



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:40 AM UTC

PDB ID : 1S6Q / pdb_00001s6q
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE (RT) IN
COMPLEX WITH JANSSEN-R147681
Authors : Das, K.; Arnold, E.
Deposited on : 2004-01-26
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

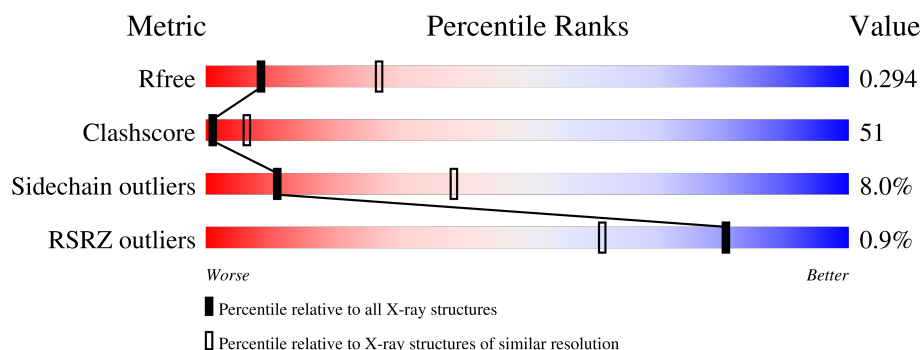
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	560	29%62%7% .
2	B	430	36%53%10% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8052 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 POL polyprotein [Contains: Reverse transcriptase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	61	0	0
			4498	2913	748	830	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366

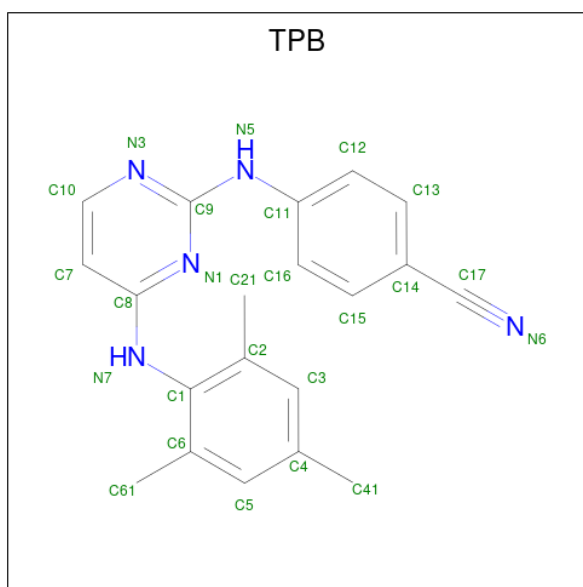
- Molecule 2 is a protein called POL polyprotein [Contains: Reverse transcriptase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	24	0	0
			3529	2300	584	638	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-[4-(2,4,6-TRIMETHYL-PHENYLAMINO)-PYRIMIDIN-2-YLAMINO]-BE NZONITRILE (CCD ID: TPB) (formula: C₂₀H₁₉N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			25	20	5		

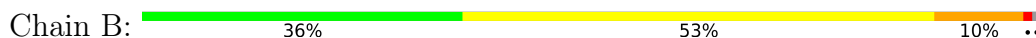
3 Residue-property plots

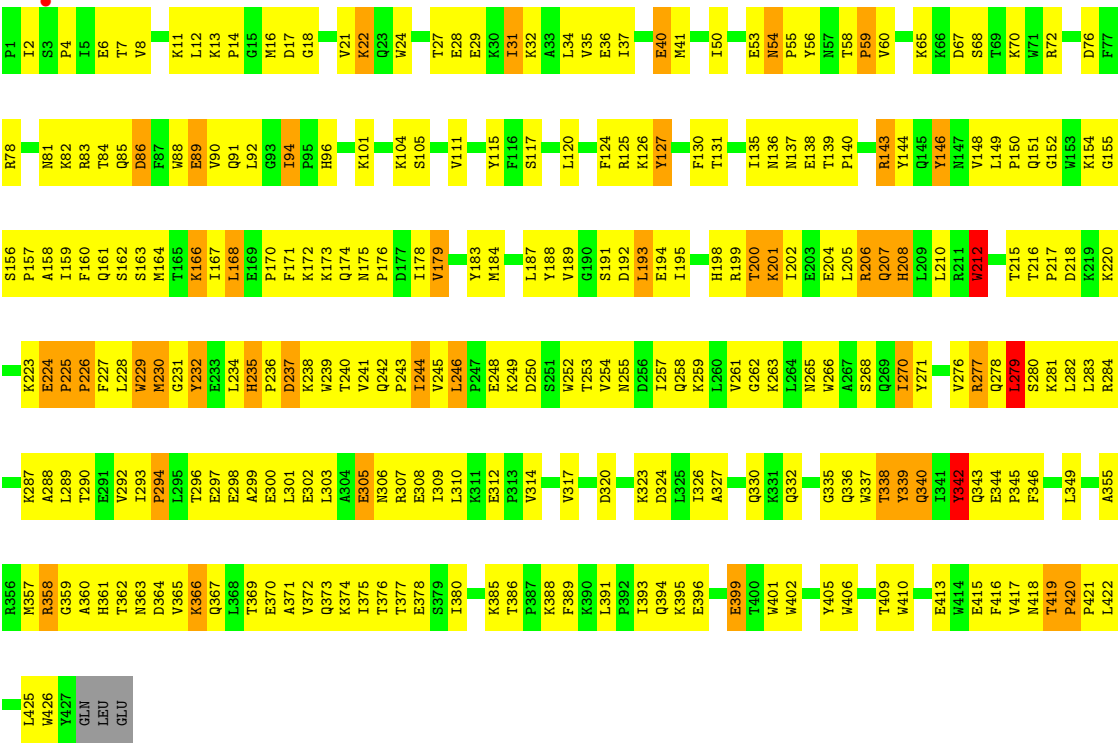
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: POL polyprotein [Contains: Reverse transcriptase]



- Molecule 2: POL polyprotein [Contains: Reverse transcriptase]





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	228.30Å 69.60Å 105.30Å 90.00° 106.30° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.6 (20.00-3.00) 94.5 (20.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.246 , 0.294 0.250 , 0.294	Depositor DCC
R_{free} test set	1544 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	84.0	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8052	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: TPB

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	0.73	2/4616 (0.0%)	1.22	49/6271 (0.8%)
2	B	0.85	2/3634 (0.1%)	1.34	52/4940 (1.1%)
All	All	0.79	4/8250 (0.0%)	1.28	101/11211 (0.9%)

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	1
2	B	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	HIS	CA-C	6.45	1.57	1.52
2	B	179	VAL	CA-CB	-5.76	1.47	1.54
2	B	230	MET	SD-CE	5.49	1.93	1.79
1	A	381	VAL	CA-CB	-5.02	1.48	1.54

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	225	PRO	N-CA-C	13.89	127.65	110.70
2	B	420	PRO	N-CA-C	12.72	126.22	110.70
2	B	235	HIS	CA-C-N	11.97	133.36	119.47
2	B	235	HIS	C-N-CA	11.97	133.36	119.47
1	A	550	LYS	N-CA-C	-11.75	98.55	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	GLN	N-CA-C	-11.48	99.80	114.04
2	B	89	GLU	N-CA-C	-11.43	98.76	113.17
1	A	13	LYS	CA-C-N	10.03	132.38	119.84
1	A	13	LYS	C-N-CA	10.03	132.38	119.84
1	A	137	ASN	N-CA-C	9.37	130.76	110.80
2	B	226	PRO	N-CA-C	-9.32	96.56	111.19
1	A	118	VAL	CA-C-N	9.09	129.14	119.78
1	A	118	VAL	C-N-CA	9.09	129.14	119.78
1	A	286	THR	N-CA-C	8.93	124.17	113.28
1	A	344	GLU	CA-C-N	8.74	130.76	119.84
1	A	344	GLU	C-N-CA	8.74	130.76	119.84
1	A	511	ASP	N-CA-C	-8.36	102.17	111.28
2	B	419	THR	N-CA-C	8.18	127.88	109.81
2	B	417	VAL	N-CA-C	8.00	119.44	106.72
1	A	67	ASP	N-CA-C	-7.94	101.92	112.72
2	B	172	LYS	N-CA-C	-7.68	103.89	113.18
1	A	200	THR	N-CA-C	-7.66	102.62	110.97
2	B	225	PRO	CA-C-N	-7.66	112.10	119.76
2	B	225	PRO	C-N-CA	-7.66	112.10	119.76
1	A	391	LEU	CA-C-N	7.58	129.32	119.84
1	A	391	LEU	C-N-CA	7.58	129.32	119.84
1	A	349	LEU	N-CA-C	-7.50	104.09	113.55
2	B	94	ILE	CA-C-N	7.44	127.87	119.83
2	B	94	ILE	C-N-CA	7.44	127.87	119.83
1	A	221	HIS	N-CA-C	7.43	122.31	111.02
1	A	382	ILE	N-CA-C	7.24	117.84	110.82
2	B	127	TYR	N-CA-C	7.14	120.11	111.82
1	A	26	LEU	N-CA-C	7.02	120.44	107.60
1	A	138	GLU	N-CA-C	-7.00	104.90	113.50
1	A	287	LYS	N-CA-C	6.91	122.69	112.94
1	A	16	MET	N-CA-C	6.87	119.19	110.33
1	A	273	GLY	N-CA-C	6.72	124.28	115.47
1	A	493	VAL	N-CA-C	6.61	119.63	108.86
1	A	401	TRP	N-CA-C	6.57	118.10	111.07
1	A	529	GLU	N-CA-C	-6.54	104.23	112.93
1	A	3	SER	N-CA-C	6.52	120.41	110.50
2	B	401	TRP	N-CA-C	6.45	122.23	113.97
1	A	143	ARG	N-CA-C	6.42	118.99	108.52
2	B	86	ASP	N-CA-C	-6.39	104.31	111.28
2	B	212	TRP	N-CA-C	-6.32	105.51	112.72
2	B	37	ILE	CB-CA-C	-6.28	103.84	111.88
2	B	391	LEU	N-CA-C	6.23	117.50	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	224	GLU	CA-C-N	6.20	126.76	120.38
2	B	224	GLU	C-N-CA	6.20	126.76	120.38
2	B	54	ASN	CA-C-N	6.13	125.84	119.64
2	B	54	ASN	C-N-CA	6.13	125.84	119.64
2	B	279	LEU	N-CA-C	-6.02	104.06	111.40
2	B	96	HIS	CA-C-N	6.01	127.36	119.84
2	B	96	HIS	C-N-CA	6.01	127.36	119.84
2	B	8	VAL	CA-C-N	5.95	126.25	119.83
2	B	8	VAL	C-N-CA	5.95	126.25	119.83
1	A	442	VAL	N-CA-C	5.92	117.67	109.80
1	A	169	GLU	CA-C-N	-5.90	112.83	118.97
1	A	169	GLU	C-N-CA	-5.90	112.83	118.97
1	A	524	GLN	N-CA-C	-5.89	104.78	111.14
2	B	389	PHE	N-CA-C	5.88	119.22	109.46
1	A	381	VAL	CB-CA-C	-5.87	104.12	112.22
2	B	230	MET	N-CA-C	5.86	119.19	109.46
2	B	419	THR	CA-C-N	5.82	126.38	120.38
2	B	419	THR	C-N-CA	5.82	126.38	120.38
2	B	78	ARG	N-CA-C	5.76	118.33	111.71
2	B	380	ILE	CB-CA-C	-5.71	104.43	112.14
1	A	388	LYS	N-CA-C	-5.69	100.43	109.76
1	A	285	GLY	N-CA-C	-5.67	99.74	113.18
2	B	96	HIS	N-CA-C	5.59	118.75	108.69
1	A	481	ALA	N-CA-C	-5.47	105.40	111.36
1	A	278	GLN	N-CA-C	5.47	116.92	111.07
2	B	40	GLU	N-CA-C	-5.46	104.73	111.40
1	A	222	GLN	N-CA-C	5.43	122.36	110.80
2	B	342	TYR	N-CA-C	5.43	115.45	108.34
1	A	191	SER	N-CA-C	5.42	115.44	108.34
1	A	507	GLN	N-CA-C	5.41	117.18	111.28
2	B	59	PRO	N-CA-C	5.41	119.81	111.21
2	B	146	TYR	N-CA-C	5.41	118.36	109.76
1	A	290	THR	N-CA-C	-5.40	105.92	112.88
2	B	270	ILE	N-CA-C	-5.39	107.57	112.96
1	A	157	PRO	N-CA-C	-5.37	105.08	113.78
1	A	513	SER	N-CA-C	-5.37	99.36	110.80
2	B	237	ASP	N-CA-C	-5.36	106.25	112.89
2	B	50	ILE	N-CA-C	5.36	116.90	109.29
1	A	58	THR	CA-C-N	5.27	125.19	119.76
1	A	58	THR	C-N-CA	5.27	125.19	119.76
1	A	178	ILE	N-CA-C	5.26	116.20	109.30
2	B	166	LYS	N-CA-C	-5.26	104.46	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ASN	N-CA-C	5.17	116.60	110.19
2	B	358	ARG	N-CA-C	5.13	117.97	109.46
2	B	31	ILE	CB-CA-C	-5.09	105.45	111.81
2	B	386	THR	N-CA-C	5.09	116.24	109.93
2	B	189	VAL	CA-C-N	-5.08	118.62	122.33
2	B	189	VAL	C-N-CA	-5.08	118.62	122.33
2	B	360	ALA	N-CA-C	5.07	121.59	110.80
1	A	23	GLN	N-CA-C	-5.05	100.04	110.80
2	B	168	LEU	N-CA-C	5.04	119.45	112.45
1	A	129	ALA	N-CA-C	5.03	117.60	110.10
2	B	208	HIS	N-CA-C	-5.03	103.12	111.37
2	B	143	ARG	N-CA-C	5.02	117.24	108.76

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	354	TYR	Sidechain
2	B	188	TYR	Sidechain
2	B	339	TYR	Sidechain

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	4498	0	4560	493	0
2	B	3529	0	3568	342	0
3	A	25	0	19	5	0
All	All	8052	0	8147	808	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 51.

All (808) 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:454:LYS:HD2	1:A:552:VAL:HA	1.21	1.11
2:B:362:THR:HG22	2:B:367:GLN:HE21	1.17	1.10
2:B:22:LYS:HE2	2:B:22:LYS:HA	1.36	1.06
2:B:357:MET:HB2	2:B:361:HIS:CE1	1.94	1.02
1:A:460:ASN:HD22	1:A:461:LYS:N	1.57	1.01
1:A:494:ASN:HD22	2:B:289:LEU:HD12	1.23	1.01
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.40	1.01
1:A:454:LYS:CD	1:A:552:VAL:HA	1.91	1.00
1:A:548:VAL:HA	1:A:551:LEU:HD12	1.40	0.99
2:B:357:MET:HB2	2:B:361:HIS:HE1	1.26	0.99
1:A:298:GLU:H	1:A:298:GLU:CD	1.71	0.99
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.42	0.99
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.26	0.99
2:B:201:LYS:NZ	2:B:204:GLU:HG2	1.78	0.97
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.47	0.97
1:A:540:LYS:HD2	2:B:265:ASN:HD21	1.27	0.97
2:B:278:GLN:HA	2:B:281:LYS:HE3	1.47	0.96
1:A:422:LEU:HD23	1:A:424:LYS:HD3	1.50	0.94
2:B:139:THR:CG2	2:B:140:PRO:HD2	1.96	0.94
2:B:263:LYS:HE3	2:B:425:LEU:HB3	1.47	0.94
1:A:288:ALA:HB1	1:A:291:GLU:HB3	1.45	0.93
1:A:90:VAL:HG23	1:A:91:GLN:HG2	1.51	0.93
1:A:315:HIS:NE2	1:A:347:LYS:HD3	1.83	0.92
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.34	0.92
1:A:460:ASN:ND2	1:A:461:LYS:H	1.68	0.91
2:B:241:VAL:HG12	2:B:243:PRO:HD3	1.48	0.91
1:A:222:GLN:HG2	1:A:223:LYS:H	1.31	0.91
1:A:460:ASN:HD22	1:A:461:LYS:H	0.90	0.90
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.18	0.90
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.37	0.89
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.36	0.89
2:B:362:THR:CG2	2:B:367:GLN:HE21	1.84	0.89
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.56	0.88
1:A:543:GLY:HA3	2:B:284:ARG:HH11	1.39	0.88
1:A:106:VAL:HG12	1:A:107:THR:H	1.38	0.88
2:B:255:ASN:O	2:B:258:GLN:HB2	1.74	0.88
1:A:53:GLU:H	1:A:55:PRO:HD3	1.39	0.87
1:A:53:GLU:C	1:A:55:PRO:HD3	1.99	0.87
2:B:101:LYS:O	2:B:236:PRO:HB2	1.75	0.87
2:B:2:ILE:O	2:B:4:PRO:HD3	1.75	0.86
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.09	0.86
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LYS:HE3	1:A:24:TRP:HZ2	1.40	0.86
2:B:201:LYS:HZ3	2:B:204:GLU:HG2	1.41	0.86
2:B:149:LEU:HD21	2:B:159:ILE:HD12	1.56	0.85
1:A:21:VAL:HG21	1:A:59:PRO:HD3	1.59	0.85
1:A:494:ASN:ND2	2:B:289:LEU:HD12	1.93	0.84
1:A:13:LYS:HD2	1:A:16:MET:HE3	1.60	0.84
1:A:454:LYS:HD2	1:A:552:VAL:CA	2.07	0.84
1:A:317:VAL:HG12	1:A:348:ASN:O	1.78	0.83
2:B:371:ALA:O	2:B:375:ILE:HG13	1.79	0.83
1:A:224:GLU:HB3	1:A:225:PRO:CD	2.09	0.83
2:B:257:ILE:O	2:B:261:VAL:HG23	1.79	0.83
2:B:216:THR:O	2:B:218:ASP:N	2.12	0.82
1:A:33:ALA:O	1:A:37:ILE:HG12	1.80	0.82
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.61	0.82
2:B:65:LYS:HZ1	2:B:409:THR:HG23	1.42	0.82
2:B:278:GLN:NE2	2:B:298:GLU:HB2	1.94	0.82
2:B:195:ILE:CD1	2:B:199:ARG:HE	1.92	0.81
2:B:244:ILE:HD13	2:B:244:ILE:H	1.43	0.81
1:A:254:VAL:HG13	1:A:283:LEU:HD11	1.63	0.81
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.46	0.81
2:B:362:THR:HG22	2:B:367:GLN:NE2	1.97	0.80
2:B:27:THR:O	2:B:31:ILE:HD12	1.81	0.80
2:B:278:GLN:HE22	2:B:298:GLU:HB2	1.44	0.79
1:A:238:LYS:HD3	1:A:315:HIS:ND1	1.97	0.79
2:B:277:ARG:H	2:B:277:ARG:HD3	1.48	0.79
1:A:288:ALA:HB1	1:A:291:GLU:CB	2.12	0.79
1:A:411:ILE:HD12	1:A:412:PRO:HD2	1.63	0.78
1:A:244:ILE:HD11	1:A:310:LEU:HD13	1.64	0.78
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.14	0.78
1:A:3:SER:HB2	1:A:5:ILE:HG13	1.66	0.77
2:B:366:LYS:O	2:B:370:GLU:HG3	1.84	0.77
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.67	0.76
1:A:104:LYS:HE2	1:A:104:LYS:N	1.99	0.76
2:B:215:THR:HB	2:B:217:PRO:HD3	1.66	0.76
2:B:310:LEU:O	2:B:310:LEU:HD23	1.86	0.76
2:B:249:LYS:HD2	2:B:252:TRP:CZ3	2.21	0.76
1:A:460:ASN:ND2	1:A:461:LYS:N	2.29	0.76
2:B:369:THR:HG22	2:B:373:GLN:NE2	2.00	0.76
1:A:506:ILE:HG21	1:A:533:LEU:CD1	2.16	0.76
1:A:503:LEU:CD2	1:A:535:TRP:HB2	2.16	0.76
2:B:369:THR:O	2:B:373:GLN:HG3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:HG13	1:A:481:ALA:HB1	1.68	0.75
1:A:222:GLN:HG2	1:A:223:LYS:N	2.00	0.75
1:A:435:VAL:HG13	2:B:290:THR:HG21	1.68	0.75
2:B:303:LEU:O	2:B:307:ARG:HB2	1.86	0.75
1:A:224:GLU:HB3	1:A:225:PRO:HD3	1.67	0.75
1:A:257:ILE:O	1:A:261:VAL:HG23	1.86	0.75
1:A:326:ILE:HD12	1:A:326:ILE:N	2.01	0.75
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.01	0.75
1:A:542:ILE:HG22	1:A:544:GLY:H	1.52	0.74
1:A:34:LEU:HB2	1:A:132:ILE:CD1	2.18	0.74
1:A:79:GLU:HG3	1:A:83:ARG:HH12	1.52	0.74
2:B:345:PRO:HB2	2:B:346:PHE:CD1	2.23	0.74
2:B:157:PRO:HG2	2:B:158:ALA:H	1.53	0.74
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.70	0.74
1:A:457:TYR:HD2	1:A:457:TYR:O	1.71	0.73
2:B:65:LYS:HD3	2:B:72:ARG:HD2	1.70	0.73
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.24	0.73
1:A:438:GLU:HG3	1:A:460:ASN:HD21	1.54	0.73
2:B:257:ILE:HG23	2:B:283:LEU:HD21	1.69	0.73
1:A:506:ILE:HG21	1:A:533:LEU:HD12	1.71	0.73
1:A:3:SER:HB3	1:A:212:TRP:O	1.89	0.72
1:A:506:ILE:HD11	1:A:521:ILE:HG21	1.71	0.72
2:B:156:SER:N	2:B:157:PRO:HD2	2.04	0.72
1:A:106:VAL:HG12	1:A:107:THR:N	2.04	0.71
1:A:17:ASP:O	1:A:83:ARG:HD3	1.90	0.71
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.26	0.71
1:A:458:VAL:HG13	1:A:464:GLN:HG2	1.70	0.71
2:B:332:GLN:HB2	2:B:336:GLN:O	1.90	0.71
2:B:31:ILE:O	2:B:35:VAL:HG23	1.90	0.71
1:A:509:GLN:N	1:A:510:PRO:HD3	2.06	0.71
2:B:201:LYS:O	2:B:204:GLU:HB3	1.90	0.70
2:B:139:THR:HG22	2:B:140:PRO:CD	2.18	0.70
1:A:229:TRP:O	1:A:232:TYR:N	2.24	0.70
2:B:339:TYR:C	2:B:340:GLN:OE1	2.34	0.70
2:B:419:THR:H	2:B:420:PRO:HD2	1.56	0.70
2:B:201:LYS:HZ2	2:B:204:GLU:HG2	1.58	0.69
1:A:328:GLU:HG2	1:A:390:LYS:CB	2.21	0.69
1:A:470:THR:O	1:A:471:ASN:HB3	1.91	0.69
1:A:18:GLY:HA3	1:A:56:TYR:CD2	2.28	0.69
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.74	0.69
1:A:120:LEU:HB2	1:A:148:VAL:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:ILE:HB	2:B:342:TYR:CE1	2.27	0.68
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.28	0.68
1:A:510:PRO:O	1:A:522:ILE:HD13	1.92	0.68
2:B:359:GLY:O	2:B:361:HIS:N	2.24	0.68
1:A:297:GLU:HB2	1:A:298:GLU:OE2	1.93	0.68
1:A:215:THR:HG22	1:A:216:THR:N	2.08	0.68
2:B:161:GLN:O	2:B:162:SER:C	2.37	0.68
1:A:34:LEU:HB2	1:A:132:ILE:HD11	1.76	0.68
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.08	0.68
1:A:224:GLU:CB	1:A:225:PRO:CD	2.72	0.67
1:A:179:VAL:HG22	1:A:190:GLY:O	1.95	0.67
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.22	0.67
2:B:364:ASP:O	2:B:367:GLN:N	2.28	0.67
2:B:366:LYS:HG3	2:B:405:TYR:CG	2.29	0.67
1:A:279:LEU:HD23	1:A:299:ALA:HB1	1.76	0.67
2:B:125:ARG:O	2:B:127:TYR:N	2.27	0.67
1:A:503:LEU:HG	1:A:507:GLN:NE2	2.10	0.67
1:A:96:HIS:CD2	1:A:98:ALA:H	2.13	0.67
2:B:263:LYS:HE3	2:B:425:LEU:CB	2.25	0.67
2:B:282:LEU:HG	2:B:293:ILE:HD12	1.78	0.66
1:A:298:GLU:CD	1:A:298:GLU:N	2.51	0.66
1:A:438:GLU:OE1	1:A:463:ARG:NH2	2.28	0.66
2:B:298:GLU:HB3	2:B:301:LEU:HD13	1.78	0.66
2:B:303:LEU:O	2:B:307:ARG:HD2	1.94	0.66
2:B:422:LEU:HA	2:B:425:LEU:HD12	1.76	0.66
1:A:328:GLU:CG	1:A:390:LYS:HB2	2.25	0.66
1:A:410:TRP:HB2	2:B:365:VAL:HG21	1.78	0.66
2:B:86:ASP:O	2:B:89:GLU:HG2	1.95	0.66
2:B:32:LYS:O	2:B:36:GLU:HG2	1.96	0.66
1:A:540:LYS:CD	2:B:265:ASN:HD21	2.03	0.66
1:A:457:TYR:HD2	1:A:457:TYR:C	2.04	0.65
1:A:544:GLY:O	1:A:548:VAL:HG23	1.96	0.65
1:A:288:ALA:CB	1:A:291:GLU:HB3	2.24	0.65
1:A:498:ASP:HB2	1:A:538:ALA:HA	1.77	0.65
1:A:23:GLN:HG2	1:A:25:PRO:HD2	1.79	0.65
1:A:393:ILE:HG23	1:A:414:TRP:CZ3	2.31	0.65
1:A:402:TRP:HE3	1:A:402:TRP:O	1.79	0.65
2:B:224:GLU:O	2:B:226:PRO:HD3	1.96	0.65
2:B:245:VAL:HG12	2:B:246:LEU:N	2.11	0.65
2:B:246:LEU:HD21	2:B:310:LEU:HD13	1.77	0.65
2:B:268:SER:HA	2:B:271:TYR:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:PRO:O	1:A:117:SER:HA	1.95	0.65
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.79	0.65
1:A:115:TYR:CE2	1:A:151:GLN:HA	2.32	0.64
2:B:175:ASN:OD1	2:B:201:LYS:HE3	1.98	0.64
2:B:345:PRO:HB2	2:B:346:PHE:CE1	2.33	0.64
1:A:124:PHE:CD2	1:A:124:PHE:O	2.51	0.64
1:A:254:VAL:HG13	1:A:283:LEU:CD1	2.27	0.64
1:A:540:LYS:O	1:A:540:LYS:HG3	1.96	0.64
1:A:77:PHE:CD2	1:A:80:LEU:HD23	2.33	0.64
1:A:278:GLN:HG2	1:A:302:GLU:OE2	1.97	0.64
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.32	0.64
1:A:514:GLU:O	1:A:516:GLU:N	2.29	0.64
2:B:178:ILE:HG22	2:B:191:SER:HB3	1.78	0.64
2:B:246:LEU:HD21	2:B:310:LEU:CD1	2.28	0.64
1:A:399:GLU:HG3	1:A:402:TRP:HE1	1.61	0.64
1:A:164:MET:HE2	1:A:187:LEU:HD13	1.80	0.64
2:B:171:PHE:HE1	2:B:178:ILE:HD11	1.63	0.64
2:B:278:GLN:OE1	2:B:297:GLU:HB3	1.98	0.64
2:B:335:GLY:O	2:B:355:ALA:HA	1.98	0.64
1:A:495:ILE:HB	1:A:533:LEU:HD23	1.81	0.63
1:A:206:ARG:HH21	1:A:217:PRO:C	2.06	0.63
1:A:458:VAL:HG13	1:A:464:GLN:CG	2.28	0.63
2:B:22:LYS:HA	2:B:22:LYS:CE	2.16	0.63
1:A:304:ALA:O	1:A:307:ARG:HB2	1.99	0.63
1:A:34:LEU:CB	1:A:132:ILE:HD12	2.28	0.63
1:A:173:LYS:O	1:A:176:PRO:HD3	1.98	0.63
1:A:85:GLN:HE22	2:B:53:GLU:HB2	1.62	0.63
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.34	0.63
2:B:282:LEU:HG	2:B:293:ILE:CD1	2.29	0.63
1:A:457:TYR:C	1:A:457:TYR:CD2	2.77	0.63
2:B:149:LEU:HD13	2:B:156:SER:HA	1.80	0.63
2:B:372:VAL:HG12	2:B:373:GLN:N	2.13	0.63
1:A:108:VAL:HG13	1:A:227:PHE:CE1	2.33	0.63
1:A:548:VAL:O	1:A:551:LEU:HB2	1.99	0.63
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.81	0.62
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.80	0.62
1:A:506:ILE:HG22	1:A:507:GLN:N	2.14	0.62
1:A:417:VAL:O	1:A:417:VAL:HG12	1.98	0.62
1:A:440:PHE:CD2	1:A:459:THR:HG22	2.35	0.62
2:B:342:TYR:CD1	2:B:342:TYR:C	2.77	0.62
1:A:10:VAL:HG12	1:A:11:LYS:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LYS:NZ	2:B:409:THR:HG23	2.15	0.62
2:B:171:PHE:O	2:B:175:ASN:HB2	2.00	0.62
2:B:206:ARG:HG2	2:B:206:ARG:HH11	1.65	0.62
2:B:418:ASN:O	2:B:419:THR:HG23	1.99	0.62
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.82	0.62
2:B:125:ARG:O	2:B:126:LYS:C	2.41	0.62
1:A:282:LEU:O	1:A:284:ARG:N	2.33	0.61
2:B:59:PRO:HB2	2:B:76:ASP:HB3	1.82	0.61
2:B:255:ASN:OD1	2:B:259:LYS:HE3	2.00	0.61
1:A:164:MET:CE	1:A:187:LEU:HD13	2.30	0.61
1:A:155:GLY:O	1:A:159:ILE:HG13	2.00	0.61
1:A:465:LYS:HG3	1:A:466:VAL:N	2.15	0.61
2:B:246:LEU:N	2:B:246:LEU:HD23	2.16	0.61
1:A:3:SER:CB	1:A:5:ILE:HG13	2.31	0.61
1:A:138:GLU:OE1	1:A:138:GLU:O	2.19	0.61
2:B:253:THR:HA	2:B:292:VAL:HA	1.82	0.61
1:A:335:GLY:HA2	1:A:367:GLN:NE2	2.14	0.61
2:B:171:PHE:CE1	2:B:178:ILE:HD11	2.35	0.61
1:A:53:GLU:H	1:A:55:PRO:CD	2.13	0.60
1:A:497:THR:CG2	1:A:499:SER:HB3	2.31	0.60
2:B:402:TRP:O	2:B:406:TRP:HB2	2.02	0.60
2:B:253:THR:O	2:B:257:ILE:HG22	2.00	0.60
1:A:21:VAL:HG22	1:A:58:THR:HA	1.83	0.60
2:B:257:ILE:CG2	2:B:283:LEU:HD21	2.31	0.60
1:A:54:ASN:N	1:A:55:PRO:HD3	2.17	0.60
1:A:75:VAL:HG12	1:A:76:ASP:N	2.17	0.60
1:A:65:LYS:HG2	1:A:68:SER:HB3	1.83	0.60
1:A:344:GLU:OE1	1:A:344:GLU:HA	2.02	0.60
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.84	0.59
2:B:241:VAL:HG12	2:B:243:PRO:CD	2.29	0.59
1:A:241:VAL:HG12	1:A:242:GLN:N	2.16	0.59
2:B:91:GLN:O	2:B:92:LEU:HD23	2.01	0.59
2:B:215:THR:CB	2:B:217:PRO:HD3	2.32	0.59
1:A:10:VAL:HG12	1:A:11:LYS:H	1.67	0.59
1:A:220:LYS:HE3	1:A:221:HIS:CD2	2.37	0.59
1:A:34:LEU:HB2	1:A:132:ILE:HD12	1.84	0.59
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.37	0.59
1:A:194:GLU:O	1:A:196:GLY:N	2.35	0.59
1:A:536:VAL:HG11	1:A:542:ILE:CD1	2.32	0.59
1:A:540:LYS:HD2	2:B:265:ASN:ND2	2.08	0.59
2:B:160:PHE:O	2:B:161:GLN:C	2.46	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LYS:HG2	1:A:24:TRP:CZ2	2.38	0.59
1:A:101:LYS:H	1:A:101:LYS:HD2	1.67	0.59
1:A:56:TYR:N	1:A:56:TYR:CD1	2.70	0.58
1:A:106:VAL:CG1	1:A:107:THR:H	2.13	0.58
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.85	0.58
2:B:220:LYS:NZ	2:B:231:GLY:HA3	2.18	0.58
1:A:55:PRO:HB2	1:A:143:ARG:NH2	2.19	0.58
2:B:18:GLY:HA3	2:B:127:TYR:CE1	2.37	0.58
2:B:296:THR:O	2:B:297:GLU:C	2.46	0.58
1:A:35:VAL:O	1:A:39:THR:HG23	2.04	0.58
1:A:441:TYR:HB2	1:A:458:VAL:O	2.03	0.58
2:B:248:GLU:HA	2:B:307:ARG:HH22	1.68	0.58
2:B:104:LYS:HA	2:B:237:ASP:OD2	2.03	0.58
2:B:168:LEU:C	2:B:170:PRO:HD2	2.29	0.58
2:B:193:LEU:O	2:B:194:GLU:C	2.44	0.58
1:A:34:LEU:HD12	1:A:132:ILE:HG13	1.85	0.58
1:A:468:PRO:O	1:A:469:LEU:HD23	2.03	0.58
2:B:163:SER:O	2:B:167:ILE:HG13	2.04	0.58
1:A:131:THR:OG1	1:A:143:ARG:NE	2.36	0.58
1:A:315:HIS:CE1	1:A:347:LYS:HD3	2.39	0.58
2:B:306:ASN:HA	2:B:309:ILE:HG22	1.85	0.58
1:A:96:HIS:HD2	1:A:97:PRO:N	2.02	0.57
2:B:342:TYR:C	2:B:342:TYR:HD1	2.12	0.57
2:B:364:ASP:O	2:B:367:GLN:HB2	2.03	0.57
1:A:246:LEU:HD13	1:A:303:LEU:HD11	1.86	0.57
1:A:270:ILE:HG13	1:A:314:VAL:HG12	1.84	0.57
1:A:335:GLY:O	1:A:355:ALA:HA	2.04	0.57
2:B:278:GLN:HE22	2:B:298:GLU:CB	2.17	0.57
1:A:373:GLN:HG2	2:B:394:GLN:HE22	1.69	0.57
2:B:200:THR:O	2:B:201:LYS:C	2.48	0.57
2:B:206:ARG:HG2	2:B:206:ARG:NH1	2.19	0.57
2:B:207:GLN:O	2:B:208:HIS:C	2.48	0.57
1:A:62:ALA:HB1	1:A:71:TRP:HD1	1.70	0.57
1:A:399:GLU:HG3	1:A:402:TRP:NE1	2.19	0.57
2:B:115:TYR:O	2:B:117:SER:N	2.38	0.57
2:B:228:LEU:C	2:B:230:MET:H	2.11	0.57
1:A:19:PRO:O	1:A:56:TYR:HB3	2.05	0.57
1:A:306:ASN:O	1:A:310:LEU:HG	2.04	0.57
1:A:33:ALA:O	1:A:36:GLU:HB2	2.04	0.57
1:A:476:LYS:HD3	1:A:517:LEU:HD22	1.87	0.57
1:A:398:TRP:CZ2	1:A:411:ILE:HB	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:LYS:O	2:B:176:PRO:HD3	2.05	0.57
1:A:454:LYS:CG	1:A:552:VAL:HA	2.35	0.56
1:A:368:LEU:O	1:A:372:VAL:HG23	2.06	0.56
1:A:101:LYS:HD2	1:A:101:LYS:N	2.20	0.56
1:A:254:VAL:HG21	1:A:288:ALA:HB3	1.86	0.56
1:A:276:VAL:HG12	1:A:276:VAL:O	2.04	0.56
2:B:155:GLY:O	2:B:159:ILE:HG13	2.04	0.56
2:B:419:THR:N	2:B:420:PRO:HD2	2.21	0.56
1:A:100:LEU:HD21	3:A:701:TPB:H211	1.88	0.56
1:A:372:VAL:HG11	1:A:411:ILE:CD1	2.36	0.56
1:A:518:VAL:O	1:A:522:ILE:HG13	2.05	0.56
2:B:161:GLN:O	2:B:164:MET:N	2.39	0.56
2:B:293:ILE:HB	2:B:294:PRO:HD2	1.88	0.56
1:A:506:ILE:HG21	1:A:533:LEU:HD11	1.88	0.56
2:B:13:LYS:O	2:B:16:MET:HB2	2.06	0.56
2:B:175:ASN:N	2:B:176:PRO:CD	2.69	0.56
1:A:315:HIS:HE2	1:A:347:LYS:HD3	1.69	0.56
2:B:94:ILE:HG12	2:B:161:GLN:CD	2.31	0.56
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.87	0.56
2:B:115:TYR:OH	2:B:184:MET:O	2.23	0.56
2:B:120:LEU:HD13	2:B:149:LEU:HD23	1.88	0.56
1:A:173:LYS:C	1:A:175:ASN:H	2.14	0.55
1:A:398:TRP:NE1	1:A:411:ILE:HG21	2.21	0.55
2:B:244:ILE:H	2:B:244:ILE:CD1	2.16	0.55
2:B:266:TRP:CZ3	2:B:426:TRP:CD1	2.94	0.55
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.41	0.55
2:B:215:THR:C	2:B:217:PRO:HD3	2.30	0.55
2:B:278:GLN:O	2:B:281:LYS:HG2	2.06	0.55
1:A:178:ILE:HD11	1:A:201:LYS:HG2	1.89	0.55
2:B:298:GLU:HB3	2:B:301:LEU:HB3	1.88	0.55
2:B:377:THR:O	2:B:378:GLU:C	2.48	0.55
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.89	0.55
1:A:53:GLU:N	1:A:55:PRO:HD3	2.16	0.55
1:A:241:VAL:CG1	1:A:242:GLN:N	2.69	0.55
1:A:244:ILE:HD11	1:A:310:LEU:HD22	1.88	0.55
1:A:353:LYS:O	1:A:374:LYS:NZ	2.38	0.55
1:A:317:VAL:O	1:A:349:LEU:HD12	2.07	0.55
1:A:457:TYR:O	1:A:457:TYR:CD2	2.58	0.55
1:A:81:ASN:C	1:A:83:ARG:H	2.15	0.55
1:A:92:LEU:HD13	2:B:22:LYS:HD2	1.88	0.55
2:B:215:THR:C	2:B:217:PRO:CD	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:ASP:O	2:B:68:SER:O	2.25	0.55
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.42	0.55
2:B:244:ILE:HD13	2:B:244:ILE:N	2.19	0.55
1:A:202:ILE:O	1:A:205:LEU:HB3	2.07	0.54
1:A:497:THR:HG22	1:A:498:ASP:N	2.21	0.54
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.90	0.54
1:A:12:LEU:O	1:A:13:LYS:C	2.51	0.54
1:A:449:GLU:N	1:A:449:GLU:CD	2.66	0.54
1:A:479:LEU:O	1:A:521:ILE:HD11	2.08	0.54
2:B:174:GLN:O	2:B:175:ASN:CG	2.51	0.54
1:A:543:GLY:CA	2:B:284:ARG:HH11	2.16	0.54
2:B:56:TYR:HE2	2:B:126:LYS:HD2	1.73	0.54
1:A:58:THR:HG22	1:A:59:PRO:CD	2.37	0.54
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.43	0.54
1:A:543:GLY:HA3	2:B:284:ARG:NH1	2.16	0.54
2:B:330:GLN:NE2	2:B:338:THR:O	2.37	0.54
1:A:402:TRP:O	1:A:402:TRP:CE3	2.60	0.54
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.43	0.54
1:A:542:ILE:HG22	1:A:543:GLY:N	2.21	0.54
2:B:296:THR:HG22	2:B:297:GLU:N	2.22	0.54
1:A:84:THR:HG21	1:A:153:TRP:NE1	2.16	0.54
1:A:128:THR:CB	1:A:146:TYR:HB2	2.38	0.53
1:A:362:THR:HG23	1:A:366:LYS:HD3	1.90	0.53
1:A:547:GLN:O	1:A:551:LEU:HG	2.08	0.53
2:B:278:GLN:HA	2:B:281:LYS:CE	2.30	0.53
2:B:306:ASN:O	2:B:308:GLU:N	2.41	0.53
2:B:388:LYS:HG3	2:B:413:GLU:HB2	1.89	0.53
1:A:290:THR:O	1:A:290:THR:HG22	2.08	0.53
1:A:220:LYS:HE3	1:A:221:HIS:NE2	2.23	0.53
1:A:394:GLN:O	1:A:395:LYS:C	2.51	0.53
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.43	0.53
1:A:282:LEU:C	1:A:284:ARG:H	2.17	0.53
1:A:309:ILE:HG22	1:A:310:LEU:N	2.24	0.53
1:A:111:VAL:O	1:A:114:ALA:HB3	2.08	0.53
2:B:104:LYS:HB2	2:B:192:ASP:OD1	2.09	0.53
2:B:198:HIS:O	2:B:200:THR:N	2.42	0.53
1:A:112:GLY:HA2	1:A:185:ASP:OD1	2.09	0.53
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.91	0.53
1:A:10:VAL:CG1	1:A:11:LYS:H	2.21	0.52
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.89	0.52
2:B:139:THR:HG23	2:B:140:PRO:HD2	1.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:MET:HE3	2:B:361:HIS:CE1	2.44	0.52
2:B:362:THR:HG23	2:B:366:LYS:NZ	2.25	0.52
1:A:103:LYS:C	1:A:104:LYS:HE2	2.33	0.52
2:B:277:ARG:H	2:B:277:ARG:CD	2.21	0.52
1:A:104:LYS:HG2	1:A:192:ASP:HA	1.92	0.52
1:A:215:THR:HG22	1:A:216:THR:H	1.73	0.52
1:A:497:THR:HG22	1:A:499:SER:HB3	1.91	0.52
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.45	0.52
1:A:389:PHE:HB3	1:A:391:LEU:HD21	1.92	0.52
1:A:395:LYS:O	1:A:396:GLU:C	2.53	0.52
1:A:66:LYS:C	1:A:68:SER:H	2.18	0.52
1:A:34:LEU:HB3	1:A:132:ILE:HD12	1.91	0.52
1:A:376:THR:O	1:A:380:ILE:HG13	2.10	0.52
1:A:411:ILE:O	1:A:411:ILE:HG23	2.10	0.52
2:B:375:ILE:O	2:B:376:THR:C	2.53	0.52
1:A:215:THR:CG2	1:A:216:THR:N	2.73	0.51
1:A:509:GLN:H	1:A:510:PRO:HD3	1.74	0.51
2:B:2:ILE:O	2:B:4:PRO:CD	2.53	0.51
1:A:77:PHE:O	1:A:80:LEU:N	2.29	0.51
2:B:31:ILE:HG22	2:B:35:VAL:CG2	2.41	0.51
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.45	0.51
1:A:31:ILE:HG21	1:A:134:SER:O	2.11	0.51
1:A:241:VAL:HG13	1:A:266:TRP:NE1	2.26	0.51
1:A:244:ILE:HD11	1:A:310:LEU:CD1	2.36	0.51
2:B:306:ASN:C	2:B:308:GLU:N	2.69	0.51
1:A:35:VAL:O	1:A:35:VAL:HG12	2.08	0.51
1:A:510:PRO:HB2	1:A:522:ILE:HD11	1.92	0.51
2:B:210:LEU:HD12	2:B:210:LEU:O	2.10	0.51
2:B:421:PRO:HG2	2:B:422:LEU:H	1.74	0.51
1:A:3:SER:OG	1:A:5:ILE:CD1	2.58	0.51
1:A:102:LYS:O	1:A:103:LYS:HD3	2.10	0.51
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.76	0.51
2:B:131:THR:OG1	2:B:143:ARG:HG2	2.11	0.51
2:B:330:GLN:HE21	2:B:338:THR:C	2.19	0.51
2:B:388:LYS:NZ	2:B:415:GLU:OE1	2.43	0.51
2:B:72:ARG:NH2	2:B:151:GLN:OE1	2.43	0.51
2:B:157:PRO:HG2	2:B:158:ALA:N	2.25	0.51
2:B:200:THR:C	2:B:202:ILE:N	2.65	0.51
2:B:226:PRO:O	2:B:228:LEU:N	2.44	0.51
1:A:301:LEU:HD12	1:A:301:LEU:O	2.10	0.51
2:B:198:HIS:C	2:B:200:THR:N	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LYS:HB2	1:A:16:MET:HG3	1.93	0.51
1:A:225:PRO:HA	1:A:226:PRO:C	2.36	0.51
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.75	0.51
1:A:350:LYS:HG2	1:A:351:THR:N	2.25	0.51
1:A:308:GLU:O	1:A:311:LYS:HG2	2.11	0.50
2:B:245:VAL:CG1	2:B:246:LEU:N	2.73	0.50
2:B:385:LYS:O	2:B:385:LYS:HG3	2.10	0.50
2:B:301:LEU:HD23	2:B:301:LEU:O	2.10	0.50
1:A:30:LYS:O	1:A:32:LYS:N	2.45	0.50
1:A:91:GLN:HE21	1:A:184:MET:CE	2.24	0.50
1:A:224:GLU:O	1:A:226:PRO:O	2.29	0.50
1:A:390:LYS:O	1:A:391:LEU:HD23	2.10	0.50
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.46	0.50
2:B:296:THR:HB	2:B:299:ALA:HB2	1.93	0.50
1:A:435:VAL:CG1	2:B:290:THR:HG21	2.39	0.50
1:A:21:VAL:CG2	1:A:58:THR:HA	2.42	0.50
1:A:62:ALA:HB1	1:A:71:TRP:CD1	2.45	0.50
1:A:330:GLN:HE22	1:A:340:GLN:NE2	1.97	0.50
1:A:477:THR:C	1:A:479:LEU:H	2.20	0.50
1:A:511:ASP:OD1	1:A:512:LYS:HG2	2.12	0.50
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.94	0.50
2:B:364:ASP:O	2:B:365:VAL:C	2.55	0.50
1:A:10:VAL:CG1	1:A:11:LYS:N	2.75	0.49
1:A:208:HIS:HA	1:A:211:ARG:NH1	2.27	0.49
1:A:84:THR:HG22	1:A:124:PHE:CZ	2.46	0.49
1:A:108:VAL:HG12	1:A:188:TYR:CD2	2.47	0.49
1:A:282:LEU:C	1:A:284:ARG:N	2.70	0.49
2:B:257:ILE:HD12	2:B:282:LEU:HD23	1.94	0.49
1:A:73:LYS:NZ	1:A:130:PHE:CZ	2.74	0.49
1:A:75:VAL:HG12	1:A:76:ASP:H	1.76	0.49
1:A:382:ILE:HG23	2:B:136:ASN:ND2	2.26	0.49
1:A:100:LEU:HD22	3:A:701:TPB:N1	2.27	0.49
1:A:246:LEU:HD13	1:A:303:LEU:CD1	2.41	0.49
1:A:311:LYS:HE3	1:A:312:GLU:OE2	2.12	0.49
2:B:115:TYR:C	2:B:117:SER:H	2.18	0.49
2:B:56:TYR:CE2	2:B:126:LYS:HD2	2.47	0.49
2:B:201:LYS:HZ3	2:B:204:GLU:CG	2.19	0.49
1:A:174:GLN:O	1:A:175:ASN:CG	2.56	0.49
1:A:536:VAL:HG11	1:A:542:ILE:HG13	1.95	0.49
2:B:34:LEU:O	2:B:35:VAL:C	2.54	0.49
1:A:3:SER:HB3	1:A:212:TRP:C	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:HA	1:A:318:TYR:HD1	1.76	0.49
1:A:59:PRO:O	1:A:75:VAL:HG13	2.13	0.49
1:A:330:GLN:NE2	1:A:340:GLN:HE22	1.98	0.49
1:A:440:PHE:CE1	1:A:489:SER:CB	2.96	0.49
2:B:278:GLN:C	2:B:281:LYS:HG2	2.36	0.49
1:A:3:SER:C	1:A:5:ILE:H	2.20	0.49
2:B:327:ALA:HA	2:B:340:GLN:O	2.12	0.49
1:A:410:TRP:HB2	2:B:365:VAL:CG2	2.42	0.48
1:A:513:SER:O	1:A:519:ASN:ND2	2.46	0.48
2:B:54:ASN:HD21	2:B:126:LYS:HA	1.78	0.48
2:B:278:GLN:HA	2:B:281:LYS:HG2	1.94	0.48
1:A:132:ILE:HG23	1:A:132:ILE:O	2.12	0.48
1:A:208:HIS:CE1	1:A:212:TRP:HE1	2.31	0.48
1:A:301:LEU:O	1:A:305:GLU:HG3	2.13	0.48
1:A:449:GLU:N	1:A:449:GLU:OE1	2.46	0.48
3:A:701:TPB:N1	3:A:701:TPB:H16	2.27	0.48
2:B:195:ILE:CG1	2:B:199:ARG:HE	2.24	0.48
2:B:337:TRP:N	2:B:337:TRP:CD1	2.81	0.48
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.48	0.48
1:A:131:THR:OG1	1:A:143:ARG:CD	2.61	0.48
1:A:210:LEU:O	1:A:210:LEU:HD12	2.14	0.48
1:A:497:THR:HG22	1:A:499:SER:N	2.28	0.48
1:A:503:LEU:HD22	1:A:535:TRP:CB	2.36	0.48
2:B:223:LYS:C	2:B:225:PRO:HD3	2.37	0.48
2:B:418:ASN:O	2:B:419:THR:CG2	2.62	0.48
1:A:38:CYS:HB3	1:A:144:TYR:CZ	2.49	0.48
1:A:293:ILE:HG23	1:A:294:PRO:HD2	1.96	0.48
2:B:216:THR:N	2:B:217:PRO:CD	2.76	0.48
2:B:305:GLU:O	2:B:308:GLU:HB3	2.14	0.48
2:B:332:GLN:HE21	2:B:338:THR:HG1	1.61	0.48
2:B:115:TYR:N	2:B:115:TYR:CD2	2.78	0.48
2:B:193:LEU:HD12	2:B:198:HIS:N	2.29	0.48
2:B:279:LEU:O	2:B:282:LEU:HB3	2.13	0.48
1:A:394:GLN:NE2	1:A:395:LYS:H	2.11	0.48
1:A:492:GLU:CD	1:A:530:LYS:HD2	2.38	0.48
2:B:149:LEU:HD13	2:B:156:SER:CA	2.44	0.48
2:B:226:PRO:O	2:B:227:PHE:C	2.56	0.48
1:A:54:ASN:N	1:A:55:PRO:CD	2.76	0.48
1:A:77:PHE:CZ	1:A:150:PRO:HB3	2.49	0.48
1:A:100:LEU:HD22	3:A:701:TPB:C9	2.44	0.48
1:A:242:GLN:HE21	1:A:244:ILE:HG22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.49	0.48
2:B:136:ASN:O	2:B:137:ASN:C	2.56	0.48
1:A:98:ALA:HB1	1:A:350:LYS:HB2	1.96	0.48
1:A:396:GLU:O	1:A:400:THR:OG1	2.27	0.48
1:A:442:VAL:HG13	1:A:481:ALA:CB	2.42	0.48
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.43	0.47
1:A:493:VAL:HG22	1:A:494:ASN:N	2.29	0.47
1:A:54:ASN:O	1:A:55:PRO:C	2.57	0.47
1:A:108:VAL:CG1	1:A:227:PHE:CE1	2.97	0.47
1:A:27:THR:O	1:A:28:GLU:C	2.56	0.47
1:A:326:ILE:N	1:A:326:ILE:CD1	2.71	0.47
1:A:477:THR:C	1:A:479:LEU:N	2.71	0.47
1:A:91:GLN:O	1:A:92:LEU:C	2.56	0.47
1:A:255:ASN:HD22	1:A:289:LEU:HD11	1.78	0.47
1:A:416:PHE:CE2	1:A:418:ASN:HB2	2.50	0.47
1:A:470:THR:O	1:A:471:ASN:CB	2.57	0.47
2:B:195:ILE:CG1	2:B:199:ARG:HG3	2.45	0.47
2:B:394:GLN:HE21	2:B:396:GLU:HB2	1.79	0.47
1:A:100:LEU:HD21	3:A:701:TPB:C21	2.44	0.47
1:A:121:ASP:O	1:A:122:GLU:C	2.56	0.47
1:A:483:TYR:CE2	1:A:487:GLN:CD	2.92	0.47
2:B:276:VAL:O	2:B:279:LEU:N	2.42	0.47
2:B:297:GLU:HG2	2:B:298:GLU:HG2	1.96	0.47
1:A:65:LYS:HG2	1:A:68:SER:CA	2.45	0.47
1:A:178:ILE:HD11	1:A:201:LYS:CG	2.45	0.47
1:A:420:PRO:HA	1:A:421:PRO:C	2.40	0.47
2:B:416:PHE:CD2	2:B:416:PHE:N	2.82	0.47
1:A:18:GLY:CA	1:A:56:TYR:CD2	2.98	0.47
1:A:483:TYR:HB2	1:A:521:ILE:CG1	2.45	0.47
2:B:266:TRP:HB2	2:B:422:LEU:HD23	1.97	0.47
2:B:320:ASP:O	2:B:343:GLN:NE2	2.33	0.47
1:A:19:PRO:O	1:A:56:TYR:CB	2.63	0.47
1:A:242:GLN:O	1:A:242:GLN:HG3	2.14	0.47
1:A:397:THR:O	1:A:400:THR:HB	2.14	0.47
2:B:85:GLN:O	2:B:85:GLN:HG2	2.13	0.47
1:A:30:LYS:O	1:A:33:ALA:N	2.48	0.47
1:A:92:LEU:CD1	2:B:22:LYS:HD2	2.44	0.47
1:A:156:SER:O	1:A:157:PRO:C	2.56	0.47
2:B:156:SER:N	2:B:157:PRO:CD	2.76	0.47
1:A:229:TRP:O	1:A:231:GLY:N	2.48	0.47
1:A:288:ALA:HB2	1:A:291:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:THR:HG22	1:A:363:ASN:N	2.30	0.47
1:A:507:GLN:O	1:A:509:GLN:HG3	2.14	0.47
2:B:65:LYS:NZ	2:B:409:THR:CG2	2.78	0.46
2:B:85:GLN:O	2:B:85:GLN:CG	2.62	0.46
2:B:323:LYS:NZ	2:B:344:GLU:OE1	2.27	0.46
2:B:388:LYS:HE2	2:B:415:GLU:OE1	2.15	0.46
1:A:162:SER:O	1:A:163:SER:C	2.58	0.46
2:B:357:MET:HE3	2:B:361:HIS:ND1	2.31	0.46
1:A:77:PHE:CE1	1:A:150:PRO:HB3	2.50	0.46
1:A:115:TYR:O	1:A:149:LEU:HB2	2.15	0.46
1:A:509:GLN:N	1:A:510:PRO:CD	2.78	0.46
2:B:90:VAL:O	2:B:91:GLN:C	2.56	0.46
1:A:120:LEU:HD23	1:A:125:ARG:CG	2.45	0.46
1:A:277:ARG:NH2	1:A:514:GLU:OE1	2.44	0.46
2:B:254:VAL:O	2:B:258:GLN:HG3	2.15	0.46
1:A:30:LYS:O	1:A:31:ILE:C	2.59	0.46
1:A:483:TYR:O	1:A:487:GLN:HG3	2.16	0.46
2:B:146:TYR:CD1	2:B:150:PRO:HB3	2.50	0.46
2:B:345:PRO:C	2:B:346:PHE:CD1	2.94	0.46
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.81	0.46
2:B:309:ILE:HG13	2:B:312:GLU:OE2	2.15	0.46
1:A:19:PRO:HG2	1:A:80:LEU:HA	1.97	0.46
1:A:182:GLN:O	1:A:182:GLN:HG3	2.15	0.46
1:A:397:THR:HG21	1:A:424:LYS:HA	1.98	0.46
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.51	0.46
2:B:300:GLU:OE1	2:B:300:GLU:HA	2.15	0.46
2:B:305:GLU:HG3	2:B:306:ASN:N	2.31	0.46
1:A:77:PHE:O	1:A:78:ARG:C	2.58	0.45
2:B:171:PHE:CD1	2:B:171:PHE:C	2.94	0.45
2:B:266:TRP:CG	2:B:422:LEU:HD23	2.51	0.45
2:B:370:GLU:O	2:B:371:ALA:C	2.58	0.45
2:B:191:SER:OG	2:B:198:HIS:ND1	2.36	0.45
2:B:332:GLN:HA	2:B:332:GLN:OE1	2.16	0.45
1:A:82:LYS:O	1:A:82:LYS:HG2	2.17	0.45
1:A:513:SER:O	1:A:519:ASN:OD1	2.34	0.45
2:B:287:LYS:C	2:B:288:ALA:O	2.58	0.45
1:A:96:HIS:CD2	1:A:97:PRO:N	2.83	0.45
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.51	0.45
2:B:238:LYS:O	2:B:240:THR:N	2.49	0.45
1:A:38:CYS:SG	1:A:144:TYR:CE2	3.10	0.45
1:A:211:ARG:HG3	1:A:211:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:TRP:C	1:A:536:VAL:HG23	2.42	0.45
2:B:183:TYR:O	2:B:184:MET:HB2	2.16	0.45
2:B:296:THR:CG2	2:B:297:GLU:N	2.79	0.45
1:A:24:TRP:CD1	1:A:24:TRP:N	2.84	0.45
1:A:96:HIS:CE1	1:A:350:LYS:HE2	2.51	0.45
1:A:131:THR:HG1	1:A:143:ARG:HE	1.64	0.45
1:A:376:THR:HG23	1:A:386:THR:HG22	1.97	0.45
1:A:500:GLN:H	1:A:500:GLN:HG3	1.49	0.45
2:B:84:THR:O	2:B:86:ASP:N	2.49	0.45
1:A:278:GLN:HB2	1:A:302:GLU:OE1	2.17	0.45
1:A:342:TYR:CD1	1:A:342:TYR:C	2.94	0.45
1:A:438:GLU:HG3	1:A:460:ASN:ND2	2.27	0.45
2:B:58:THR:HA	2:B:59:PRO:HD3	1.81	0.45
1:A:22:LYS:HE3	1:A:24:TRP:CZ2	2.33	0.45
1:A:32:LYS:O	1:A:36:GLU:HG3	2.17	0.45
1:A:115:TYR:OH	1:A:151:GLN:HB2	2.17	0.45
1:A:356:ARG:NH1	1:A:358:ARG:HD2	2.32	0.45
2:B:179:VAL:HG23	2:B:179:VAL:O	2.15	0.45
2:B:362:THR:HG23	2:B:366:LYS:HZ3	1.82	0.45
1:A:125:ARG:C	1:A:127:TYR:N	2.76	0.45
1:A:379:SER:HA	1:A:383:TRP:CE3	2.52	0.45
2:B:198:HIS:C	2:B:200:THR:H	2.25	0.45
2:B:301:LEU:O	2:B:305:GLU:HB3	2.17	0.44
1:A:115:TYR:OH	1:A:151:GLN:CB	2.65	0.44
1:A:215:THR:CG2	1:A:216:THR:H	2.30	0.44
1:A:22:LYS:HB3	1:A:24:TRP:NE1	2.32	0.44
1:A:125:ARG:C	1:A:127:TYR:H	2.25	0.44
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.53	0.44
2:B:280:SER:O	2:B:283:LEU:N	2.46	0.44
1:A:151:GLN:O	1:A:151:GLN:HG3	2.17	0.44
1:A:167:ILE:O	1:A:170:PRO:HD2	2.17	0.44
1:A:206:ARG:HH21	1:A:217:PRO:CA	2.31	0.44
1:A:242:GLN:HG2	1:A:266:TRP:HE1	1.81	0.44
2:B:308:GLU:C	2:B:310:LEU:N	2.74	0.44
2:B:314:VAL:HG13	2:B:317:VAL:HG21	1.98	0.44
2:B:394:GLN:O	2:B:395:LYS:C	2.60	0.44
1:A:128:THR:HB	1:A:146:TYR:HB2	2.00	0.44
1:A:183:TYR:CE2	1:A:230:MET:SD	3.11	0.44
1:A:373:GLN:HG2	2:B:394:GLN:NE2	2.30	0.44
1:A:39:THR:O	1:A:40:GLU:C	2.61	0.44
1:A:50:ILE:HG12	1:A:51:GLY:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:HG13	1:A:227:PHE:HE1	1.79	0.44
1:A:543:GLY:CA	2:B:284:ARG:NH1	2.78	0.44
2:B:6:GLU:O	2:B:7:THR:O	2.35	0.44
1:A:57:ASN:HA	1:A:129:ALA:O	2.17	0.44
1:A:382:ILE:HA	2:B:136:ASN:HD22	1.83	0.44
1:A:402:TRP:CE3	1:A:402:TRP:C	2.95	0.44
1:A:483:TYR:CE2	1:A:487:GLN:NE2	2.86	0.44
2:B:164:MET:C	2:B:166:LYS:N	2.75	0.44
2:B:245:VAL:CG1	2:B:246:LEU:H	2.31	0.44
1:A:30:LYS:C	1:A:32:LYS:N	2.76	0.44
1:A:35:VAL:O	1:A:35:VAL:CG1	2.65	0.44
1:A:55:PRO:HB2	1:A:143:ARG:HH22	1.82	0.44
1:A:283:LEU:C	1:A:285:GLY:H	2.26	0.44
2:B:76:ASP:O	2:B:76:ASP:CG	2.56	0.44
2:B:202:ILE:C	2:B:204:GLU:N	2.73	0.44
2:B:242:GLN:O	2:B:243:PRO:C	2.59	0.44
2:B:262:GLY:O	2:B:263:LYS:C	2.60	0.44
1:A:106:VAL:O	1:A:107:THR:OG1	2.36	0.44
1:A:259:LYS:HG2	1:A:263:LYS:HE3	2.00	0.44
1:A:328:GLU:HA	1:A:390:LYS:O	2.17	0.44
1:A:438:GLU:OE2	1:A:461:LYS:HB2	2.17	0.44
2:B:229:TRP:CD1	2:B:229:TRP:N	2.85	0.44
2:B:363:ASN:O	2:B:367:GLN:NE2	2.51	0.44
2:B:232:TYR:CE1	2:B:234:LEU:HD21	2.53	0.43
1:A:254:VAL:O	1:A:258:GLN:HG3	2.18	0.43
2:B:298:GLU:O	2:B:302:GLU:N	2.51	0.43
1:A:65:LYS:HG2	1:A:68:SER:CB	2.47	0.43
1:A:77:PHE:CD2	1:A:80:LEU:CD2	3.01	0.43
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.45	0.43
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.48	0.43
1:A:536:VAL:HG11	1:A:542:ILE:HD12	2.01	0.43
2:B:216:THR:O	2:B:216:THR:HG22	2.17	0.43
2:B:306:ASN:C	2:B:308:GLU:H	2.26	0.43
1:A:369:THR:O	1:A:370:GLU:C	2.59	0.43
1:A:442:VAL:CG1	1:A:443:ASP:N	2.80	0.43
2:B:242:GLN:O	2:B:242:GLN:CD	2.61	0.43
1:A:51:GLY:O	1:A:52:PRO:C	2.61	0.43
1:A:81:ASN:C	1:A:83:ARG:N	2.77	0.43
1:A:84:THR:CG2	1:A:124:PHE:HZ	2.31	0.43
1:A:302:GLU:O	1:A:303:LEU:C	2.60	0.43
1:A:324:ASP:O	1:A:343:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ARG:HG3	2:B:72:ARG:HH11	1.82	0.43
2:B:178:ILE:HG22	2:B:191:SER:CB	2.48	0.43
1:A:17:ASP:OD2	1:A:56:TYR:HE2	2.02	0.43
1:A:111:VAL:O	1:A:114:ALA:CB	2.66	0.43
1:A:361:HIS:HD2	1:A:513:SER:HB2	1.84	0.43
1:A:476:LYS:HD3	1:A:517:LEU:CD2	2.49	0.43
2:B:84:THR:HG21	2:B:124:PHE:CZ	2.53	0.43
1:A:5:ILE:HG22	1:A:6:GLU:O	2.18	0.43
1:A:447:ASN:ND2	1:A:450:THR:HG23	2.34	0.43
2:B:249:LYS:HD2	2:B:252:TRP:HZ3	1.76	0.43
1:A:195:ILE:O	1:A:199:ARG:HG3	2.18	0.43
2:B:27:THR:HG22	2:B:29:GLU:H	1.84	0.43
2:B:152:GLY:O	2:B:184:MET:HE1	2.18	0.43
1:A:283:LEU:C	1:A:285:GLY:N	2.75	0.43
1:A:30:LYS:HD3	1:A:62:ALA:HB3	2.01	0.43
1:A:161:GLN:HE21	1:A:182:GLN:CD	2.26	0.43
1:A:341:ILE:O	1:A:349:LEU:HB3	2.19	0.43
2:B:418:ASN:C	2:B:419:THR:HG23	2.43	0.43
1:A:194:GLU:O	1:A:195:ILE:C	2.62	0.42
1:A:363:ASN:OD1	1:A:364:ASP:N	2.51	0.42
1:A:371:ALA:O	1:A:372:VAL:C	2.61	0.42
1:A:397:THR:HB	1:A:398:TRP:H	1.66	0.42
1:A:400:THR:O	1:A:403:THR:HB	2.19	0.42
1:A:497:THR:HG21	1:A:499:SER:HB3	2.00	0.42
2:B:12:LEU:HD11	2:B:127:TYR:CE2	2.54	0.42
2:B:53:GLU:OE1	2:B:53:GLU:N	2.44	0.42
1:A:9:PRO:O	1:A:9:PRO:HG2	2.18	0.42
2:B:104:LYS:HB3	2:B:192:ASP:HA	2.00	0.42
2:B:194:GLU:O	2:B:195:ILE:C	2.61	0.42
1:A:183:TYR:OH	1:A:230:MET:SD	2.74	0.42
2:B:11:LYS:NZ	2:B:14:PRO:HG3	2.34	0.42
2:B:362:THR:HG22	2:B:363:ASN:O	2.19	0.42
1:A:317:VAL:HG22	1:A:318:TYR:H	1.84	0.42
2:B:171:PHE:CE2	2:B:205:LEU:HB2	2.53	0.42
1:A:13:LYS:N	1:A:83:ARG:O	2.51	0.42
1:A:23:GLN:HG2	1:A:25:PRO:CD	2.48	0.42
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.91	0.42
1:A:101:LYS:NZ	2:B:138:GLU:OE2	2.48	0.42
1:A:173:LYS:C	1:A:175:ASN:N	2.77	0.42
1:A:389:PHE:CD1	1:A:391:LEU:HD21	2.54	0.42
1:A:411:ILE:HD12	1:A:412:PRO:CD	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:GLN:NE2	2:B:298:GLU:CB	2.74	0.42
1:A:169:GLU:O	1:A:170:PRO:C	2.60	0.42
1:A:222:GLN:CG	1:A:223:LYS:H	2.16	0.42
2:B:81:ASN:O	2:B:82:LYS:C	2.63	0.42
2:B:105:SER:OG	2:B:235:HIS:CE1	2.72	0.42
2:B:324:ASP:O	2:B:343:GLN:HG2	2.20	0.42
1:A:100:LEU:O	1:A:318:TYR:HB3	2.20	0.42
1:A:201:LYS:O	1:A:202:ILE:C	2.60	0.42
1:A:465:LYS:HE2	1:A:488:ASP:OD2	2.20	0.42
2:B:18:GLY:CA	2:B:127:TYR:CE1	3.03	0.42
2:B:302:GLU:HA	2:B:305:GLU:HB3	2.00	0.42
1:A:57:ASN:ND2	1:A:58:THR:H	2.18	0.42
1:A:62:ALA:HA	1:A:72:ARG:O	2.20	0.42
2:B:249:LYS:HB2	2:B:252:TRP:CZ3	2.55	0.42
2:B:323:LYS:HB2	2:B:343:GLN:NE2	2.35	0.42
2:B:388:LYS:HG3	2:B:413:GLU:CB	2.50	0.42
1:A:41:MET:HB3	1:A:47:ILE:HG12	2.01	0.42
1:A:183:TYR:CZ	1:A:230:MET:SD	3.13	0.42
1:A:469:LEU:HD11	1:A:480:GLN:HG2	2.02	0.42
2:B:266:TRP:CD1	2:B:422:LEU:HD23	2.54	0.42
2:B:422:LEU:HD12	2:B:425:LEU:HD12	2.01	0.42
1:A:445:ALA:HB2	1:A:549:ASP:OD1	2.20	0.42
1:A:542:ILE:CG2	1:A:543:GLY:N	2.83	0.42
2:B:312:GLU:O	2:B:312:GLU:CG	2.68	0.42
2:B:357:MET:H	2:B:357:MET:HG3	1.66	0.42
2:B:359:GLY:C	2:B:361:HIS:H	2.25	0.42
1:A:244:ILE:CD1	1:A:310:LEU:HD13	2.41	0.41
1:A:267:ALA:O	1:A:271:TYR:HB2	2.19	0.41
2:B:148:VAL:O	2:B:150:PRO:HD3	2.20	0.41
2:B:270:ILE:HG23	2:B:346:PHE:O	2.19	0.41
1:A:104:LYS:HB2	1:A:192:ASP:HA	2.01	0.41
1:A:492:GLU:HG2	1:A:530:LYS:HD2	2.02	0.41
2:B:17:ASP:O	2:B:83:ARG:NE	2.37	0.41
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.01	0.41
1:A:519:ASN:O	1:A:523:GLU:HG3	2.21	0.41
2:B:90:VAL:HG12	2:B:91:GLN:N	2.34	0.41
2:B:195:ILE:O	2:B:199:ARG:HG3	2.21	0.41
2:B:212:TRP:CE3	2:B:212:TRP:HA	2.55	0.41
2:B:306:ASN:HA	2:B:309:ILE:CG2	2.50	0.41
2:B:317:VAL:HG12	2:B:349:LEU:CD2	2.50	0.41
2:B:326:ILE:HB	2:B:342:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:LYS:HG2	2:B:399:GLU:OE1	2.21	0.41
1:A:344:GLU:HA	1:A:345:PRO:HD3	1.66	0.41
1:A:440:PHE:HE1	1:A:489:SER:CB	2.33	0.41
1:A:451:LYS:O	1:A:471:ASN:N	2.52	0.41
1:A:540:LYS:O	1:A:540:LYS:CG	2.66	0.41
2:B:220:LYS:HZ1	2:B:231:GLY:HA3	1.85	0.41
2:B:235:HIS:HA	2:B:236:PRO:HD2	1.67	0.41
2:B:254:VAL:O	2:B:257:ILE:HG23	2.20	0.41
1:A:356:ARG:HH11	1:A:358:ARG:HD2	1.84	0.41
1:A:506:ILE:CG2	1:A:533:LEU:HD12	2.44	0.41
2:B:246:LEU:HD21	2:B:310:LEU:HD11	2.02	0.41
2:B:298:GLU:O	2:B:301:LEU:HB3	2.20	0.41
1:A:19:PRO:CG	1:A:80:LEU:HA	2.50	0.41
1:A:39:THR:C	1:A:41:MET:N	2.76	0.41
2:B:53:GLU:O	2:B:55:PRO:HD3	2.20	0.41
2:B:200:THR:O	2:B:204:GLU:N	2.48	0.41
2:B:358:ARG:O	2:B:361:HIS:NE2	2.53	0.41
1:A:340:GLN:CB	1:A:351:THR:HG22	2.50	0.41
1:A:433:PRO:HG3	2:B:255:ASN:ND2	2.36	0.41
1:A:460:ASN:HD22	1:A:460:ASN:N	2.19	0.41
1:A:474:ASN:HD22	1:A:474:ASN:H	1.68	0.41
2:B:363:ASN:OD1	2:B:366:LYS:HB2	2.21	0.41
1:A:94:ILE:CD1	1:A:230:MET:HE2	2.50	0.41
1:A:189:VAL:HG21	1:A:205:LEU:CD2	2.50	0.41
1:A:201:LYS:O	1:A:204:GLU:HB2	2.21	0.41
1:A:477:THR:O	1:A:480:GLN:N	2.51	0.41
2:B:296:THR:H	2:B:299:ALA:HB3	1.85	0.41
1:A:12:LEU:CD1	1:A:127:TYR:CE1	3.04	0.41
1:A:22:LYS:HE2	1:A:22:LYS:HB2	1.89	0.41
1:A:356:ARG:O	1:A:356:ARG:HG3	2.21	0.41
1:A:372:VAL:O	1:A:376:THR:OG1	2.39	0.41
1:A:395:LYS:HE2	1:A:399:GLU:OE1	2.21	0.41
2:B:31:ILE:HG22	2:B:35:VAL:HG21	2.03	0.41
2:B:40:GLU:O	2:B:41:MET:C	2.63	0.41
2:B:200:THR:O	2:B:202:ILE:N	2.54	0.41
2:B:362:THR:CG2	2:B:366:LYS:NZ	2.84	0.41
2:B:366:LYS:HA	2:B:405:TYR:CD1	2.56	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD2	1.82	0.41
1:A:511:ASP:CG	1:A:512:LYS:N	2.79	0.41
2:B:16:MET:HG3	2:B:83:ARG:HG2	2.03	0.41
2:B:24:TRP:HZ3	2:B:59:PRO:CB	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PRO:C	1:A:99:GLY:N	2.79	0.40
1:A:253:THR:O	1:A:254:VAL:C	2.63	0.40
1:A:270:ILE:O	1:A:272:PRO:HD3	2.20	0.40
1:A:407:GLN:HG2	2:B:393:ILE:HA	2.03	0.40
1:A:515:SER:O	1:A:517:LEU:N	2.54	0.40
1:A:17:ASP:O	1:A:83:ARG:CD	2.65	0.40
1:A:172:LYS:HB3	1:A:172:LYS:HE2	1.70	0.40
1:A:241:VAL:HG12	1:A:242:GLN:O	2.21	0.40
1:A:394:GLN:O	1:A:397:THR:N	2.52	0.40
1:A:536:VAL:HG11	1:A:542:ILE:CG1	2.51	0.40
2:B:54:ASN:ND2	2:B:126:LYS:HA	2.35	0.40
2:B:216:THR:N	2:B:217:PRO:HD3	2.36	0.40
1:A:201:LYS:O	1:A:204:GLU:N	2.54	0.40
1:A:246:LEU:HA	1:A:246:LEU:HD23	1.78	0.40
1:A:275:LYS:C	1:A:276:VAL:HG23	2.46	0.40
1:A:283:LEU:O	1:A:285:GLY:N	2.54	0.40
1:A:498:ASP:HA	1:A:536:VAL:O	2.21	0.40
2:B:184:MET:HE2	2:B:184:MET:HB3	1.86	0.40
2:B:245:VAL:HG12	2:B:246:LEU:O	2.22	0.40
2:B:276:VAL:O	2:B:277:ARG:C	2.64	0.40
1:A:3:SER:OG	1:A:5:ILE:HD12	2.21	0.40
1:A:31:ILE:O	1:A:35:VAL:HG23	2.21	0.40
1:A:535:TRP:O	1:A:536:VAL:HG23	2.21	0.40
1:A:3:SER:HB2	1:A:4:PRO:HD2	2.03	0.40
1:A:55:PRO:HB2	1:A:143:ARG:CZ	2.52	0.40
1:A:124:PHE:CE2	1:A:153:TRP:CZ2	3.09	0.40
2:B:12:LEU:HD12	2:B:12:LEU:H	1.86	0.40
2:B:195:ILE:HG13	2:B:199:ARG:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	258/500 (52%)	240 (93%)	18 (7%)	14	44
2	B	268/392 (68%)	244 (91%)	24 (9%)	9	34
All	All	526/892 (59%)	484 (92%)	42 (8%)	11	38

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
1	A	104	LYS
1	A	132	ILE
1	A	136	ASN
1	A	138	GLU
1	A	142	ILE
1	A	162	SER
1	A	172	LYS
1	A	177	ASP
1	A	207	GLN
1	A	216	THR
1	A	228	LEU
1	A	269	GLN
1	A	274	ILE
1	A	298	GLU
1	A	326	ILE
1	A	347	LYS
1	A	358	ARG
2	B	22	LYS
2	B	70	LYS
2	B	193	LEU
2	B	200	THR
2	B	201	LYS
2	B	206	ARG
2	B	207	GLN
2	B	212	TRP
2	B	229	TRP
2	B	232	TYR
2	B	239	TRP
2	B	244	ILE
2	B	246	LEU

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Mol	Chain	Res	Type
2	B	250	ASP
2	B	277	ARG
2	B	279	LEU
2	B	294	PRO
2	B	305	GLU
2	B	338	THR
2	B	340	GLN
2	B	342	TYR
2	B	366	LYS
2	B	374	LYS
2	B	399	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	96	HIS
1	A	136	ASN
1	A	151	GLN
1	A	161	GLN
1	A	235	HIS
1	A	242	GLN
1	A	255	ASN
1	A	269	GLN
1	A	330	GLN
1	A	361	HIS
2	B	23	GLN
2	B	182	GLN
2	B	207	GLN
2	B	258	GLN
2	B	348	ASN
2	B	367	GLN
2	B	394	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
3	TPB	A	701	-	27,27,27	3.30	15 (55%)	35,37,37	2.23	9 (25%)

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
3	TPB	A	701	-	-	0/10/10/10	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	TPB	C9-N3	6.75	1.44	1.34
3	A	701	TPB	C5-C6	5.40	1.47	1.39
3	A	701	TPB	C10-N3	5.07	1.45	1.34
3	A	701	TPB	C5-C4	4.85	1.46	1.39
3	A	701	TPB	C16-C11	4.54	1.46	1.39
3	A	701	TPB	C1-C6	4.52	1.46	1.40
3	A	701	TPB	C8-N7	4.45	1.46	1.38
3	A	701	TPB	C16-C15	4.01	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	TPB	C13-C12	3.99	1.45	1.38
3	A	701	TPB	C3-C2	3.94	1.45	1.39
3	A	701	TPB	C9-N5	3.59	1.44	1.36
3	A	701	TPB	C15-C14	3.35	1.46	1.39
3	A	701	TPB	C1-C2	3.30	1.44	1.40
3	A	701	TPB	C61-C6	2.34	1.55	1.51
3	A	701	TPB	C12-C11	2.30	1.43	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	TPB	N3-C9-N1	-8.97	117.75	126.42
3	A	701	TPB	C1-N7-C8	-3.55	117.71	124.11
3	A	701	TPB	C10-N3-C9	3.37	118.23	115.42
3	A	701	TPB	C7-C10-N3	-3.04	120.24	123.97
3	A	701	TPB	C61-C6-C1	2.96	125.03	121.42
3	A	701	TPB	C6-C1-N7	2.68	124.03	119.38
3	A	701	TPB	C15-C14-C17	2.45	123.96	119.97
3	A	701	TPB	C13-C14-C17	-2.34	116.16	119.97
3	A	701	TPB	C3-C2-C1	2.08	120.64	118.25

There are no chirality outliers.

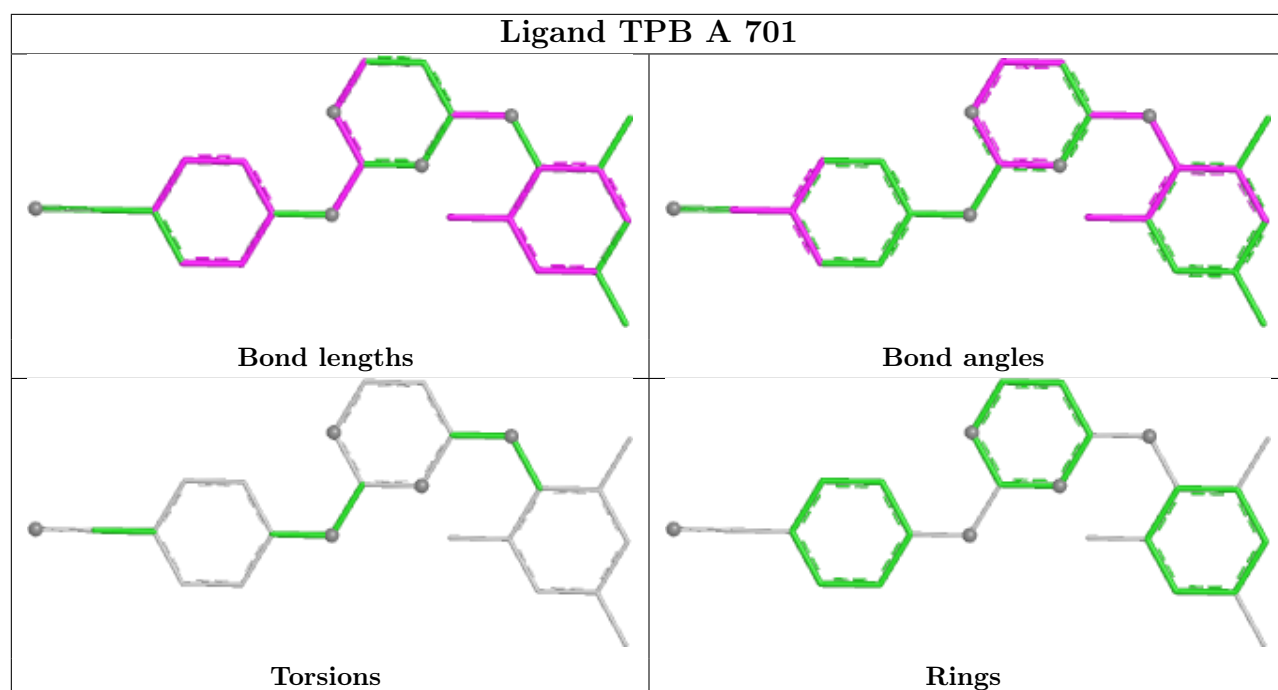
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	TPB	5	0

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 [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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	552/560 (98%)	-0.12	8 (1%)	73 51	47, 94, 121, 122	18 (3%)
2	B	427/430 (99%)	-0.24	1 (0%)	91 83	32, 79, 121, 122	7 (1%)
All	All	979/990 (98%)	-0.17	9 (0%)	81 61	32, 89, 121, 122	25 (2%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	548	VAL	4.7
1	A	549	ASP	4.4
1	A	221	HIS	3.6
1	A	545	ASN	3.2
1	A	544	GLY	2.8
2	B	3	SER	2.5
1	A	551	LEU	2.2
1	A	444	GLY	2.1
1	A	547	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

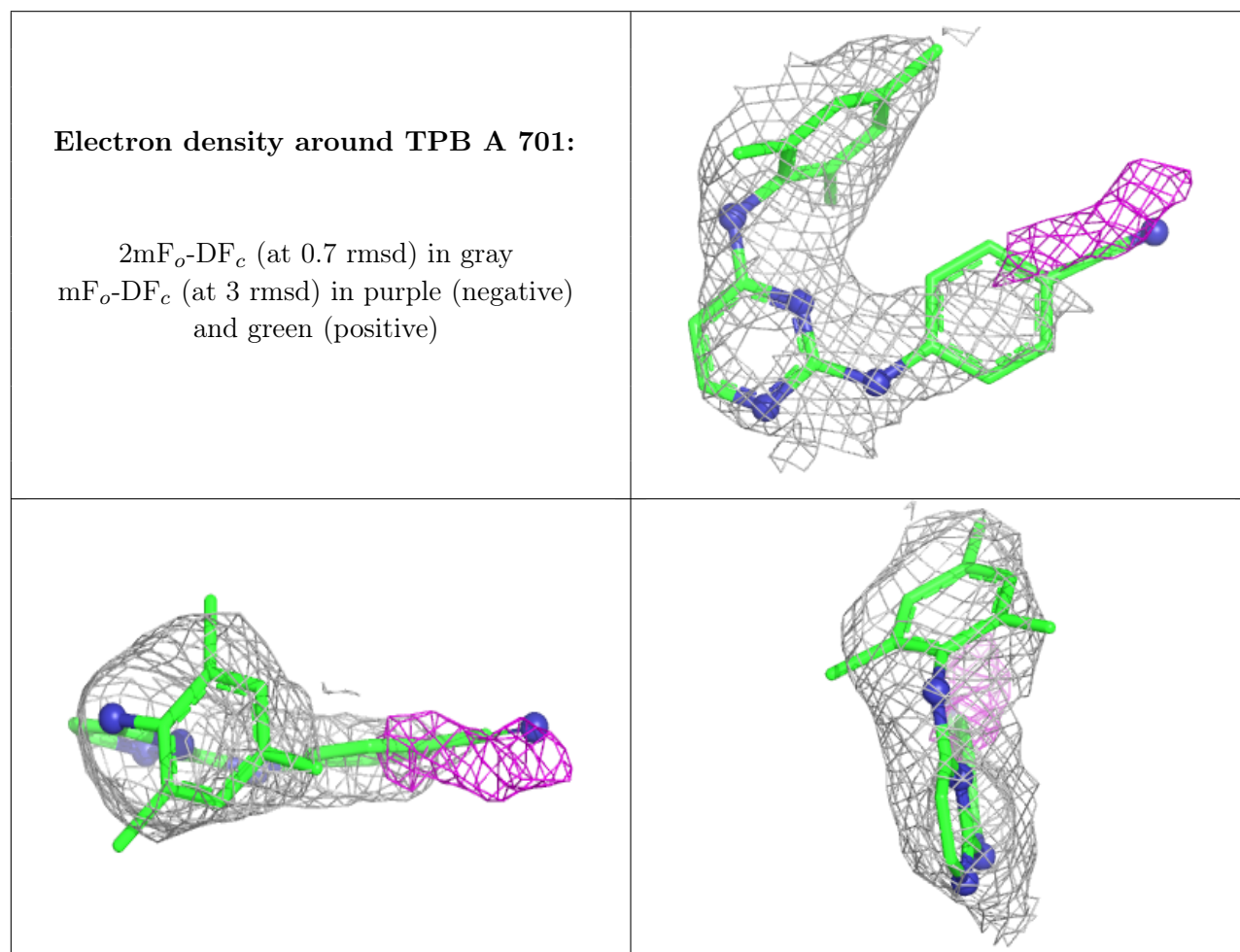
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TPB	A	701	25/25	0.91	0.12	55,70,77,83	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.