



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:34 AM UTC

PDB ID : 3CST / pdb_00003cst
Title : Crystal structure of PI3K p110gamma catalytical domain in complex with organoruthenium inhibitor E5E2
Authors : Xie, P.; Marmorstein, R.
Deposited on : 2008-04-10
Resolution : 3.20 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 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

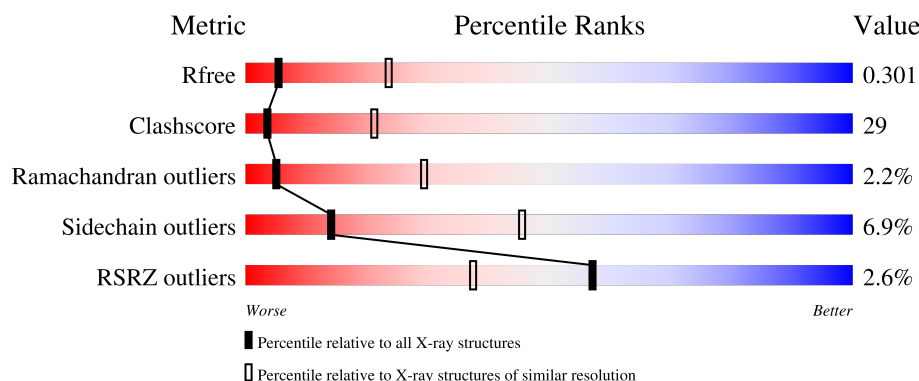
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	966	

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	E52	A	1	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6824 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.

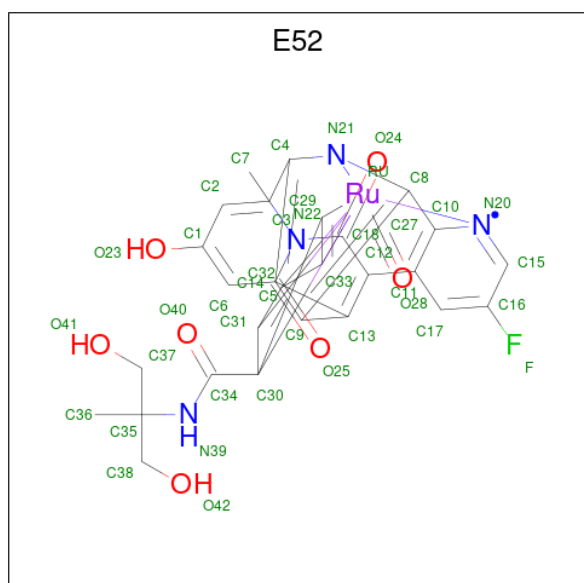
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	836	Total	C	N	O	S	0	0	0
			6782	4350	1157	1239	36			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	expression tag	UNP P48736
A	1103	HIS	-	expression tag	UNP P48736
A	1104	HIS	-	expression tag	UNP P48736
A	1105	HIS	-	expression tag	UNP P48736
A	1106	HIS	-	expression tag	UNP P48736
A	1107	HIS	-	expression tag	UNP P48736
A	1108	HIS	-	expression tag	UNP P48736

- Molecule 2 is Methylated Ruthenium Pyridocarbazole (CCD ID: E52) (formula: $C_{29}H_{23}FN_4O_7Ru$).

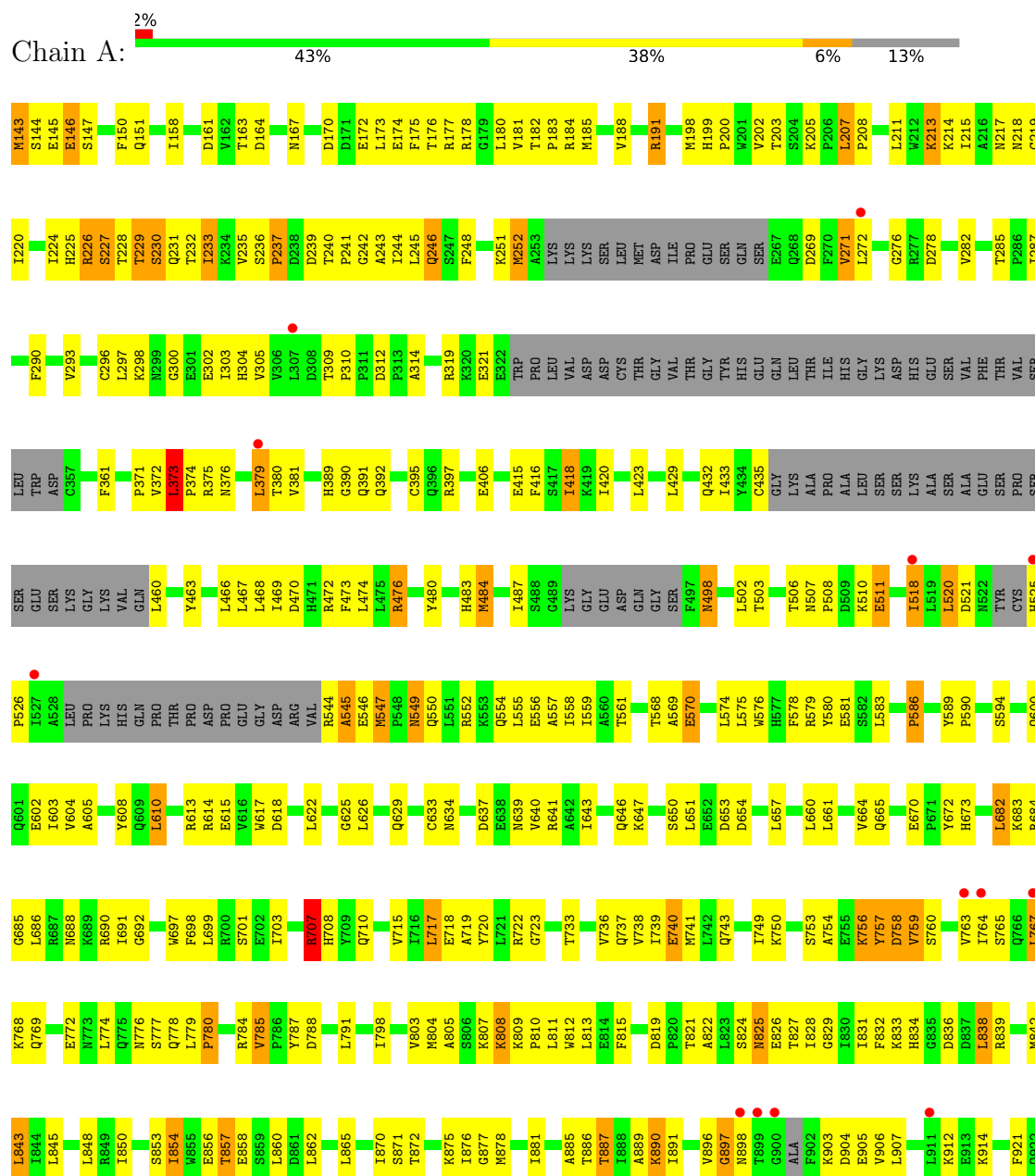


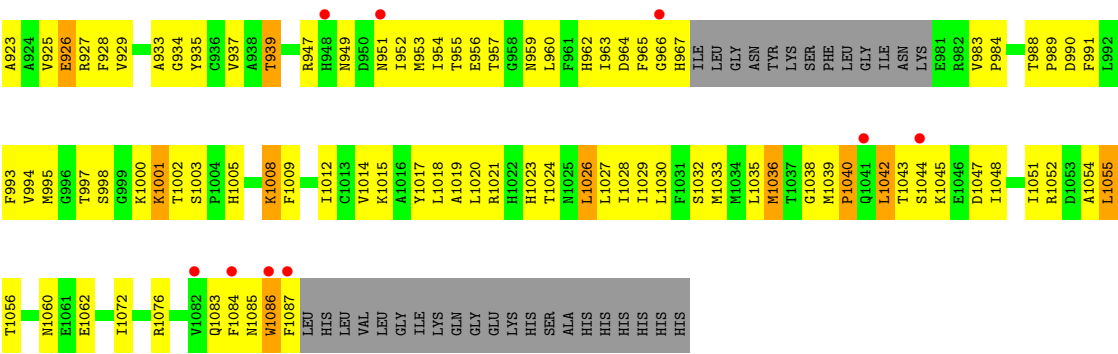
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	Ru	0	0
			42	29	1	4	7	1		

3 Residue-property plots [i](#)

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

- Molecule 1: Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.11Å 68.32Å 107.03Å 90.00° 95.14° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.2 (50.00-3.20) 95.1 (50.00-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.264 , 0.305 0.256 , 0.301	Depositor DCC
R_{free} test set	1838 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å ²)	81.8	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6824	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: E52

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	0.68	0/6926	1.09	33/9365 (0.4%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	LEU	N-CA-C	-8.01	103.49	113.18
1	A	707	ARG	N-CA-C	-7.60	103.08	111.36
1	A	594	SER	N-CA-C	-7.55	103.87	113.23
1	A	808	LYS	N-CA-C	-7.00	101.09	110.55
1	A	604	VAL	N-CA-C	-6.97	103.04	110.36
1	A	708	HIS	N-CA-C	6.89	120.78	112.38
1	A	503	THR	N-CA-C	6.89	121.08	110.20
1	A	581	GLU	N-CA-C	-6.82	103.78	111.14
1	A	1008	LYS	N-CA-C	-6.53	104.24	111.36
1	A	418	ILE	N-CA-C	6.45	117.36	109.30
1	A	904	ASP	N-CA-C	6.39	119.23	111.82
1	A	547	MET	N-CA-C	6.26	117.28	109.57
1	A	549	ASN	N-CA-C	6.07	118.42	111.02
1	A	634	ASN	N-CA-C	5.96	120.28	112.89
1	A	738	VAL	N-CA-C	5.95	116.41	110.23
1	A	191	ARG	N-CA-C	5.93	118.85	109.96
1	A	163	THR	N-CA-C	-5.82	106.16	113.72
1	A	484	MET	N-CA-C	5.75	117.95	110.53
1	A	788	ASP	CA-C-N	5.69	126.95	119.84
1	A	788	ASP	C-N-CA	5.69	126.95	119.84
1	A	423	LEU	CA-C-N	5.61	126.85	119.84
1	A	423	LEU	C-N-CA	5.61	126.85	119.84
1	A	1019	ALA	N-CA-C	-5.50	105.37	111.36
1	A	511	GLU	N-CA-C	5.44	117.07	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	569	ALA	N-CA-C	-5.44	105.25	111.07
1	A	246	GLN	N-CA-C	-5.33	105.05	112.45
1	A	785	VAL	CA-C-N	5.16	126.29	119.84
1	A	785	VAL	C-N-CA	5.16	126.29	119.84
1	A	650	SER	N-CA-C	5.14	119.19	113.02
1	A	1036	MET	N-CA-C	5.14	117.78	111.82
1	A	145	GLU	N-CA-C	-5.09	106.17	112.38
1	A	1055	LEU	N-CA-C	-5.06	107.13	113.15
1	A	991	PHE	N-CA-C	-5.01	105.90	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6782	0	6811	402	0
2	A	42	0	19	22	0
All	All	6824	0	6830	402	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 29.

All (402) 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:890:LYS:HD3	2:A:1:E52:O42	1.43	1.17
1:A:890:LYS:CE	2:A:1:E52:H38A	1.77	1.14
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.30	1.14
1:A:544:ARG:HH21	1:A:546:GLU:HB3	1.13	1.10
1:A:890:LYS:HE2	2:A:1:E52:H38A	1.33	1.06
1:A:805:ALA:O	2:A:1:E52:H37A	1.56	1.05
1:A:525:HIS:HB3	1:A:526:PRO:HD3	1.33	1.04
1:A:805:ALA:HB3	2:A:1:E52:H36A	1.42	0.99
1:A:373:LEU:HD22	1:A:406:GLU:HG2	1.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ILE:HD12	1:A:233:ILE:HD13	1.48	0.96
1:A:181:VAL:HG12	1:A:185:MET:HE2	1.55	0.89
1:A:804:MET:HE3	1:A:810:PRO:CG	2.01	0.89
1:A:890:LYS:CD	2:A:1:E52:O42	2.24	0.86
1:A:554:GLN:O	1:A:558:ILE:HD13	1.76	0.85
1:A:890:LYS:NZ	2:A:1:E52:H38A	1.90	0.85
1:A:143:MET:HG2	1:A:147:SER:OG	1.76	0.84
1:A:207:LEU:HD23	1:A:208:PRO:HD2	1.60	0.84
1:A:896:VAL:HG12	1:A:897:GLY:H	1.40	0.84
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.25	0.83
1:A:804:MET:HE3	1:A:810:PRO:HG2	1.61	0.83
1:A:474:LEU:HD23	1:A:525:HIS:N	1.93	0.82
1:A:890:LYS:HD2	2:A:1:E52:O28	1.78	0.82
1:A:544:ARG:NH2	1:A:546:GLU:HB3	1.92	0.82
1:A:217:ASN:HD22	1:A:219:CYS:HB2	1.45	0.82
1:A:890:LYS:CE	2:A:1:E52:C38	2.57	0.81
1:A:1060:ASN:HD21	1:A:1062:GLU:HB2	1.45	0.81
1:A:240:THR:O	1:A:244:ILE:HG23	1.81	0.80
1:A:379:LEU:HD13	1:A:380:THR:H	1.46	0.79
1:A:1002:THR:HG22	1:A:1003:SER:H	1.48	0.79
1:A:217:ASN:ND2	1:A:219:CYS:HB2	1.97	0.78
1:A:768:LYS:O	1:A:772:GLU:HG2	1.84	0.78
1:A:733:THR:O	1:A:737:GLN:HG3	1.85	0.77
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.67	0.76
1:A:395:CYS:SG	1:A:418:ILE:HG13	2.25	0.76
1:A:824:SER:OG	1:A:826:GLU:HG3	1.85	0.75
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.69	0.75
1:A:885:ALA:O	2:A:1:E52:C2	2.34	0.75
1:A:890:LYS:HE2	2:A:1:E52:C38	2.12	0.75
1:A:568:THR:HG22	1:A:570:GLU:H	1.51	0.74
1:A:1042:LEU:HD23	1:A:1048:ILE:HD11	1.68	0.74
1:A:167:ASN:ND2	1:A:506:THR:O	2.20	0.74
1:A:812:TRP:O	1:A:812:TRP:CD1	2.41	0.74
1:A:231:GLN:HG3	1:A:232:THR:H	1.53	0.73
1:A:947:ARG:NH2	1:A:963:ILE:O	2.22	0.73
1:A:839:ARG:HA	1:A:842:MET:CE	2.19	0.72
1:A:233:ILE:H	1:A:233:ILE:HD12	1.55	0.72
1:A:1043:THR:C	1:A:1045:LYS:H	1.97	0.71
1:A:804:MET:HE2	1:A:831:ILE:HD12	1.72	0.71
1:A:839:ARG:HA	1:A:842:MET:HE2	1.72	0.71
1:A:198:MET:SD	1:A:282:VAL:HG11	2.31	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.72	0.71
1:A:885:ALA:N	2:A:1:E52:O23	2.22	0.71
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.72	0.71
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.05	0.71
1:A:833:LYS:O	1:A:876:ILE:HD12	1.90	0.71
1:A:373:LEU:CD2	1:A:406:GLU:HG2	2.20	0.70
1:A:750:LYS:HE3	1:A:809:LYS:H	1.55	0.70
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.09	0.70
1:A:463:TYR:HD2	1:A:487:ILE:HD11	1.57	0.69
1:A:890:LYS:HZ3	2:A:1:E52:H38A	1.56	0.69
1:A:180:LEU:O	1:A:183:PRO:HD2	1.92	0.69
1:A:1020:LEU:HD22	1:A:1027:LEU:HD11	1.74	0.69
1:A:765:SER:O	1:A:769:GLN:HG3	1.93	0.68
1:A:576:TRP:O	1:A:579:ARG:HD3	1.94	0.68
1:A:758:ASP:OD1	1:A:759:VAL:N	2.26	0.68
1:A:887:THR:HG22	1:A:889:ALA:H	1.59	0.68
1:A:207:LEU:CD2	1:A:208:PRO:HD2	2.24	0.68
1:A:251:LYS:O	1:A:251:LYS:HD3	1.94	0.67
1:A:1056:THR:HG23	1:A:1056:THR:O	1.95	0.67
1:A:576:TRP:CZ3	1:A:579:ARG:HD2	2.30	0.67
1:A:372:VAL:HG12	1:A:374:PRO:HD2	1.77	0.67
1:A:580:TYR:HE2	1:A:613:ARG:HD3	1.60	0.67
1:A:657:LEU:HD11	1:A:690:ARG:HD3	1.76	0.67
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.60	0.66
1:A:805:ALA:O	2:A:1:E52:C37	2.41	0.66
1:A:812:TRP:O	1:A:812:TRP:HD1	1.76	0.66
1:A:525:HIS:CB	1:A:526:PRO:HD3	2.17	0.66
1:A:661:LEU:HD21	1:A:843:LEU:HD13	1.76	0.66
1:A:483:HIS:CD2	1:A:510:LYS:HG3	2.30	0.66
1:A:468:LEU:C	1:A:469:ILE:HD12	2.19	0.66
1:A:811:LEU:HB3	1:A:813:LEU:HD21	1.78	0.66
1:A:544:ARG:HH21	1:A:546:GLU:CB	2.00	0.66
1:A:997:THR:HG22	1:A:998:SER:N	2.11	0.66
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.78	0.65
1:A:829:GLY:CA	1:A:881:ILE:HD12	2.27	0.65
1:A:1008:LYS:O	1:A:1012:ILE:HG13	1.97	0.65
1:A:213:LYS:HD3	1:A:214:LYS:N	2.12	0.65
1:A:1043:THR:O	1:A:1045:LYS:N	2.29	0.65
1:A:158:ILE:HG12	1:A:717:LEU:HD13	1.78	0.64
1:A:568:THR:HG22	1:A:570:GLU:N	2.11	0.64
1:A:379:LEU:CD1	1:A:380:THR:H	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:ALA:O	2:A:1:E52:C1	2.45	0.64
1:A:240:THR:HG22	1:A:242:GLY:H	1.63	0.64
1:A:373:LEU:N	1:A:374:PRO:HD2	2.14	0.63
1:A:829:GLY:C	1:A:881:ILE:HD12	2.22	0.63
1:A:860:LEU:HD11	1:A:1015:LYS:HG2	1.79	0.63
1:A:1002:THR:HG22	1:A:1003:SER:N	2.14	0.63
1:A:660:LEU:O	1:A:664:VAL:HG23	1.99	0.63
1:A:184:ARG:HH11	1:A:184:ARG:HB2	1.63	0.62
1:A:736:VAL:O	1:A:740:GLU:HB2	1.99	0.62
1:A:467:LEU:O	1:A:476:ARG:HD2	2.00	0.62
1:A:525:HIS:HB3	1:A:526:PRO:CD	2.19	0.62
1:A:640:VAL:O	1:A:643:ILE:HG12	2.00	0.62
1:A:949:ASN:HB2	1:A:1083:GLN:NE2	2.13	0.62
1:A:1000:LYS:HA	1:A:1076:ARG:NH1	2.15	0.62
1:A:576:TRP:CE3	1:A:579:ARG:HD2	2.35	0.62
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.35	0.62
1:A:741:MET:HE1	1:A:778:GLN:C	2.24	0.61
1:A:896:VAL:CG2	1:A:903:LYS:HG3	2.30	0.61
1:A:1000:LYS:HA	1:A:1076:ARG:CZ	2.31	0.61
1:A:182:THR:HB	1:A:183:PRO:HD3	1.82	0.61
1:A:876:ILE:HG13	1:A:877:GLY:N	2.15	0.61
1:A:1021:ARG:HE	1:A:1056:THR:CG2	2.13	0.61
1:A:1009:PHE:HE2	1:A:1072:ILE:HD12	1.65	0.60
1:A:576:TRP:CH2	1:A:579:ARG:HD2	2.36	0.60
1:A:1042:LEU:HD13	1:A:1042:LEU:O	2.02	0.60
1:A:622:LEU:HD21	1:A:651:LEU:CD2	2.32	0.60
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.01	0.60
1:A:188:VAL:O	1:A:191:ARG:HG2	2.02	0.59
1:A:147:SER:HA	1:A:319:ARG:NH2	2.18	0.59
1:A:887:THR:HG22	1:A:889:ALA:N	2.17	0.59
1:A:278:ASP:OD1	1:A:784:ARG:NH2	2.35	0.59
1:A:583:LEU:CD1	1:A:610:LEU:HD22	2.33	0.59
1:A:180:LEU:C	1:A:183:PRO:HD2	2.27	0.58
1:A:379:LEU:HB3	1:A:435:CYS:SG	2.43	0.58
1:A:804:MET:HE3	1:A:810:PRO:HG3	1.85	0.58
1:A:1052:ARG:HG2	1:A:1052:ARG:HH11	1.68	0.58
1:A:779:LEU:HD23	1:A:780:PRO:O	2.03	0.58
1:A:955:THR:HG1	1:A:959:ASN:H	1.51	0.58
1:A:760:SER:O	1:A:763:VAL:HG12	2.04	0.57
1:A:469:ILE:HD12	1:A:469:ILE:N	2.18	0.57
1:A:583:LEU:HD12	1:A:610:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:LEU:CD1	1:A:1042:LEU:H	2.17	0.57
1:A:890:LYS:HD3	2:A:1:E52:C38	2.34	0.57
1:A:739:ILE:O	1:A:743:GLN:HG3	2.05	0.57
1:A:312:ASP:OD2	1:A:314:ALA:HB3	2.03	0.57
1:A:220:ILE:HD11	1:A:237:PRO:HG3	1.86	0.57
1:A:302:GLU:HB2	1:A:304:HIS:HE1	1.70	0.56
1:A:935:TYR:O	1:A:939:THR:HB	2.05	0.56
1:A:296:CYS:SG	1:A:303:ILE:HD13	2.46	0.56
1:A:891:ILE:HG22	1:A:906:VAL:HG12	1.87	0.56
1:A:1000:LYS:HG2	1:A:1076:ARG:HB3	1.86	0.56
1:A:1055:LEU:O	1:A:1056:THR:C	2.49	0.56
1:A:1029:ILE:O	1:A:1033:MET:HG3	2.05	0.56
1:A:1043:THR:C	1:A:1045:LYS:N	2.64	0.56
1:A:233:ILE:H	1:A:233:ILE:CD1	2.19	0.56
1:A:887:THR:HA	1:A:953:MET:HG2	1.87	0.55
1:A:1017:TYR:CE2	1:A:1021:ARG:HD2	2.41	0.55
1:A:214:LYS:O	1:A:215:ILE:HD13	2.07	0.55
1:A:832:PHE:CZ	1:A:878:MET:HE2	2.42	0.55
1:A:614:ARG:O	1:A:615:GLU:C	2.49	0.55
1:A:896:VAL:HG12	1:A:897:GLY:N	2.17	0.55
1:A:226:ARG:O	1:A:227:SER:HB2	2.07	0.54
1:A:373:LEU:H	1:A:374:PRO:CD	2.20	0.54
1:A:218:ASN:OD1	1:A:218:ASN:O	2.26	0.54
1:A:1001:LYS:NZ	1:A:1001:LYS:HB3	2.23	0.54
1:A:233:ILE:HD12	1:A:233:ILE:N	2.20	0.54
1:A:498:ASN:OD1	1:A:498:ASN:C	2.50	0.54
1:A:271:VAL:HG23	1:A:282:VAL:HG12	1.90	0.54
1:A:903:LYS:HB2	1:A:906:VAL:CG2	2.37	0.54
1:A:373:LEU:N	1:A:374:PRO:CD	2.71	0.53
1:A:246:GLN:C	1:A:248:PHE:H	2.14	0.53
1:A:202:VAL:HG12	1:A:203:THR:N	2.21	0.53
1:A:614:ARG:HH11	1:A:646:GLN:HE22	1.56	0.53
1:A:1042:LEU:O	1:A:1042:LEU:HD22	2.08	0.53
1:A:235:VAL:HG12	1:A:236:SER:N	2.23	0.53
1:A:750:LYS:HE3	1:A:809:LYS:N	2.23	0.53
1:A:807:LYS:H	1:A:807:LYS:HD2	1.72	0.53
1:A:825:ASN:N	1:A:825:ASN:ND2	2.55	0.53
1:A:890:LYS:NZ	2:A:1:E52:C38	2.69	0.53
1:A:756:LYS:O	1:A:758:ASP:OD2	2.27	0.53
1:A:988:THR:HB	1:A:989:PRO:HD2	1.91	0.53
1:A:371:PRO:HG2	1:A:511:GLU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:ILE:O	1:A:854:ILE:HD13	2.09	0.53
1:A:622:LEU:HD21	1:A:651:LEU:HD21	1.90	0.53
1:A:170:ASP:OD1	1:A:170:ASP:C	2.51	0.53
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.57	0.52
1:A:176:THR:O	1:A:180:LEU:HG	2.10	0.52
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.77	0.52
1:A:641:ARG:HE	1:A:670:GLU:CD	2.17	0.52
1:A:1026:LEU:HD22	1:A:1026:LEU:O	2.08	0.52
1:A:151:GLN:OE1	1:A:722:ARG:NH2	2.42	0.52
1:A:174:GLU:HB3	1:A:178:ARG:HH12	1.75	0.52
1:A:229:THR:O	1:A:230:SER:HB3	2.09	0.52
1:A:1026:LEU:O	1:A:1030:LEU:HG	2.09	0.52
1:A:661:LEU:HD21	1:A:843:LEU:CD1	2.40	0.52
1:A:1043:THR:N	1:A:1047:ASP:OD2	2.36	0.52
1:A:741:MET:HE1	1:A:778:GLN:HB3	1.92	0.52
1:A:544:ARG:O	1:A:545:ALA:HB3	2.10	0.52
1:A:576:TRP:CD2	1:A:579:ARG:HD2	2.44	0.52
1:A:239:ASP:HB3	1:A:244:ILE:HG22	1.92	0.52
1:A:549:ASN:HD22	1:A:550:GLN:NE2	2.08	0.52
1:A:143:MET:N	1:A:143:MET:HE2	2.25	0.52
1:A:544:ARG:CG	1:A:545:ALA:H	2.23	0.52
1:A:997:THR:CG2	1:A:998:SER:N	2.72	0.52
1:A:214:LYS:HZ2	1:A:300:GLY:HA2	1.72	0.51
1:A:690:ARG:HG3	1:A:690:ARG:HH11	1.74	0.51
1:A:805:ALA:HB3	2:A:1:E52:C36	2.30	0.51
1:A:890:LYS:CD	2:A:1:E52:C38	2.87	0.51
1:A:161:ASP:O	1:A:164:ASP:HB3	2.10	0.51
1:A:1038:GLY:HA3	1:A:1039:MET:HE2	1.93	0.51
1:A:804:MET:CE	1:A:831:ILE:HD12	2.40	0.51
1:A:964:ASP:C	1:A:966:GLY:H	2.18	0.51
1:A:1060:ASN:ND2	1:A:1062:GLU:HB2	2.22	0.51
1:A:583:LEU:O	1:A:583:LEU:HD23	2.11	0.51
1:A:1042:LEU:CD2	1:A:1048:ILE:HD11	2.40	0.51
1:A:685:GLY:O	1:A:688:ASN:O	2.28	0.51
1:A:953:MET:HE1	2:A:1:E52:C5	2.41	0.51
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.42	0.50
1:A:657:LEU:HD21	1:A:691:ILE:HD12	1.92	0.50
1:A:208:PRO:HG2	1:A:211:LEU:HB2	1.92	0.50
1:A:379:LEU:HD13	1:A:380:THR:HG22	1.93	0.50
1:A:220:ILE:CD1	1:A:237:PRO:HG3	2.42	0.50
1:A:779:LEU:O	1:A:780:PRO:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:MET:HE2	1:A:871:SER:HB3	1.94	0.50
1:A:1009:PHE:CE2	1:A:1072:ILE:HD12	2.46	0.50
1:A:202:VAL:CG1	1:A:203:THR:N	2.75	0.50
1:A:474:LEU:HA	1:A:525:HIS:N	2.27	0.50
1:A:839:ARG:HA	1:A:842:MET:HE3	1.93	0.50
1:A:202:VAL:HG11	1:A:285:THR:HG21	1.94	0.50
1:A:293:VAL:O	1:A:297:LEU:HG	2.11	0.50
1:A:905:GLU:HG2	1:A:993:PHE:CZ	2.47	0.50
1:A:912:LYS:HA	1:A:921:PHE:CD1	2.46	0.49
1:A:933:ALA:O	1:A:937:VAL:HG23	2.12	0.49
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.93	0.49
1:A:202:VAL:CG1	1:A:285:THR:HG21	2.42	0.49
1:A:576:TRP:CE2	1:A:579:ARG:HD2	2.47	0.49
1:A:831:ILE:HG12	1:A:881:ILE:HG12	1.94	0.49
1:A:923:ALA:O	1:A:926:GLU:HB3	2.12	0.49
1:A:235:VAL:HG12	1:A:236:SER:H	1.77	0.49
1:A:372:VAL:CG1	1:A:374:PRO:HD2	2.41	0.49
1:A:576:TRP:CZ2	1:A:579:ARG:HD2	2.48	0.49
1:A:1002:THR:O	1:A:1003:SER:HB3	2.13	0.49
1:A:1042:LEU:HD22	1:A:1042:LEU:C	2.37	0.49
1:A:653:ASP:O	1:A:654:ASP:C	2.53	0.49
1:A:767:LEU:HD12	1:A:803:VAL:HG23	1.95	0.49
1:A:229:THR:HG22	1:A:230:SER:H	1.76	0.49
1:A:544:ARG:HG2	1:A:545:ALA:N	2.27	0.49
1:A:896:VAL:HG21	1:A:903:LYS:HG3	1.94	0.49
1:A:691:ILE:HD12	1:A:691:ILE:N	2.28	0.48
1:A:834:HIS:HA	1:A:875:LYS:O	2.13	0.48
1:A:150:PHE:HB2	1:A:319:ARG:NH1	2.28	0.48
1:A:397:ARG:NE	1:A:415:GLU:O	2.46	0.48
1:A:547:MET:HG2	1:A:578:PHE:CD2	2.48	0.48
1:A:1042:LEU:H	1:A:1042:LEU:HD12	1.79	0.48
1:A:1054:ALA:C	1:A:1056:THR:H	2.21	0.48
1:A:252:MET:HE3	1:A:252:MET:HA	1.96	0.48
1:A:361:PHE:HA	1:A:420:ILE:HD11	1.95	0.48
1:A:466:LEU:CD1	1:A:476:ARG:HD3	2.43	0.48
1:A:470:ASP:OD2	1:A:474:LEU:HB2	2.13	0.48
1:A:555:LEU:O	1:A:559:ILE:HG12	2.14	0.48
1:A:896:VAL:HG22	1:A:903:LYS:HG3	1.96	0.48
1:A:912:LYS:HD2	1:A:912:LYS:O	2.13	0.48
1:A:927:ARG:HG3	1:A:927:ARG:HH11	1.78	0.48
1:A:199:HIS:O	1:A:200:PRO:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:THR:HG22	1:A:1045:LYS:H	1.78	0.48
1:A:243:ALA:HA	1:A:246:GLN:HG3	1.95	0.48
1:A:833:LYS:HG3	1:A:834:HIS:N	2.29	0.48
1:A:890:LYS:CD	2:A:1:E52:O28	2.56	0.47
1:A:757:TYR:HA	1:A:809:LYS:NZ	2.29	0.47
1:A:1032:SER:HB3	1:A:1048:ILE:HG23	1.96	0.47
1:A:1026:LEU:HD22	1:A:1030:LEU:HG	1.96	0.47
1:A:657:LEU:HG	1:A:691:ILE:HD11	1.97	0.47
1:A:213:LYS:NZ	1:A:214:LYS:HB2	2.30	0.47
1:A:718:GLU:O	1:A:719:ALA:C	2.56	0.47
1:A:184:ARG:HH11	1:A:184:ARG:CB	2.28	0.47
1:A:233:ILE:HD11	1:A:248:PHE:CD1	2.50	0.47
1:A:373:LEU:H	1:A:374:PRO:HD2	1.76	0.47
1:A:1032:SER:HB3	1:A:1048:ILE:CG2	2.45	0.47
1:A:637:ASP:OD1	1:A:639:ASN:N	2.47	0.47
1:A:764:ILE:O	1:A:768:LYS:HG3	2.15	0.47
1:A:954:ILE:HG23	1:A:954:ILE:O	2.14	0.47
1:A:829:GLY:HA3	1:A:881:ILE:HD12	1.96	0.47
1:A:962:HIS:C	1:A:963:ILE:HG23	2.40	0.47
1:A:433:ILE:HG13	1:A:484:MET:HE1	1.96	0.46
1:A:467:LEU:HD13	1:A:672:TYR:CE2	2.50	0.46
1:A:928:PHE:HE1	1:A:960:LEU:HD12	1.79	0.46
1:A:1060:ASN:ND2	1:A:1062:GLU:H	2.13	0.46
1:A:241:PRO:HG2	1:A:290:PHE:CZ	2.50	0.46
1:A:589:TYR:HD1	1:A:589:TYR:H	1.64	0.46
1:A:544:ARG:CG	1:A:545:ALA:N	2.76	0.46
1:A:557:ALA:O	1:A:561:THR:HG23	2.15	0.46
1:A:1052:ARG:HG2	1:A:1052:ARG:NH1	2.31	0.46
1:A:1085:ASN:O	1:A:1087:PHE:N	2.49	0.46
1:A:661:LEU:HB2	1:A:698:PHE:CE1	2.50	0.46
1:A:774:LEU:C	1:A:776:ASN:N	2.73	0.46
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.50	0.46
1:A:685:GLY:HA2	1:A:691:ILE:HG22	1.98	0.46
1:A:583:LEU:HD23	1:A:583:LEU:C	2.41	0.45
1:A:1084:PHE:O	1:A:1087:PHE:CE1	2.69	0.45
1:A:828:ILE:N	1:A:828:ILE:HD12	2.31	0.45
1:A:862:LEU:HD11	1:A:1012:ILE:HG22	1.99	0.45
1:A:389:HIS:O	1:A:392:GLN:HB3	2.16	0.45
1:A:887:THR:O	1:A:891:ILE:HG12	2.17	0.45
1:A:239:ASP:O	1:A:287:ILE:HG12	2.17	0.45
1:A:699:LEU:O	1:A:703:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:ARG:HG3	1:A:927:ARG:NH1	2.31	0.45
1:A:174:GLU:OE1	1:A:178:ARG:NH1	2.50	0.45
1:A:819:ASP:OD1	1:A:821:THR:OG1	2.31	0.45
1:A:614:ARG:HD2	1:A:618:ASP:OD1	2.17	0.45
1:A:240:THR:HG23	1:A:241:PRO:HD2	1.99	0.45
1:A:925:VAL:O	1:A:929:VAL:HG23	2.17	0.45
1:A:1021:ARG:NE	1:A:1056:THR:CG2	2.80	0.45
1:A:276:GLY:HA3	1:A:822:ALA:HA	1.98	0.44
1:A:373:LEU:O	1:A:374:PRO:C	2.59	0.44
1:A:633:CYS:SG	1:A:1036:MET:HE1	2.57	0.44
1:A:625:GLY:O	1:A:629:GLN:HG3	2.17	0.44
1:A:697:TRP:CH2	1:A:739:ILE:HD13	2.52	0.44
1:A:174:GLU:OE2	1:A:177:ARG:NH1	2.48	0.44
1:A:198:MET:O	1:A:199:HIS:C	2.59	0.44
1:A:214:LYS:HZ1	1:A:300:GLY:HA2	1.77	0.44
1:A:741:MET:CE	1:A:778:GLN:HB3	2.48	0.44
1:A:1035:LEU:CD1	1:A:1048:ILE:HD13	2.22	0.44
1:A:239:ASP:HB3	1:A:244:ILE:CG2	2.47	0.44
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.83	0.44
1:A:469:ILE:N	1:A:469:ILE:CD1	2.81	0.44
1:A:838:LEU:HD12	1:A:838:LEU:HA	1.76	0.44
1:A:480:TYR:HB2	1:A:518:ILE:HD11	1.98	0.44
1:A:498:ASN:OD1	1:A:498:ASN:O	2.35	0.44
1:A:815:PHE:O	1:A:827:THR:HB	2.18	0.44
1:A:857:THR:O	1:A:858:GLU:HG2	2.18	0.44
1:A:219:CYS:HA	1:A:235:VAL:O	2.18	0.44
1:A:698:PHE:O	1:A:701:SER:HB3	2.18	0.44
1:A:472:ARG:O	1:A:473:PHE:HB2	2.17	0.43
1:A:951:ASN:C	1:A:952:ILE:HD12	2.43	0.43
1:A:1014:VAL:O	1:A:1018:LEU:HG	2.18	0.43
1:A:205:LYS:NZ	1:A:654:ASP:OD2	2.51	0.43
1:A:1023:HIS:O	1:A:1024:THR:C	2.60	0.43
1:A:1056:THR:O	1:A:1056:THR:CG2	2.64	0.43
1:A:476:ARG:HB3	1:A:520:LEU:HD23	2.00	0.43
1:A:172:GLU:O	1:A:175:PHE:HB3	2.17	0.43
1:A:487:ILE:HD12	1:A:487:ILE:N	2.33	0.43
1:A:507:ASN:HA	1:A:508:PRO:HD3	1.89	0.43
1:A:589:TYR:CD1	1:A:589:TYR:N	2.86	0.43
1:A:429:LEU:HB2	1:A:468:LEU:CD2	2.44	0.43
1:A:807:LYS:H	1:A:807:LYS:CD	2.31	0.43
1:A:480:TYR:O	1:A:518:ILE:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:NH2	1:A:321:GLU:OE1	2.48	0.43
1:A:602:GLU:O	1:A:605:ALA:HB3	2.19	0.43
1:A:637:ASP:OD1	1:A:637:ASP:C	2.61	0.43
1:A:1086:TRP:O	1:A:1087:PHE:CD1	2.71	0.43
1:A:518:ILE:HD13	1:A:518:ILE:N	2.34	0.43
1:A:1017:TYR:CZ	1:A:1021:ARG:HD2	2.54	0.43
1:A:1042:LEU:CD1	1:A:1042:LEU:N	2.79	0.43
1:A:296:CYS:HB2	1:A:303:ILE:HD11	2.00	0.42
1:A:785:VAL:HG23	1:A:791:LEU:O	2.19	0.42
1:A:825:ASN:N	1:A:825:ASN:HD22	2.16	0.42
1:A:1039:MET:SD	1:A:1039:MET:N	2.92	0.42
1:A:807:LYS:HD2	1:A:807:LYS:N	2.35	0.42
1:A:886:THR:HB	1:A:891:ILE:HD11	2.01	0.42
1:A:995:MET:O	1:A:1005:HIS:HB2	2.18	0.42
1:A:233:ILE:HD11	1:A:248:PHE:HD1	1.83	0.42
1:A:777:SER:O	1:A:778:GLN:HG2	2.18	0.42
1:A:965:PHE:O	1:A:966:GLY:C	2.62	0.42
1:A:1021:ARG:NE	1:A:1056:THR:HG22	2.28	0.42
1:A:1086:TRP:C	1:A:1087:PHE:CD1	2.98	0.42
1:A:707:ARG:HA	1:A:710:GLN:OE1	2.20	0.42
1:A:739:ILE:HG22	1:A:878:MET:HE1	2.01	0.42
1:A:753:SER:CB	1:A:809:LYS:HG3	2.50	0.42
1:A:692:GLY:HA3	1:A:720:TYR:OH	2.20	0.42
1:A:213:LYS:HD3	1:A:214:LYS:H	1.81	0.42
1:A:683:LYS:O	1:A:684:ARG:C	2.62	0.42
1:A:756:LYS:HE3	1:A:756:LYS:HB2	1.85	0.42
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.50	0.42
1:A:990:ASP:O	1:A:994:VAL:HG23	2.20	0.42
1:A:853:SER:O	1:A:856:GLU:HB3	2.19	0.41
1:A:856:GLU:C	1:A:858:GLU:H	2.28	0.41
1:A:184:ARG:CB	1:A:184:ARG:NH1	2.83	0.41
1:A:614:ARG:HH11	1:A:646:GLN:NE2	2.17	0.41
1:A:739:ILE:HG13	1:A:740:GLU:N	2.34	0.41
1:A:787:TYR:CD1	1:A:787:TYR:C	2.98	0.41
1:A:207:LEU:HD22	1:A:211:LEU:HB2	2.02	0.41
1:A:309:THR:HA	1:A:310:PRO:HD3	1.96	0.41
1:A:1043:THR:HG22	1:A:1045:LYS:N	2.36	0.41
1:A:741:MET:HE1	1:A:778:GLN:O	2.20	0.41
1:A:181:VAL:O	1:A:184:ARG:HB3	2.20	0.41
1:A:862:LEU:HB3	1:A:934:GLY:HA3	2.03	0.41
1:A:552:ARG:O	1:A:556:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:SER:C	1:A:146:GLU:N	2.75	0.41
1:A:173:LEU:HD23	1:A:673:HIS:CD2	2.55	0.41
1:A:463:TYR:HD2	1:A:487:ILE:CD1	2.31	0.41
1:A:610:LEU:HD23	1:A:610:LEU:HA	1.95	0.41
1:A:779:LEU:O	1:A:780:PRO:O	2.38	0.41
1:A:808:LYS:HE3	1:A:836:ASP:OD1	2.21	0.41
1:A:955:THR:HB	1:A:957:THR:HG22	2.03	0.41
1:A:787:TYR:HA	1:A:870:ILE:HD11	2.03	0.41
1:A:812:TRP:CD1	1:A:812:TRP:C	2.97	0.41
1:A:682:LEU:HD22	1:A:686:LEU:HD11	2.02	0.40
1:A:236:SER:O	1:A:239:ASP:N	2.48	0.40
1:A:246:GLN:C	1:A:248:PHE:N	2.79	0.40
1:A:600:GLN:CB	1:A:603:ILE:HD12	2.51	0.40
1:A:664:VAL:O	1:A:665:GLN:C	2.63	0.40
1:A:690:ARG:HG3	1:A:690:ARG:NH1	2.36	0.40
1:A:953:MET:HE1	2:A:1:E52:C9	2.51	0.40
1:A:177:ARG:HG2	1:A:715:VAL:HG13	2.03	0.40
1:A:914:LYS:HD2	1:A:956:GLU:OE2	2.21	0.40
1:A:1028:ILE:HG12	1:A:1051:ILE:HG23	2.04	0.40
1:A:390:GLY:O	1:A:391:GLN:C	2.63	0.40
1:A:391:GLN:HG3	1:A:502:LEU:HD21	2.02	0.40
1:A:547:MET:SD	1:A:552:ARG:HA	2.61	0.40
1:A:589:TYR:HB2	1:A:590:PRO:HD3	2.03	0.40
1:A:921:PHE:O	1:A:925:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	818/966 (85%)	715 (87%)	85 (10%)	18 (2%)	5	29

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	A	1086	TRP
1	A	227	SER
1	A	230	SER
1	A	758	ASP
1	A	1040	PRO
1	A	1044	SER
1	A	545	ALA
1	A	780	PRO
1	A	798	ILE
1	A	373	LEU
1	A	754	ALA
1	A	756	LYS
1	A	759	VAL
1	A	857	THR
1	A	723	GLY
1	A	897	GLY
1	A	237	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	752/864 (87%)	700 (93%)	52 (7%)	14 45

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	MET
1	A	146	GLU
1	A	207	LEU
1	A	213	LYS
1	A	226	ARG
1	A	228	THR
1	A	229	THR

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Mol	Chain	Res	Type
1	A	233	ILE
1	A	252	MET
1	A	269	ASP
1	A	271	VAL
1	A	298	LYS
1	A	373	LEU
1	A	375	ARG
1	A	379	LEU
1	A	381	VAL
1	A	476	ARG
1	A	498	ASN
1	A	518	ILE
1	A	520	LEU
1	A	521	ASP
1	A	570	GLU
1	A	574	LEU
1	A	575	LEU
1	A	586	PRO
1	A	610	LEU
1	A	626	LEU
1	A	647	LYS
1	A	682	LEU
1	A	707	ARG
1	A	717	LEU
1	A	740	GLU
1	A	749	ILE
1	A	757	TYR
1	A	767	LEU
1	A	825	ASN
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	854	ILE
1	A	865	LEU
1	A	887	THR
1	A	890	LYS
1	A	898	ASN
1	A	907	LEU
1	A	926	GLU
1	A	939	THR
1	A	967	HIS

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Mol	Chain	Res	Type
1	A	1001	LYS
1	A	1026	LEU
1	A	1042	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	217	ASN
1	A	218	ASN
1	A	225	HIS
1	A	291	GLN
1	A	295	HIS
1	A	299	ASN
1	A	304	HIS
1	A	389	HIS
1	A	483	HIS
1	A	498	ASN
1	A	549	ASN
1	A	550	GLN
1	A	554	GLN
1	A	634	ASN
1	A	646	GLN
1	A	705	GLN
1	A	737	GLN
1	A	766	GLN
1	A	769	GLN
1	A	773	ASN
1	A	778	GLN
1	A	825	ASN
1	A	840	GLN
1	A	962	HIS
1	A	967	HIS
1	A	1041	GLN
1	A	1060	ASN
1	A	1083	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	$\# Z > 2$
2	E52	A	1	-	31,52,52	2.89	13 (41%)	34,109,109	3.35	16 (47%)

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	E52	A	1	-	-	3/11/215/215	0/12/11/11

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	E52	C11-C10	6.81	1.52	1.40
2	A	1	E52	F-C16	-6.65	1.21	1.35
2	A	1	E52	C2-C1	5.49	1.49	1.39
2	A	1	E52	C6-C5	5.06	1.48	1.39
2	A	1	E52	C9-C13	4.58	1.48	1.40
2	A	1	E52	C14-N22	-4.15	1.34	1.39
2	A	1	E52	C15-C16	4.03	1.47	1.39
2	A	1	E52	C3-C2	2.85	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	E52	C5-C4	2.59	1.45	1.41
2	A	1	E52	C13-C14	2.57	1.54	1.49
2	A	1	E52	C6-C1	2.48	1.42	1.39
2	A	1	E52	C18-N22	-2.18	1.36	1.39
2	A	1	E52	C13-C12	-2.09	1.35	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	E52	C18-N22-C14	9.35	120.22	112.32
2	A	1	E52	O25-C14-C13	6.26	138.66	129.15
2	A	1	E52	C9-C5-C4	5.29	111.81	106.49
2	A	1	E52	C11-C10-C8	-5.19	116.84	121.36
2	A	1	E52	C5-C9-C8	-5.03	99.38	106.44
2	A	1	E52	C13-C14-N22	-4.89	99.68	105.55
2	A	1	E52	C7-N22-C18	-4.78	117.90	123.53
2	A	1	E52	C5-C6-C1	-4.46	113.89	120.33
2	A	1	E52	C6-C5-C9	-3.82	124.07	134.34
2	A	1	E52	C6-C5-C4	3.66	124.01	119.67
2	A	1	E52	C10-C11-C17	-3.48	114.39	118.58
2	A	1	E52	C3-C2-C1	3.45	123.53	119.88
2	A	1	E52	C5-C9-C13	3.29	145.30	134.87
2	A	1	E52	O25-C14-N22	-3.22	121.66	124.89
2	A	1	E52	C12-C18-N22	-3.04	101.90	105.55
2	A	1	E52	O24-C18-N22	2.71	127.61	124.89

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	E52	C38-C35-N39-C34
2	A	1	E52	C36-C35-N39-C34
2	A	1	E52	C37-C35-N39-C34

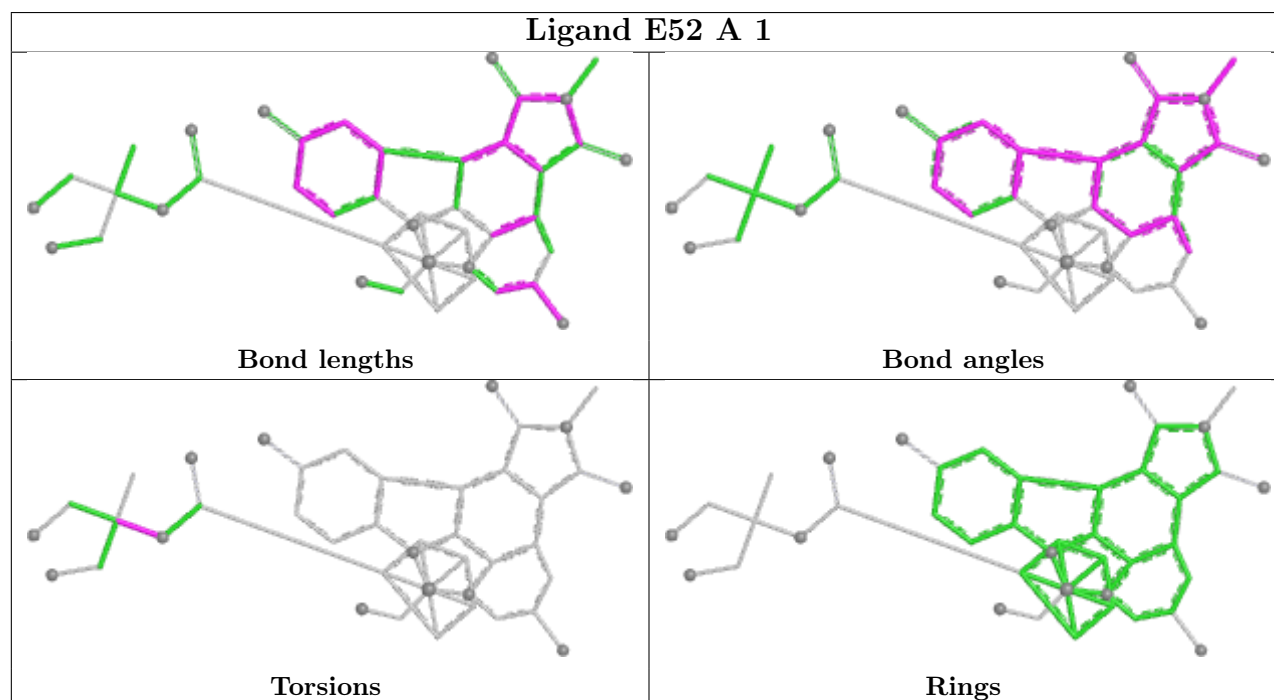
There are no ring outliers.

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	E52	22	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	836/966 (86%)	0.24	22 (2%) 57 37	46, 98, 156, 194	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	899	THR	4.8
1	A	948	HIS	4.4
1	A	900	GLY	4.4
1	A	1087	PHE	3.7
1	A	518	ILE	3.5
1	A	1086	TRP	3.3
1	A	379	LEU	3.1
1	A	898	ASN	3.0
1	A	1044	SER	3.0
1	A	767	LEU	2.9
1	A	527	ILE	2.5
1	A	307	LEU	2.5
1	A	1082	VAL	2.5
1	A	764	ILE	2.5
1	A	966	GLY	2.5
1	A	272	LEU	2.4
1	A	525	HIS	2.3
1	A	763	VAL	2.3
1	A	1041	GLN	2.3
1	A	1084	PHE	2.2
1	A	911	LEU	2.2
1	A	951	ASN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

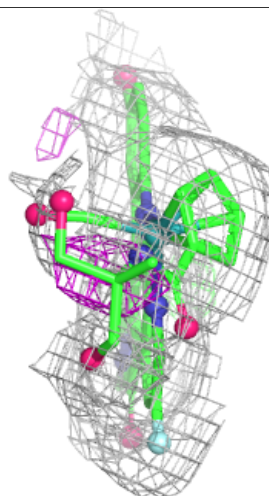
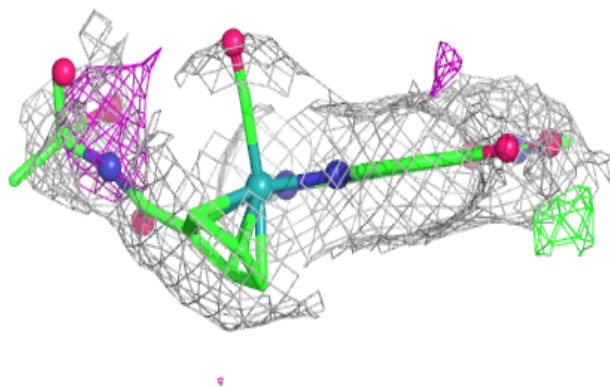
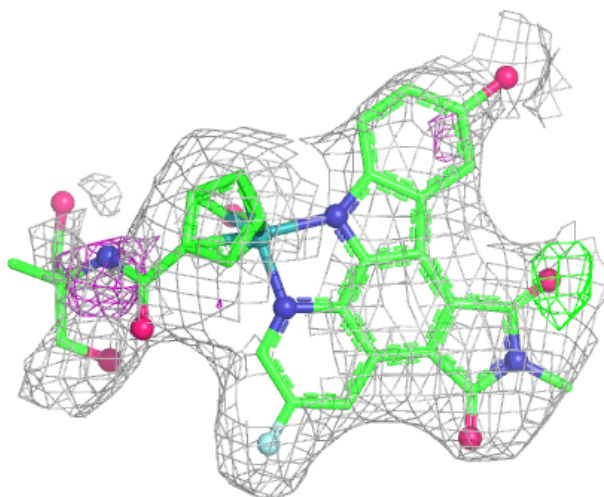
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	E52	A	1	42/42	0.94	0.12	94,104,119,119	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 E52 A 1:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.