2.5
1	A	563	SER	2.5
1	B	60	LEU	2.5
1	B	663	ASP	2.5
1	A	1433	THR	2.5
1	B	1059	THR	2.5
1	B	152	ASP	2.5
1	A	1343	VAL	2.5
1	A	122	GLN	2.5
1	A	1269	GLU	2.5
1	B	1243	ASN	2.5
1	A	163	ILE	2.4
1	A	220	ILE	2.4
1	B	1370	PRO	2.4
1	A	154	ALA	2.4
1	B	1433	THR	2.4
1	B	59	LYS	2.4
1	B	241	ARG	2.4
1	B	371	ASP	2.4
1	A	1339	GLU	2.4
1	A	189	ALA	2.4
1	A	52	LYS	2.4
1	A	383	PRO	2.4
1	A	315	ALA	2.4
1	B	39	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	666	ILE	2.4
1	A	1045	GLU	2.4
1	A	1490	PHE	2.3
1	A	1487	THR	2.3
1	B	1278	MET	2.3
1	B	1066	HIS	2.3
1	B	209	VAL	2.3
1	B	254	ASP	2.3
1	B	28	SER	2.3
1	B	648	THR	2.3
1	B	976	GLU	2.3
1	A	1340	ASP	2.3
1	B	1045	GLU	2.3
1	A	1261	LEU	2.3
1	A	558	ARG	2.3
1	A	214	CYS	2.3
1	A	149	VAL	2.3
1	B	17	LEU	2.2
1	B	1484	SER	2.2
1	A	430	PHE	2.2
1	B	1046	GLU	2.2
1	A	413	PRO	2.2
1	A	386	SER	2.2
1	B	1274	GLN	2.2
1	A	61	CYS	2.2
1	B	497	VAL	2.2
1	A	106	GLU	2.2
1	B	218	TRP	2.2
1	A	130	LYS	2.2
1	B	731	SER	2.2
1	B	1388	LYS	2.2
1	A	314	LEU	2.2
1	A	9	LEU	2.2
1	A	774	PRO	2.2
1	B	1398	SER	2.2
1	B	311	GLY	2.1
1	B	306	LYS	2.1
1	B	314	LEU	2.1
1	A	1110	ASP	2.1
1	B	1485	ILE	2.1
1	B	549	PHE	2.1
1	A	150	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	300	ASN	2.1
1	A	1228	THR	2.1
1	B	243	PHE	2.1
1	B	827	ASP	2.1
1	A	1231	GLN	2.1
1	A	1270	ALA	2.1
1	B	164	GLN	2.1
1	B	1432	ASP	2.1
1	A	65	ARG	2.1
1	B	1280	ASN	2.1
1	A	133	THR	2.1
1	A	176	VAL	2.1
1	B	389	ARG	2.1
1	B	308	LEU	2.0
1	B	1184	SER	2.0
1	B	273	THR	2.0
1	B	1277	PHE	2.0
1	A	1484	SER	2.0
1	B	560	LEU	2.0
1	B	417	LYS	2.0
1	A	742	ARG	2.0
1	A	1452	ASN	2.0
1	A	37	CYS	2.0
1	A	1185	LYS	2.0
1	A	1385	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

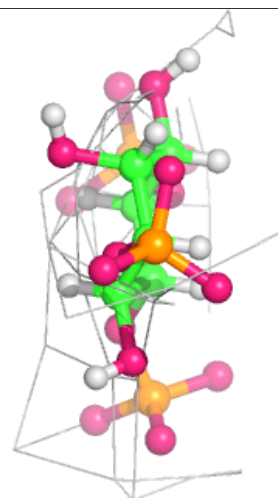
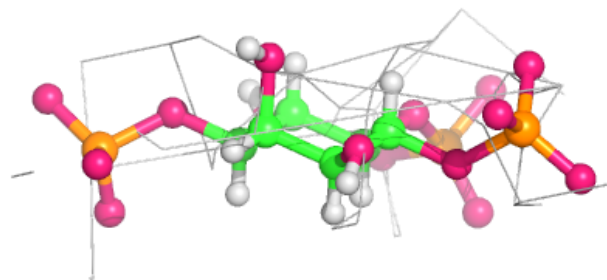
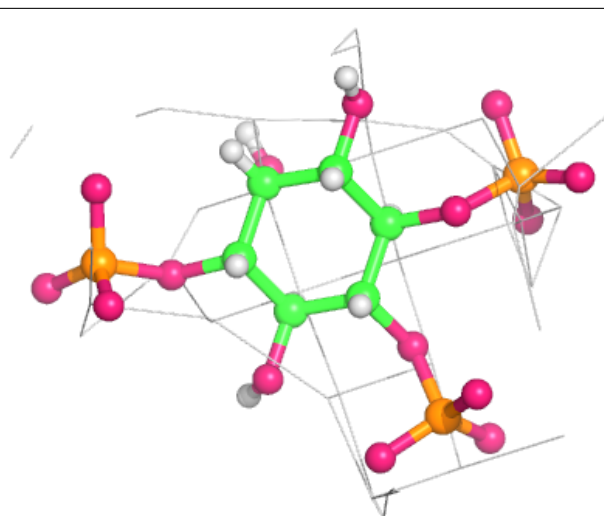
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

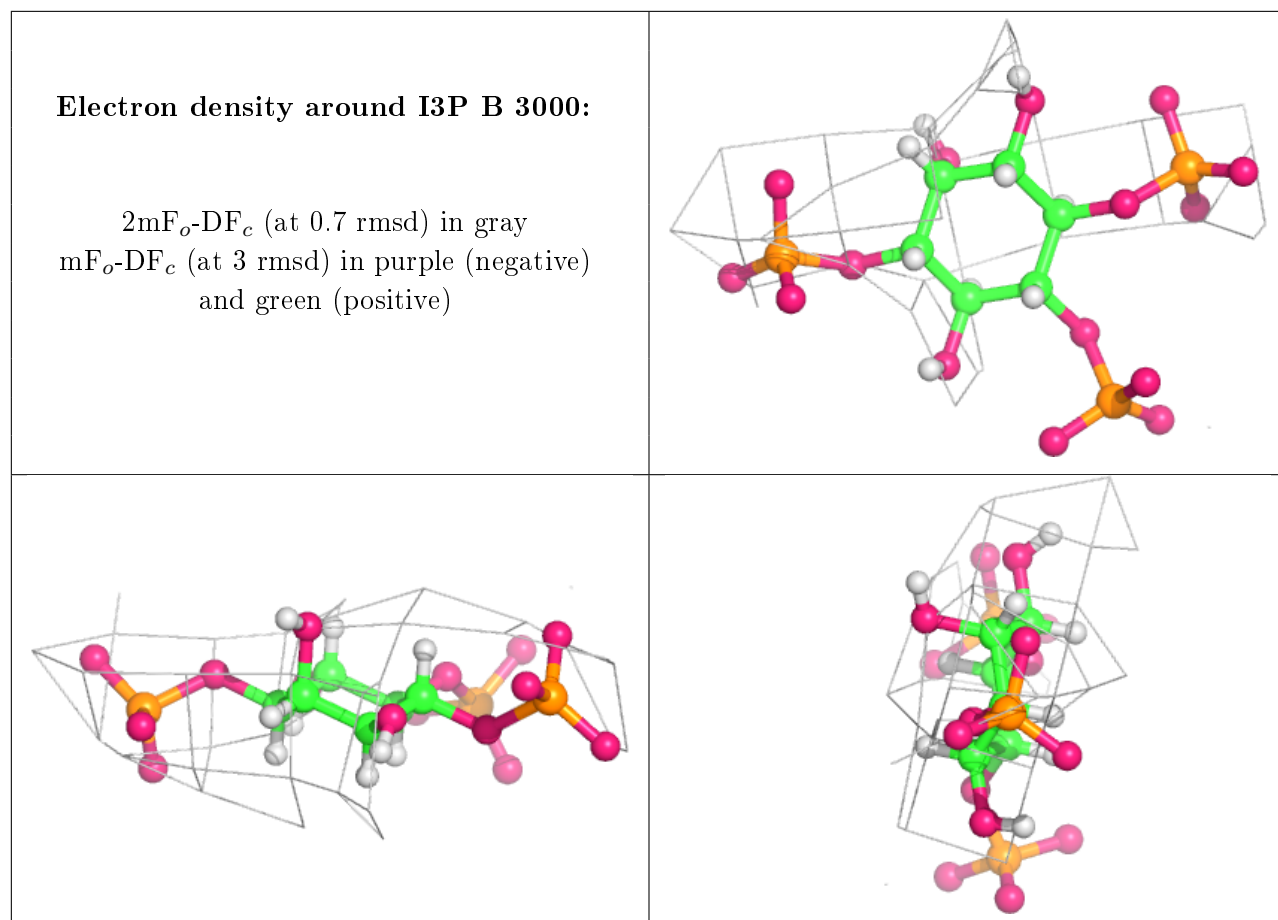
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	I3P	A	3000	24/24	0.72	0.65	174,174,174,174	0
2	I3P	B	3000	24/24	0.87	0.45	174,174,174,174	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around I3P A 3000:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.