



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:04 PM UTC

PDB ID : 4W2R / pdb_00004w2r
Title : Structure of Hs/AcPRC2 in complex with 5,8-dichloro-2-[(4-methoxy-6-methyl-2-oxo-1,2-dihydropyridin-3-yl)methyl]-7-[(R)-methoxy(oxetan-3-yl)methyl]-3,4-dihydroisoquinolin-1(2H)-one
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Deposited on : 2017-09-25
Resolution : 2.81 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

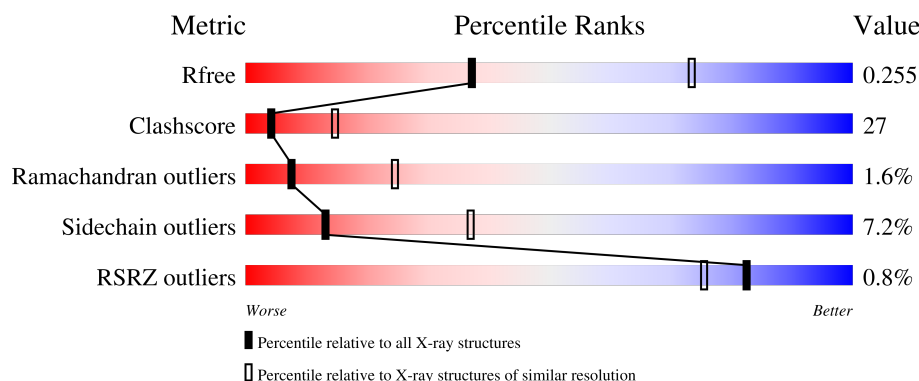
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	643	% 38% 29% 5% 28%
1	B	643	% 40% 28% . 28%
2	E	362	% 58% 37% ..
2	F	362	58% 37% ..

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Mol	Chain	Length	Quality of chain
3	S	191	
3	T	191	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15566 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 Enhancer of zeste 2 polycomb repressive complex 2 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3769	2365	678	688	38			
1	B	465	Total	C	N	O	S	0	0	0
			3777	2368	679	692	38			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	389	LEU	-	linker	UNP G1KPH4
A	390	GLY	-	linker	UNP G1KPH4
A	391	GLY	-	linker	UNP G1KPH4
A	392	GLY	-	linker	UNP G1KPH4
A	393	GLY	-	linker	UNP G1KPH4
A	394	SER	-	linker	UNP G1KPH4
A	395	GLY	-	linker	UNP G1KPH4
A	396	GLY	-	linker	UNP G1KPH4
A	397	GLY	-	linker	UNP G1KPH4
A	398	GLY	-	linker	UNP G1KPH4
A	399	SER	-	linker	UNP G1KPH4
A	400	GLY	-	linker	UNP G1KPH4
A	401	GLY	-	linker	UNP G1KPH4
A	402	GLY	-	linker	UNP G1KPH4
A	403	GLY	-	linker	UNP G1KPH4
A	404	SER	-	linker	UNP G1KPH4
A	405	ALA	-	linker	UNP G1KPH4
A	406	ALA	-	linker	UNP G1KPH4
A	407	ALA	-	linker	UNP G1KPH4
B	389	LEU	-	linker	UNP G1KPH4
B	390	GLY	-	linker	UNP G1KPH4
B	391	GLY	-	linker	UNP G1KPH4
B	392	GLY	-	linker	UNP G1KPH4
B	393	GLY	-	linker	UNP G1KPH4
B	394	SER	-	linker	UNP G1KPH4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	395	GLY	-	linker	UNP G1KPH4
B	396	GLY	-	linker	UNP G1KPH4
B	397	GLY	-	linker	UNP G1KPH4
B	398	GLY	-	linker	UNP G1KPH4
B	399	SER	-	linker	UNP G1KPH4
B	400	GLY	-	linker	UNP G1KPH4
B	401	GLY	-	linker	UNP G1KPH4
B	402	GLY	-	linker	UNP G1KPH4
B	403	GLY	-	linker	UNP G1KPH4
B	404	SER	-	linker	UNP G1KPH4
B	405	ALA	-	linker	UNP G1KPH4
B	406	ALA	-	linker	UNP G1KPH4
B	407	ALA	-	linker	UNP G1KPH4

- Molecule 2 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	358	Total	C	N	O	S	0	0	0
			2898	1834	509	534	21			
2	F	359	Total	C	N	O	S	0	0	0
			2906	1840	510	535	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	66	MET	-	expression tag	UNP O75530
F	66	MET	-	expression tag	UNP O75530

- Molecule 3 is a protein called Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	128	Total	C	N	O	S	0	0	0
			1070	675	185	198	12			
3	T	128	Total	C	N	O	S	0	0	0
			1070	675	185	198	12			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	535	MET	-	expression tag	UNP Q15022
S	536	ASP	-	expression tag	UNP Q15022
S	537	TYR	-	expression tag	UNP Q15022

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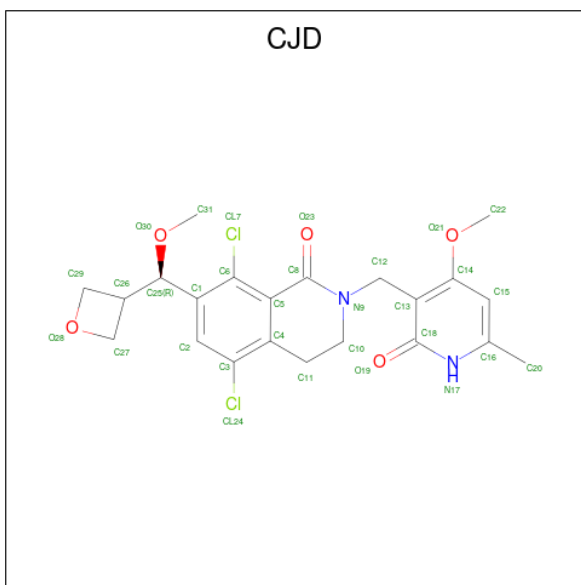
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Chain	Residue	Modelled	Actual	Comment	Reference
S	538	LYS	-	expression tag	UNP Q15022
S	539	ASP	-	expression tag	UNP Q15022
S	540	ASP	-	expression tag	UNP Q15022
S	541	ASP	-	expression tag	UNP Q15022
S	542	ASP	-	expression tag	UNP Q15022
S	543	LYS	-	expression tag	UNP Q15022
S	544	GLY	-	expression tag	UNP Q15022
S	583	ASP	SER	conflict	UNP Q15022
T	535	MET	-	expression tag	UNP Q15022
T	536	ASP	-	expression tag	UNP Q15022
T	537	TYR	-	expression tag	UNP Q15022
T	538	LYS	-	expression tag	UNP Q15022
T	539	ASP	-	expression tag	UNP Q15022
T	540	ASP	-	expression tag	UNP Q15022
T	541	ASP	-	expression tag	UNP Q15022
T	542	ASP	-	expression tag	UNP Q15022
T	543	LYS	-	expression tag	UNP Q15022
T	544	GLY	-	expression tag	UNP Q15022
T	583	ASP	SER	conflict	UNP Q15022

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	Zn	0	0
			7	7		
4	B	7	Total	Zn	0	0
			7	7		

- Molecule 5 is 5,8-dichloro-2-[(4-methoxy-6-methyl-2-oxo-1,2-dihydropyridin-3-yl)methyl]-7-[(R)-methoxy(oxetan-3-yl)methyl]-3,4-dihydroisoquinolin-1(2H)-one (CCD ID: CJD) (formula: C₂₂H₂₄Cl₂N₂O₅).

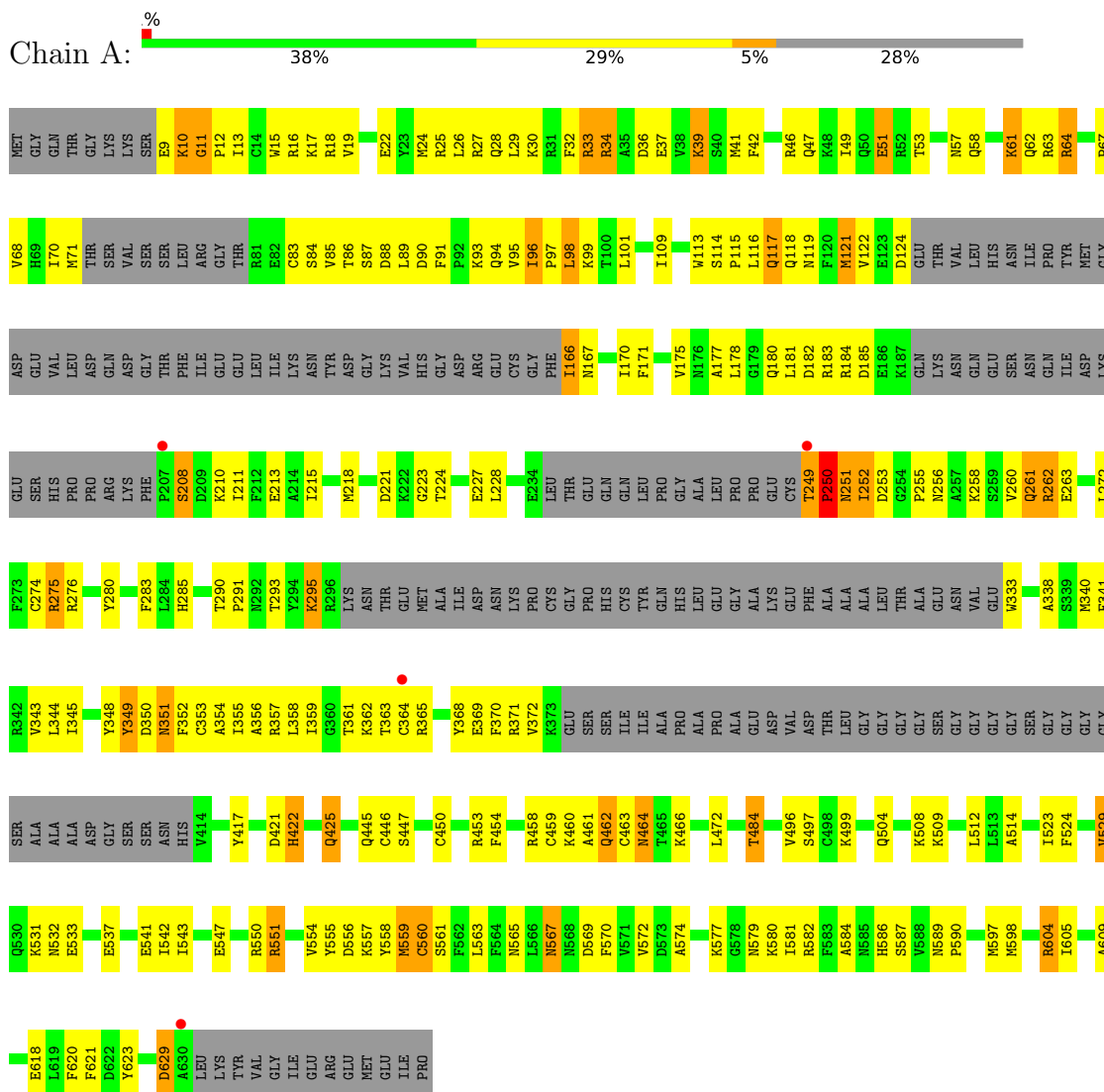


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 31	C 22	Cl 2	N 2	O 5	0	0
5	B	1	Total 31	C 22	Cl 2	N 2	O 5	0	0

3 Residue-property plots

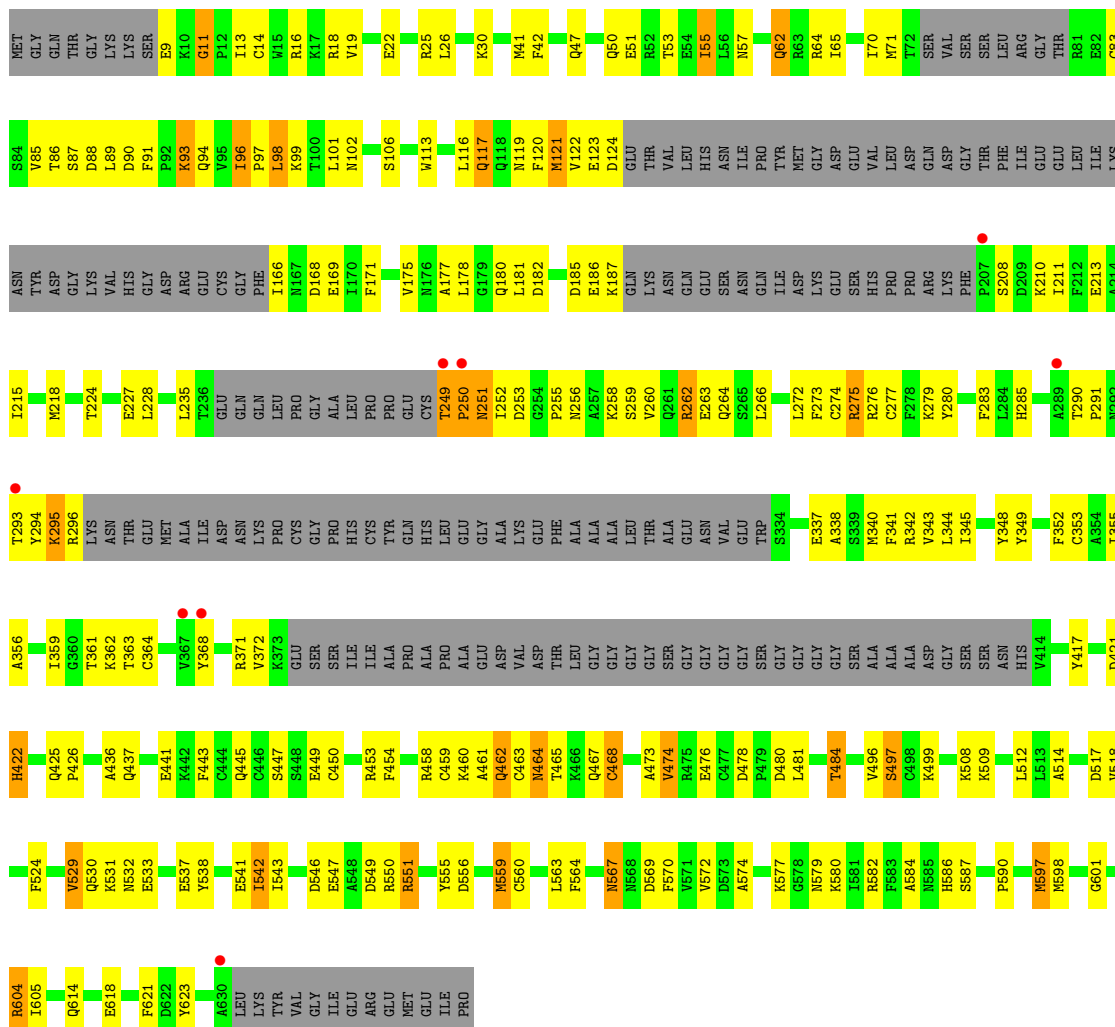
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Enhancer of zeste 2 polycomb repressive complex 2 subunit

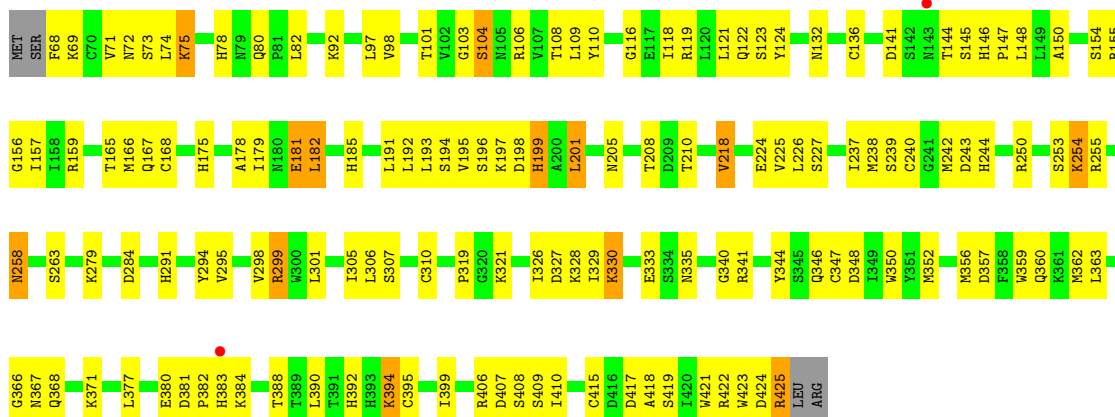


- Molecule 1: Enhancer of zeste 2 polycomb repressive complex 2 subunit



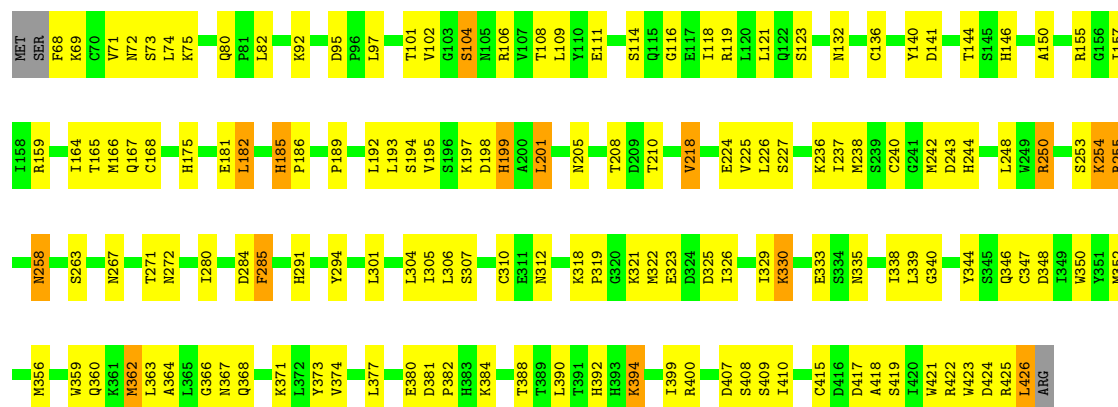


- Molecule 2: Polycomb protein EED

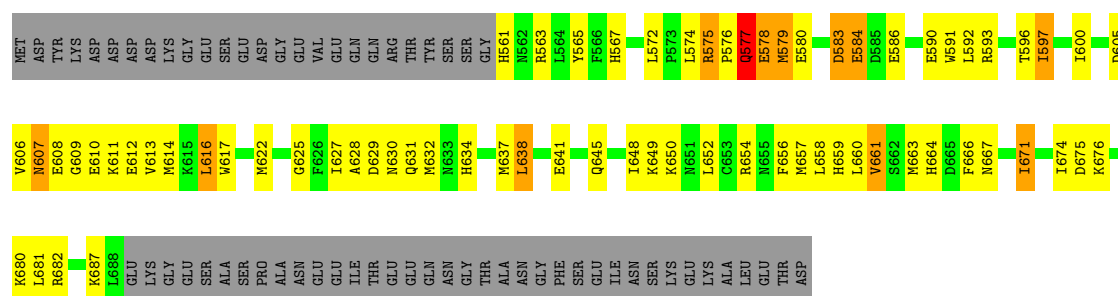
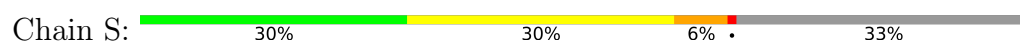


- Molecule 2: Polycomb protein EED

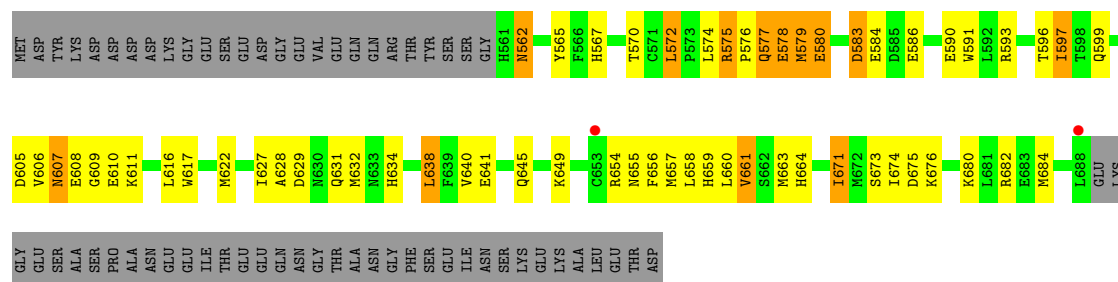




• Molecule 3: Polycomb protein SUZ12



• Molecule 3: Polycomb protein SUZ12



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.72Å 115.48Å 151.54Å 90.00° 102.40° 90.00°	Depositor
Resolution (Å)	148.01 – 2.81 148.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.8 (148.01-2.81) 99.8 (148.00-2.81)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.82Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.266 0.208 , 0.255	Depositor DCC
R_{free} test set	2944 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15566	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.37% 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: ZN, CJD

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	0.48	0/3850	0.85	11/5176 (0.2%)
1	B	0.46	0/3856	0.83	8/5184 (0.2%)
2	E	0.52	0/2972	0.84	2/4026 (0.0%)
2	F	0.48	0/2980	0.82	4/4037 (0.1%)
3	S	0.45	0/1091	0.75	1/1464 (0.1%)
3	T	0.50	0/1091	0.79	3/1464 (0.2%)
All	All	0.48	0/15840	0.83	29/21351 (0.1%)

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	2
1	B	0	1
3	T	0	1
All	All	0	4

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	PHE	CA-C-N	8.71	128.72	119.05
1	A	454	PHE	C-N-CA	8.71	128.72	119.05
1	A	249	THR	CA-C-N	7.11	128.73	119.84
1	A	249	THR	C-N-CA	7.11	128.73	119.84
3	S	608	GLU	N-CA-C	-7.00	104.55	113.23
2	E	196	SER	N-CA-C	6.54	119.12	109.24
1	A	589	ASN	CA-C-N	6.48	126.44	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	589	ASN	C-N-CA	6.48	126.44	120.03
1	B	249	THR	CA-C-N	6.46	127.92	119.84
1	B	249	THR	C-N-CA	6.46	127.92	119.84
1	B	454	PHE	CA-C-N	6.42	126.34	119.28
1	B	454	PHE	C-N-CA	6.42	126.34	119.28
3	T	608	GLU	N-CA-C	-6.15	105.77	113.28
1	B	11	GLY	CA-C-N	6.05	127.40	119.84
1	B	11	GLY	C-N-CA	6.05	127.40	119.84
2	F	185	HIS	CA-C-N	5.88	125.75	119.28
2	F	185	HIS	C-N-CA	5.88	125.75	119.28
1	A	629	ASP	N-CA-C	-5.83	103.41	111.81
2	F	104	SER	CB-CA-C	-5.55	110.16	116.54
2	E	104	SER	CB-CA-C	-5.52	110.19	116.54
1	B	285	HIS	CA-C-N	5.45	126.65	119.84
1	B	285	HIS	C-N-CA	5.45	126.65	119.84
3	T	575	ARG	CA-C-N	5.32	125.39	119.32
3	T	575	ARG	C-N-CA	5.32	125.39	119.32
2	F	280	ILE	CB-CA-C	-5.31	106.17	111.80
1	A	11	GLY	CA-C-N	5.24	124.56	118.85
1	A	11	GLY	C-N-CA	5.24	124.56	118.85
1	A	285	HIS	CA-C-N	5.19	126.33	119.84
1	A	285	HIS	C-N-CA	5.19	126.33	119.84

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	250	PRO	Peptide
1	A	559	MET	Peptide
1	B	559	MET	Peptide
3	T	577	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3769	0	3657	215	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3777	0	3673	200	0
2	E	2898	0	2812	169	0
2	F	2906	0	2823	157	0
3	S	1070	0	1052	88	0
3	T	1070	0	1052	88	0
4	A	7	0	0	0	0
4	B	7	0	0	0	0
5	A	31	0	0	0	0
5	B	31	0	0	0	0
All	All	15566	0	15069	832	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 27.

All (832) 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)
2:E:165:THR:HG22	2:E:167:GLN:HG2	1.32	1.11
2:F:340:GLY:HA3	2:F:382:PRO:HG3	1.40	1.03
2:F:165:THR:HG22	2:F:167:GLN:HG2	1.40	1.02
2:E:340:GLY:HA3	2:E:382:PRO:HG3	1.45	0.96
1:A:96:ILE:HG12	1:A:97:PRO:HD2	1.43	0.96
1:B:458:ARG:HA	1:B:484:THR:HG21	1.47	0.94
2:F:272:ASN:HA	3:T:577:GLN:HG2	1.50	0.93
1:A:30:LYS:HE2	1:A:170:ILE:HG12	1.51	0.92
1:B:293:THR:HG22	1:B:445:GLN:NE2	1.86	0.91
1:A:293:THR:HG22	1:A:445:GLN:NE2	1.85	0.91
3:S:671:ILE:O	3:S:674:ILE:HG22	1.70	0.90
1:A:458:ARG:HA	1:A:484:THR:HG21	1.54	0.90
3:T:607:ASN:O	3:T:611:LYS:HG3	1.72	0.89
3:T:628:ALA:H	3:T:631:GLN:HE21	1.13	0.88
1:B:57:ASN:HD22	2:E:406:ARG:HH21	1.14	0.88
3:T:593:ARG:O	3:T:596:THR:HG22	1.73	0.88
2:E:326:ILE:HA	2:E:329:ILE:HD12	1.56	0.86
3:T:617:TRP:HZ2	3:T:632:MET:HE1	1.41	0.86
1:B:580:LYS:HE2	3:S:584:GLU:HG3	1.56	0.84
2:E:165:THR:CG2	2:E:167:GLN:HG2	2.07	0.84
2:E:291:HIS:HE1	2:E:307:SER:OG	1.60	0.84
2:F:326:ILE:HA	2:F:329:ILE:HD12	1.59	0.83
1:B:293:THR:HG22	1:B:445:GLN:HE21	1.42	0.83
1:A:290:THR:HB	1:A:293:THR:HG23	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ARG:HD2	1:A:218:MET:HE3	1.62	0.81
2:E:294:TYR:CZ	2:E:350:TRP:HB3	2.15	0.81
1:A:567:ASN:ND2	1:A:569:ASP:H	1.77	0.81
3:S:628:ALA:H	3:S:631:GLN:HE21	1.24	0.81
1:B:57:ASN:ND2	2:E:406:ARG:HH21	1.77	0.81
1:B:290:THR:HB	1:B:293:THR:HG23	1.60	0.81
3:S:682:ARG:HG2	3:S:682:ARG:HH11	1.45	0.81
1:A:567:ASN:HD22	1:A:569:ASP:H	1.29	0.80
2:E:392:HIS:CE1	2:E:394:LYS:HB2	2.16	0.80
1:A:99:LYS:HE3	2:F:166:MET:O	1.82	0.80
1:B:262:ARG:HB2	1:B:343:VAL:HA	1.63	0.80
2:E:367:ASN:HD22	2:E:371:LYS:HB2	1.46	0.80
1:A:251:ASN:HA	3:T:607:ASN:ND2	1.96	0.80
2:E:425:ARG:HH21	2:E:425:ARG:CG	1.94	0.80
1:A:355:ILE:O	1:A:359:ILE:HG13	1.83	0.79
1:B:177:ALA:O	1:B:180:GLN:HG2	1.83	0.79
2:E:330:LYS:N	2:E:330:LYS:HD3	1.96	0.79
2:E:330:LYS:HD3	2:E:330:LYS:H	1.47	0.79
1:B:96:ILE:HG12	1:B:97:PRO:HD2	1.65	0.79
1:B:280:TYR:OH	3:S:659:HIS:HD2	1.67	0.78
3:T:578:GLU:HB3	3:T:580:GLU:HG2	1.65	0.78
3:S:659:HIS:CE1	3:S:663:MET:HE1	2.20	0.77
1:A:39:LYS:HD2	2:F:380:GLU:HB3	1.66	0.77
1:A:67:PRO:HG3	2:F:95:ASP:OD2	1.84	0.76
3:T:682:ARG:HG2	3:T:682:ARG:HH11	1.48	0.76
2:F:294:TYR:CZ	2:F:350:TRP:HB3	2.20	0.76
1:B:251:ASN:HA	3:S:607:ASN:ND2	2.01	0.75
2:E:330:LYS:HE2	2:E:333:GLU:OE1	1.87	0.75
3:S:607:ASN:HB2	3:S:610:GLU:HG2	1.67	0.75
1:B:85:VAL:HG11	2:E:74:LEU:HD23	1.69	0.75
3:S:593:ARG:O	3:S:596:THR:HG22	1.87	0.75
3:T:627:ILE:H	3:T:631:GLN:HE22	1.35	0.74
1:B:355:ILE:O	1:B:359:ILE:HG13	1.86	0.74
1:A:10:LYS:HZ1	1:A:18:ARG:NH2	1.85	0.74
1:A:16:ARG:HD2	1:A:218:MET:CE	2.16	0.74
3:T:607:ASN:HB2	3:T:610:GLU:HG2	1.68	0.74
1:A:340:MET:HE3	3:T:657:MET:HE3	1.68	0.74
2:E:333:GLU:OE2	2:E:335:ASN:HB2	1.88	0.74
2:E:250:ARG:HG3	2:E:284:ASP:CG	2.12	0.73
1:A:290:THR:HB	1:A:293:THR:CG2	2.18	0.73
2:F:197:LYS:HA	2:F:224:GLU:HG3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:71:VAL:HG12	2:F:116:GLY:HA3	1.70	0.73
3:S:607:ASN:O	3:S:611:LYS:HG3	1.89	0.73
3:S:578:GLU:HG3	3:S:580:GLU:HG2	1.70	0.73
1:B:567:ASN:HD22	1:B:567:ASN:C	1.97	0.72
3:T:628:ALA:H	3:T:631:GLN:NE2	1.87	0.72
2:E:298:VAL:O	2:E:299:ARG:HD3	1.90	0.72
1:B:340:MET:HE3	3:S:657:MET:HE3	1.70	0.72
3:T:645:GLN:HE21	3:T:649:LYS:NZ	1.87	0.72
2:E:197:LYS:HA	2:E:224:GLU:HG3	1.71	0.72
1:B:290:THR:HB	1:B:293:THR:CG2	2.20	0.71
3:T:671:ILE:O	3:T:674:ILE:HG22	1.90	0.71
1:B:71:MET:HB3	1:B:96:ILE:HD11	1.70	0.71
2:F:82:LEU:HD13	2:F:101:THR:HG21	1.72	0.71
2:F:175:HIS:HE1	2:F:194:SER:OG	1.73	0.71
2:F:392:HIS:CE1	2:F:394:LYS:HB2	2.24	0.71
3:T:627:ILE:H	3:T:631:GLN:NE2	1.86	0.71
2:E:425:ARG:HH21	2:E:425:ARG:CB	2.03	0.71
1:B:30:LYS:HE2	1:B:169:GLU:OE2	1.91	0.70
2:F:330:LYS:H	2:F:330:LYS:HD3	1.56	0.70
2:F:330:LYS:HD3	2:F:330:LYS:N	2.07	0.70
1:A:275:ARG:HH11	1:A:275:ARG:HG2	1.56	0.70
1:B:11:GLY:O	1:B:14:CYS:HB3	1.92	0.70
2:F:301:LEU:HD13	2:F:356:MET:HE1	1.74	0.70
3:T:617:TRP:CZ2	3:T:632:MET:HE1	2.26	0.70
2:E:425:ARG:HH21	2:E:425:ARG:HG2	1.55	0.69
1:B:567:ASN:ND2	1:B:570:PHE:H	1.90	0.69
1:B:57:ASN:HD22	2:E:406:ARG:NH2	1.88	0.69
2:E:208:THR:HG23	2:E:210:THR:OG1	1.92	0.69
2:E:319:PRO:HG2	2:E:329:ILE:HD13	1.74	0.69
2:F:250:ARG:HG3	2:F:284:ASP:CG	2.17	0.69
1:A:555:TYR:HE2	1:A:563:LEU:HD11	1.58	0.69
1:B:224:THR:HG22	1:B:227:GLU:HG3	1.75	0.68
1:B:425:GLN:HG2	1:B:426:PRO:HD2	1.75	0.68
1:A:262:ARG:HD2	1:A:343:VAL:HA	1.76	0.68
1:A:224:THR:HG22	1:A:227:GLU:HG3	1.75	0.68
3:S:607:ASN:HB2	3:S:610:GLU:H	1.56	0.68
1:A:293:THR:HG22	1:A:445:GLN:HE21	1.56	0.68
2:E:97:LEU:HD12	2:E:410:ILE:HD12	1.75	0.68
3:S:627:ILE:H	3:S:631:GLN:NE2	1.90	0.68
2:E:367:ASN:HB2	2:E:371:LYS:O	1.94	0.68
2:E:394:LYS:HB3	2:E:421:TRP:HH2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ASN:ND2	1:A:570:PHE:H	1.91	0.67
1:B:275:ARG:HG2	1:B:275:ARG:HH11	1.58	0.67
1:A:96:ILE:HG12	1:A:97:PRO:CD	2.21	0.67
2:E:71:VAL:HG12	2:E:116:GLY:HA3	1.75	0.67
2:E:175:HIS:HE1	2:E:194:SER:OG	1.76	0.67
1:A:67:PRO:HG3	2:F:95:ASP:CG	2.20	0.67
3:S:575:ARG:HH11	3:S:575:ARG:CB	2.07	0.67
1:B:361:THR:O	1:B:362:LYS:HG2	1.94	0.67
2:E:144:THR:HG22	2:E:146:HIS:CD2	2.30	0.66
2:F:82:LEU:HD13	2:F:101:THR:CG2	2.25	0.66
2:F:253:SER:HB2	2:F:254:LYS:HE2	1.75	0.66
1:A:39:LYS:CD	2:F:380:GLU:HB3	2.24	0.66
1:A:30:LYS:O	1:A:34:ARG:HB3	1.95	0.66
1:A:39:LYS:CA	1:A:39:LYS:HE2	2.24	0.66
2:E:167:GLN:HA	2:E:167:GLN:OE1	1.95	0.66
1:A:177:ALA:O	1:A:180:GLN:HG2	1.95	0.66
1:B:524:PHE:CE1	1:B:618:GLU:HB2	2.30	0.66
1:A:422:HIS:H	1:A:422:HIS:CD2	2.12	0.66
1:B:567:ASN:ND2	1:B:569:ASP:H	1.94	0.66
1:A:577:LYS:HE2	2:F:218:VAL:HG12	1.77	0.66
1:B:94:GLN:HE22	2:E:119:ARG:HA	1.60	0.65
2:F:218:VAL:HG11	3:T:591:TRP:CZ3	2.32	0.65
2:F:254:LYS:CD	2:F:254:LYS:H	2.09	0.65
2:E:301:LEU:HD13	2:E:356:MET:HE1	1.77	0.65
3:S:628:ALA:H	3:S:631:GLN:NE2	1.94	0.65
3:T:660:LEU:HB3	3:T:674:ILE:HG13	1.78	0.65
1:A:422:HIS:H	1:A:422:HIS:HD2	1.45	0.65
2:F:140:TYR:CZ	2:F:189:PRO:HG3	2.32	0.64
2:E:254:LYS:CD	2:E:254:LYS:H	2.09	0.64
1:A:171:PHE:O	1:A:175:VAL:HG23	1.96	0.64
1:B:249:THR:N	1:B:250:PRO:HD3	2.13	0.64
1:B:83:CYS:HB2	2:E:106:ARG:NH2	2.12	0.64
1:B:458:ARG:CA	1:B:484:THR:HG21	2.26	0.64
2:F:330:LYS:HE2	2:F:333:GLU:OE1	1.97	0.64
3:T:607:ASN:HB2	3:T:610:GLU:H	1.62	0.64
1:A:567:ASN:HD22	1:A:567:ASN:C	2.06	0.64
2:E:68:PHE:HA	2:E:424:ASP:O	1.97	0.64
3:S:617:TRP:HZ2	3:S:632:MET:HE1	1.63	0.64
1:A:531:LYS:HG2	1:A:532:ASN:ND2	2.13	0.63
1:A:178:LEU:HD12	1:A:215:ILE:HD11	1.80	0.63
2:E:425:ARG:HG2	2:E:425:ARG:NH2	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:195:VAL:HG22	2:F:201:LEU:HD13	1.79	0.63
2:E:71:VAL:HG12	2:E:116:GLY:CA	2.29	0.63
1:A:64:ARG:HA	2:F:92:LYS:NZ	2.14	0.63
3:T:578:GLU:HG3	3:T:579:MET:H	1.64	0.63
1:B:101:LEU:HD22	2:E:168:CYS:HB2	1.81	0.63
1:B:62:GLN:HE21	1:B:62:GLN:N	1.97	0.62
2:F:165:THR:CG2	2:F:167:GLN:HG2	2.23	0.62
2:F:346:GLN:O	2:F:368:GLN:HG2	1.98	0.62
2:F:144:THR:HG22	2:F:146:HIS:CD2	2.34	0.62
3:S:607:ASN:CB	3:S:610:GLU:HG2	2.27	0.62
1:A:41:MET:SD	2:F:318:LYS:HE3	2.40	0.62
1:B:275:ARG:HG2	1:B:275:ARG:NH1	2.13	0.62
2:E:195:VAL:HG22	2:E:201:LEU:HD13	1.81	0.62
3:T:578:GLU:HG3	3:T:579:MET:N	2.12	0.62
1:A:338:ALA:O	1:A:341:PHE:HB3	1.99	0.62
1:A:280:TYR:OH	3:T:659:HIS:HD2	1.82	0.62
2:F:425:ARG:HG2	2:F:426:LEU:H	1.64	0.62
1:B:53:THR:HG21	2:E:359:TRP:CE3	2.35	0.62
1:A:458:ARG:HA	1:A:484:THR:CG2	2.27	0.62
2:E:363:LEU:HB2	2:E:377:LEU:HD11	1.82	0.62
3:S:628:ALA:N	3:S:631:GLN:HE21	1.96	0.61
1:A:275:ARG:HG2	1:A:275:ARG:NH1	2.11	0.61
2:F:205:ASN:CG	2:F:208:THR:HG22	2.25	0.61
3:T:657:MET:O	3:T:661:VAL:HG12	2.00	0.61
1:A:86:THR:HG22	1:A:87:SER:N	2.14	0.61
2:F:291:HIS:HE1	2:F:307:SER:OG	1.84	0.61
2:E:69:LYS:O	2:E:71:VAL:HG23	2.00	0.61
1:A:262:ARG:HB2	1:A:343:VAL:HA	1.81	0.61
1:B:280:TYR:OH	3:S:659:HIS:CD2	2.53	0.61
2:F:68:PHE:HB2	2:F:390:LEU:HD11	1.83	0.61
1:A:422:HIS:CD2	1:A:422:HIS:N	2.69	0.61
1:A:512:LEU:O	1:A:523:ILE:HD12	2.01	0.60
2:F:118:ILE:HD11	2:F:422:ARG:HB2	1.83	0.60
2:F:333:GLU:OE2	2:F:335:ASN:HB2	2.01	0.60
1:A:39:LYS:CE	2:F:380:GLU:HB3	2.32	0.60
1:B:99:LYS:HE3	2:E:166:MET:O	2.01	0.60
2:E:205:ASN:CG	2:E:208:THR:HG22	2.26	0.60
2:F:254:LYS:H	2:F:254:LYS:HD3	1.66	0.60
3:T:628:ALA:N	3:T:631:GLN:HE21	1.94	0.60
3:T:606:VAL:CG1	3:T:610:GLU:HG3	2.32	0.60
1:B:89:LEU:HD22	2:E:72:ASN:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:660:LEU:HB3	3:S:674:ILE:HG13	1.83	0.60
1:A:33:ARG:HG2	1:A:33:ARG:O	2.00	0.60
1:A:224:THR:O	1:A:228:LEU:HG	2.02	0.60
1:B:459:CYS:SG	1:B:468:CYS:HB2	2.42	0.60
1:A:84:SER:HB3	1:A:95:VAL:HG22	1.83	0.60
1:A:251:ASN:OD1	1:A:252:ILE:N	2.35	0.60
1:B:42:PHE:HD2	2:E:380:GLU:O	1.85	0.60
3:S:627:ILE:H	3:S:631:GLN:HE22	1.50	0.60
1:A:94:GLN:HE22	2:F:119:ARG:HA	1.68	0.59
1:A:290:THR:HG23	1:A:421:ASP:OD1	2.01	0.59
3:T:575:ARG:HB2	3:T:576:PRO:CD	2.32	0.59
2:F:415:CYS:HB2	2:F:417:ASP:OD1	2.03	0.59
3:T:676:LYS:O	3:T:680:LYS:HG2	2.02	0.59
1:A:363:THR:O	1:A:364:CYS:C	2.46	0.59
1:B:555:TYR:HE2	1:B:563:LEU:HD11	1.68	0.59
2:F:319:PRO:HG2	2:F:329:ILE:HD13	1.85	0.59
1:B:96:ILE:CG1	1:B:97:PRO:HD2	2.32	0.59
2:F:193:LEU:HD22	2:F:237:ILE:HD13	1.84	0.59
2:F:367:ASN:HB2	2:F:371:LYS:O	2.03	0.59
2:E:181:GLU:HG3	2:E:182:LEU:H	1.68	0.59
2:F:250:ARG:HG3	2:F:284:ASP:OD2	2.02	0.59
2:F:301:LEU:HD13	2:F:356:MET:CE	2.32	0.59
2:E:82:LEU:HD22	2:E:101:THR:CG2	2.33	0.58
2:F:226:LEU:HD11	2:F:242:MET:HG2	1.85	0.58
1:A:9:GLU:N	1:A:210:LYS:HZ2	2.00	0.58
2:E:253:SER:HB2	2:E:254:LYS:HE2	1.85	0.58
1:A:537:GLU:OE1	1:A:604:ARG:HD2	2.03	0.58
1:A:177:ALA:O	1:A:181:LEU:HD13	2.03	0.58
1:B:538:TYR:HH	1:B:564:PHE:HE2	1.51	0.58
2:E:155:ARG:O	2:E:157:ILE:HG13	2.04	0.58
1:A:83:CYS:HB2	2:F:106:ARG:HH22	1.68	0.58
1:A:496:VAL:HG12	1:A:497:SER:N	2.19	0.58
2:E:193:LEU:HD22	2:E:237:ILE:HD13	1.86	0.58
1:A:464:ASN:ND2	1:A:464:ASN:H	2.02	0.58
1:B:338:ALA:O	1:B:341:PHE:HB3	2.03	0.58
3:S:612:GLU:OE2	3:S:650:LYS:HE2	2.02	0.58
3:T:645:GLN:HE21	3:T:649:LYS:HZ1	1.50	0.58
2:E:250:ARG:HG3	2:E:284:ASP:OD2	2.04	0.58
2:F:182:LEU:HG	2:F:192:LEU:HD11	1.84	0.58
2:F:208:THR:HG23	2:F:210:THR:OG1	2.03	0.58
1:A:255:PRO:HG2	1:A:256:ASN:OD1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:MET:CE	3:T:657:MET:HE3	2.32	0.58
1:A:565:ASN:ND2	1:A:629:ASP:HB2	2.18	0.58
2:F:167:GLN:OE1	2:F:167:GLN:HA	2.04	0.58
1:B:16:ARG:HD2	1:B:218:MET:HE3	1.86	0.57
1:A:572:VAL:HG11	1:A:605:ILE:HD12	1.85	0.57
1:B:363:THR:O	1:B:364:CYS:C	2.46	0.57
2:F:294:TYR:OH	2:F:310:CYS:HB3	2.04	0.57
2:E:108:THR:C	2:E:109:LEU:HD12	2.29	0.57
3:T:617:TRP:HZ2	3:T:632:MET:CE	2.17	0.57
1:B:290:THR:HG23	1:B:291:PRO:HD2	1.86	0.57
1:B:556:ASP:O	1:B:559:MET:HE2	2.05	0.57
1:A:524:PHE:CE1	1:A:618:GLU:HB2	2.39	0.57
2:E:71:VAL:HG12	2:E:71:VAL:O	2.05	0.57
1:A:15:TRP:O	1:A:19:VAL:HG23	2.04	0.57
1:A:464:ASN:H	1:A:464:ASN:HD22	1.52	0.57
1:A:290:THR:CB	1:A:293:THR:HG23	2.33	0.57
2:F:68:PHE:HA	2:F:424:ASP:O	2.04	0.57
1:A:345:ILE:O	1:A:349:TYR:HA	2.04	0.56
1:B:450:CYS:HB3	1:B:453:ARG:HG3	1.86	0.56
3:T:567:HIS:NE2	3:T:574:LEU:HD13	2.20	0.56
2:E:197:LYS:HG3	2:E:224:GLU:CD	2.29	0.56
3:T:664:HIS:CE1	3:T:671:ILE:HG12	2.40	0.56
1:A:263:GLU:O	1:A:263:GLU:HG3	2.04	0.56
1:B:259:SER:OG	1:B:342:ARG:NH2	2.37	0.56
1:B:422:HIS:CD2	1:B:422:HIS:H	2.23	0.56
2:E:425:ARG:HH21	2:E:425:ARG:HB3	1.70	0.56
1:A:417:TYR:HB2	1:A:598:MET:HE1	1.88	0.56
1:A:579:ASN:O	1:A:582:ARG:HG2	2.05	0.56
1:B:537:GLU:OE1	1:B:604:ARG:HD2	2.06	0.56
1:A:531:LYS:HG2	1:A:532:ASN:HD22	1.71	0.56
1:B:71:MET:CE	2:E:123:SER:H	2.18	0.56
1:B:168:ASP:HB3	1:B:235:LEU:CD1	2.36	0.56
1:B:251:ASN:OD1	1:B:252:ILE:N	2.38	0.56
2:F:195:VAL:HG13	2:F:225:VAL:CG1	2.36	0.56
1:B:62:GLN:N	1:B:62:GLN:NE2	2.53	0.56
1:B:590:PRO:HB3	1:B:621:PHE:HA	1.88	0.56
2:F:136:CYS:HA	2:F:150:ALA:O	2.05	0.56
3:T:579:MET:H	3:T:579:MET:HE3	1.70	0.56
1:B:121:MET:HE3	1:B:542:ILE:HB	1.87	0.56
2:E:415:CYS:HB2	2:E:417:ASP:OD1	2.06	0.56
1:B:96:ILE:HG12	1:B:97:PRO:CD	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:ASN:O	1:B:582:ARG:HG2	2.06	0.55
2:E:201:LEU:N	2:E:201:LEU:HD23	2.20	0.55
2:E:254:LYS:H	2:E:254:LYS:HD3	1.70	0.55
3:S:575:ARG:HH11	3:S:575:ARG:HB3	1.70	0.55
3:T:593:ARG:HA	3:T:622:MET:HE1	1.87	0.55
1:A:85:VAL:HG11	2:F:74:LEU:HD23	1.86	0.55
1:B:86:THR:HG22	1:B:87:SER:N	2.20	0.55
1:A:541:GLU:OE1	1:A:551:ARG:NH2	2.39	0.55
1:B:340:MET:CE	3:S:657:MET:HE3	2.35	0.55
2:F:72:ASN:OD1	2:F:73:SER:N	2.39	0.55
3:T:656:PHE:O	3:T:659:HIS:HB3	2.07	0.55
1:A:39:LYS:HE3	2:F:380:GLU:HB3	1.87	0.55
1:A:58:GLN:HA	1:A:61:LYS:HG3	1.89	0.55
2:F:321:LYS:HE2	2:F:335:ASN:ND2	2.22	0.55
1:A:368:TYR:O	1:A:372:VAL:HG23	2.06	0.55
3:T:575:ARG:HB2	3:T:576:PRO:HD2	1.88	0.55
3:S:656:PHE:O	3:S:659:HIS:HB3	2.06	0.55
2:E:390:LEU:N	2:E:390:LEU:HD22	2.22	0.55
2:F:367:ASN:HD22	2:F:371:LYS:HB2	1.71	0.55
1:B:422:HIS:CD2	1:B:422:HIS:N	2.75	0.55
1:A:249:THR:N	1:A:250:PRO:HD3	2.20	0.54
1:B:340:MET:HG3	1:B:344:LEU:HD12	1.89	0.54
2:F:227:SER:HB3	2:F:240:CYS:SG	2.48	0.54
1:A:371:ARG:HH11	1:A:371:ARG:HG2	1.73	0.54
1:A:590:PRO:HB3	1:A:621:PHE:HA	1.89	0.54
2:E:254:LYS:H	2:E:254:LYS:CE	2.21	0.54
2:F:301:LEU:HA	2:F:360:GLN:HE22	1.72	0.54
2:E:68:PHE:HB2	2:E:390:LEU:HD11	1.88	0.54
2:F:272:ASN:O	3:T:577:GLN:HB3	2.08	0.54
1:A:182:ASP:O	1:A:185:ASP:HB2	2.07	0.54
1:A:210:LYS:O	1:A:213:GLU:HG2	2.08	0.54
2:F:236:LYS:HD2	2:F:248:LEU:HD11	1.90	0.54
2:F:344:TYR:HE1	2:F:347:CYS:HB3	1.73	0.54
2:F:425:ARG:O	2:F:426:LEU:HB3	2.07	0.54
1:A:10:LYS:NZ	1:A:18:ARG:NH2	2.55	0.54
1:A:509:LYS:HE2	1:A:533:GLU:OE2	2.06	0.54
2:E:254:LYS:HE2	2:E:254:LYS:N	2.23	0.54
1:A:450:CYS:HB3	1:A:453:ARG:HG3	1.90	0.54
1:B:462:GLN:O	1:B:463:CYS:HB2	2.06	0.54
2:F:198:ASP:O	2:F:199:HIS:HB2	2.08	0.54
2:F:394:LYS:HB3	2:F:421:TRP:HH2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:648:ILE:HG13	3:S:681:LEU:HD11	1.90	0.54
3:S:682:ARG:HG2	3:S:682:ARG:NH1	2.20	0.54
2:E:319:PRO:HG2	2:E:329:ILE:CD1	2.38	0.54
3:S:567:HIS:HD2	3:S:583:ASP:OD1	1.90	0.54
1:A:96:ILE:CG1	1:A:97:PRO:HD2	2.29	0.53
1:B:290:THR:CB	1:B:293:THR:HG23	2.36	0.53
2:E:224:GLU:HB3	2:E:242:MET:HG3	1.90	0.53
1:B:117:GLN:CD	1:B:508:LYS:HZ3	2.16	0.53
2:E:226:LEU:HD11	2:E:242:MET:HG2	1.89	0.53
1:B:480:ASP:O	1:B:481:LEU:HD23	2.08	0.53
2:E:136:CYS:HA	2:E:150:ALA:O	2.08	0.53
2:E:198:ASP:O	2:E:199:HIS:HB2	2.08	0.53
3:S:676:LYS:O	3:S:680:LYS:HG2	2.09	0.53
1:A:89:LEU:HD22	2:F:72:ASN:HA	1.90	0.53
1:B:47:GLN:HE21	1:B:50:GLN:NE2	2.07	0.53
1:B:277:CYS:O	1:B:279:LYS:HE2	2.08	0.53
3:T:579:MET:N	3:T:579:MET:HE3	2.23	0.53
3:T:607:ASN:CB	3:T:610:GLU:HG2	2.37	0.53
1:B:70:ILE:HG13	1:B:71:MET:N	2.21	0.53
2:E:294:TYR:OH	2:E:310:CYS:HB3	2.08	0.53
3:T:593:ARG:HG2	3:T:622:MET:CE	2.38	0.53
3:T:682:ARG:HH11	3:T:682:ARG:CG	2.21	0.53
1:A:547:GLU:HG3	1:A:551:ARG:HD2	1.89	0.53
2:F:155:ARG:O	2:F:157:ILE:HG13	2.08	0.53
1:A:567:ASN:HD22	1:A:569:ASP:N	2.01	0.53
1:B:514:ALA:HB3	1:B:524:PHE:CE2	2.43	0.53
2:E:195:VAL:HG13	2:E:225:VAL:CG1	2.38	0.53
2:F:330:LYS:N	2:F:330:LYS:CD	2.71	0.53
1:A:39:LYS:HE2	1:A:39:LYS:HA	1.88	0.53
1:A:354:ALA:HA	1:A:357:ARG:NH1	2.24	0.53
1:B:124:ASP:HB3	1:B:550:ARG:HH21	1.74	0.53
1:B:517:ASP:OD2	3:S:563:ARG:NH2	2.42	0.53
3:S:666:PHE:O	3:S:667:ASN:HB2	2.08	0.53
2:F:69:LYS:O	2:F:71:VAL:HG23	2.09	0.53
1:B:572:VAL:HG11	1:B:605:ILE:CD1	2.39	0.53
2:F:208:THR:HG21	2:F:263:SER:O	2.09	0.53
2:F:254:LYS:O	2:F:258:ASN:HB2	2.08	0.53
1:A:119:ASN:HD22	1:A:542:ILE:HD11	1.73	0.52
1:A:345:ILE:HG22	1:A:355:ILE:CD1	2.39	0.52
1:B:64:ARG:CB	2:E:92:LYS:HZ1	2.22	0.52
1:B:530:GLN:O	1:B:531:LYS:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ARG:CA	1:A:484:THR:HG21	2.33	0.52
2:E:195:VAL:HG13	2:E:225:VAL:HB	1.91	0.52
1:B:210:LYS:O	1:B:213:GLU:HG2	2.09	0.52
2:E:154:SER:HA	2:E:178:ALA:CB	2.38	0.52
3:S:578:GLU:CG	3:S:580:GLU:HG2	2.39	0.52
3:S:645:GLN:HE21	3:S:649:LYS:NZ	2.08	0.52
1:B:42:PHE:CD2	2:E:380:GLU:O	2.62	0.52
1:B:119:ASN:HD22	1:B:542:ILE:HD11	1.75	0.52
1:B:368:TYR:O	1:B:372:VAL:HG23	2.09	0.52
1:B:71:MET:HE2	2:E:123:SER:H	1.75	0.52
2:E:394:LYS:HB3	2:E:421:TRP:CH2	2.41	0.52
1:A:83:CYS:HB2	2:F:106:ARG:NH2	2.24	0.52
3:T:658:LEU:HA	3:T:661:VAL:CG1	2.40	0.52
1:B:458:ARG:HA	1:B:484:THR:CG2	2.30	0.52
2:F:356:MET:HE2	2:F:377:LEU:CD1	2.40	0.52
3:S:578:GLU:CD	3:S:579:MET:HE3	2.34	0.52
1:B:224:THR:O	1:B:228:LEU:HG	2.10	0.52
2:E:301:LEU:HA	2:E:360:GLN:HE22	1.75	0.52
2:F:253:SER:HB2	2:F:254:LYS:CE	2.39	0.52
1:B:371:ARG:HG2	1:B:371:ARG:HH11	1.74	0.52
2:F:80:GLN:HG3	2:F:104:SER:HB2	1.92	0.52
1:B:171:PHE:O	1:B:175:VAL:HG23	2.09	0.51
1:B:574:ALA:O	1:B:582:ARG:NH1	2.42	0.51
1:A:16:ARG:HB3	1:A:218:MET:HE3	1.92	0.51
1:B:547:GLU:HG3	1:B:551:ARG:HD2	1.93	0.51
3:S:659:HIS:CE1	3:S:663:MET:CE	2.91	0.51
1:B:509:LYS:HE2	1:B:533:GLU:OE2	2.10	0.51
1:B:224:THR:CG2	1:B:227:GLU:HG3	2.39	0.51
2:F:407:ASP:OD1	2:F:409:SER:HB3	2.11	0.51
3:T:596:THR:HG23	3:T:597:ILE:N	2.25	0.51
2:E:321:LYS:HE2	2:E:335:ASN:ND2	2.26	0.51
1:A:541:GLU:O	1:A:572:VAL:HA	2.11	0.51
1:B:531:LYS:HG2	1:B:532:ASN:ND2	2.26	0.51
2:E:104:SER:O	2:E:132:ASN:HA	2.10	0.51
2:E:330:LYS:N	2:E:330:LYS:CD	2.67	0.51
2:F:201:LEU:HD23	2:F:201:LEU:N	2.25	0.51
1:A:340:MET:HG3	1:A:344:LEU:HD12	1.93	0.51
1:A:572:VAL:HG11	1:A:605:ILE:CD1	2.40	0.51
3:S:617:TRP:CZ2	3:S:632:MET:HE1	2.45	0.51
2:E:356:MET:HE2	2:E:377:LEU:CD1	2.41	0.51
1:A:87:SER:CB	1:A:91:PHE:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:346:GLN:O	2:E:368:GLN:HG2	2.11	0.51
3:S:657:MET:O	3:S:661:VAL:HG12	2.11	0.51
3:T:607:ASN:HB3	3:T:609:GLY:H	1.76	0.51
2:F:92:LYS:NZ	2:F:92:LYS:HB2	2.25	0.50
2:F:164:ILE:HG22	2:F:164:ILE:O	2.10	0.50
3:S:682:ARG:HH11	3:S:682:ARG:CG	2.20	0.50
3:T:593:ARG:O	3:T:597:ILE:HG23	2.11	0.50
1:A:34:ARG:NH2	2:F:338:ILE:O	2.45	0.50
1:B:224:THR:HG23	1:B:227:GLU:H	1.76	0.50
1:A:350:ASP:O	1:A:352:PHE:CD2	2.64	0.50
1:B:572:VAL:HG11	1:B:605:ILE:HD12	1.93	0.50
1:B:291:PRO:HA	1:B:294:TYR:CZ	2.46	0.50
1:B:464:ASN:H	1:B:464:ASN:ND2	2.09	0.50
3:S:593:ARG:HA	3:S:622:MET:HE1	1.92	0.50
1:B:64:ARG:HG2	2:E:92:LYS:HZ1	1.77	0.50
1:B:168:ASP:HB3	1:B:235:LEU:HD11	1.94	0.50
2:E:82:LEU:HD13	2:E:101:THR:HG21	1.94	0.50
2:E:417:ASP:O	2:E:418:ALA:HB3	2.12	0.50
3:S:654:ARG:O	3:S:658:LEU:HD13	2.12	0.50
3:T:617:TRP:CZ2	3:T:663:MET:HE1	2.46	0.50
2:F:272:ASN:HA	3:T:577:GLN:CG	2.34	0.50
1:B:121:MET:HE1	1:B:570:PHE:CE2	2.47	0.50
2:E:82:LEU:HD13	2:E:101:THR:CG2	2.42	0.50
1:B:263:GLU:HG3	1:B:263:GLU:O	2.12	0.50
1:B:529:VAL:HG22	1:B:533:GLU:CD	2.36	0.50
2:E:253:SER:HB2	2:E:254:LYS:CE	2.42	0.50
3:S:610:GLU:O	3:S:614:MET:HG3	2.12	0.50
2:E:154:SER:HA	2:E:178:ALA:HB1	1.93	0.50
1:A:30:LYS:HD2	1:A:170:ILE:HD11	1.94	0.49
1:A:121:MET:HE3	1:A:542:ILE:HB	1.94	0.49
1:A:555:TYR:CE2	1:A:563:LEU:HD11	2.43	0.49
3:S:637:MET:HE3	3:S:637:MET:HA	1.93	0.49
3:S:660:LEU:HD12	3:S:660:LEU:H	1.77	0.49
3:S:596:THR:O	3:S:600:ILE:HG12	2.12	0.49
3:T:673:SER:C	3:T:675:ASP:H	2.21	0.49
1:B:178:LEU:HD13	1:B:211:ILE:HG23	1.93	0.49
2:E:74:LEU:O	2:E:419:SER:HA	2.12	0.49
2:F:71:VAL:HG12	2:F:116:GLY:CA	2.39	0.49
2:F:218:VAL:HG11	3:T:591:TRP:CE3	2.47	0.49
3:S:576:PRO:C	3:S:578:GLU:N	2.71	0.49
2:E:238:MET:HE3	2:E:305:ILE:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LYS:HG2	1:A:33:ARG:NH1	2.27	0.49
1:A:341:PHE:O	1:A:345:ILE:HG23	2.13	0.49
1:B:577:LYS:HE2	2:E:218:VAL:HG12	1.94	0.49
2:F:364:ALA:HA	2:F:373:TYR:O	2.12	0.49
1:A:567:ASN:HD21	1:A:570:PHE:H	1.61	0.49
3:S:637:MET:O	3:S:641:GLU:HG3	2.12	0.49
1:A:274:CYS:SG	1:A:276:ARG:HB2	2.52	0.49
1:A:353:CYS:O	1:A:356:ALA:HB3	2.12	0.49
1:A:554:VAL:HA	1:A:557:LYS:HE2	1.94	0.49
3:S:577:GLN:O	3:S:578:GLU:HB3	2.12	0.49
1:A:275:ARG:NH1	1:A:275:ARG:O	2.46	0.49
1:B:255:PRO:HG2	1:B:256:ASN:OD1	2.12	0.49
1:B:337:GLU:OE2	1:B:361:THR:OG1	2.31	0.49
2:E:71:VAL:O	2:E:72:ASN:HB2	2.12	0.49
3:S:660:LEU:HD12	3:S:660:LEU:N	2.28	0.49
1:A:275:ARG:HH22	3:T:629:ASP:CG	2.21	0.48
1:A:425:GLN:HE22	1:B:102:ASN:HB3	1.78	0.48
3:T:682:ARG:HG2	3:T:682:ARG:NH1	2.23	0.48
2:E:291:HIS:CE1	2:E:307:SER:OG	2.52	0.48
1:A:41:MET:CE	2:F:322:MET:SD	3.02	0.48
1:B:178:LEU:HD12	1:B:215:ILE:HD11	1.95	0.48
3:S:629:ASP:C	3:S:631:GLN:H	2.22	0.48
3:S:671:ILE:C	3:S:674:ILE:HG22	2.37	0.48
1:A:365:ARG:O	1:A:369:GLU:HG3	2.14	0.48
2:E:254:LYS:O	2:E:258:ASN:HB2	2.14	0.48
2:F:195:VAL:HG13	2:F:225:VAL:HB	1.95	0.48
1:A:122:VAL:HG22	1:A:543:ILE:HG22	1.96	0.48
1:B:22:GLU:O	1:B:26:LEU:HD23	2.13	0.48
2:F:407:ASP:O	2:F:408:SER:CB	2.61	0.48
1:A:586:HIS:CG	1:A:587:SER:N	2.82	0.48
2:F:321:LYS:HE2	2:F:335:ASN:HD21	1.77	0.48
3:T:640:VAL:O	3:T:641:GLU:C	2.56	0.48
2:E:301:LEU:HD13	2:E:356:MET:CE	2.44	0.48
2:E:306:LEU:HD13	2:E:363:LEU:CD1	2.43	0.48
3:S:617:TRP:HZ2	3:S:632:MET:CE	2.25	0.48
1:B:253:ASP:OD1	3:S:654:ARG:HB2	2.14	0.48
2:E:253:SER:HB2	2:E:254:LYS:NZ	2.29	0.48
2:F:381:ASP:HB3	2:F:382:PRO:HD2	1.96	0.48
3:T:655:ASN:HA	3:T:658:LEU:HD13	1.95	0.48
1:B:71:MET:CB	1:B:96:ILE:HD11	2.42	0.47
1:B:579:ASN:OD1	1:B:579:ASN:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:82:LEU:HD22	2:E:101:THR:HG22	1.95	0.47
2:E:121:LEU:O	2:E:122:GLN:HG2	2.14	0.47
2:F:363:LEU:HD23	2:F:364:ALA:N	2.29	0.47
1:A:32:PHE:C	1:A:34:ARG:H	2.22	0.47
1:A:101:LEU:HD22	2:F:168:CYS:HB2	1.96	0.47
2:F:97:LEU:HD12	2:F:410:ILE:HD12	1.96	0.47
1:B:64:ARG:HB3	2:E:92:LYS:HZ1	1.79	0.47
2:E:109:LEU:HD12	2:E:109:LEU:N	2.29	0.47
3:S:656:PHE:O	3:S:660:LEU:HD12	2.13	0.47
3:T:645:GLN:HE21	3:T:649:LYS:HZ3	1.60	0.47
3:T:661:VAL:HA	3:T:674:ILE:HD11	1.96	0.47
1:B:496:VAL:HG12	1:B:497:SER:N	2.27	0.47
1:A:16:ARG:CD	1:A:218:MET:HE3	2.39	0.47
1:A:574:ALA:O	1:A:582:ARG:NH1	2.43	0.47
1:B:584:ALA:O	1:B:623:TYR:OH	2.31	0.47
2:F:205:ASN:OD1	2:F:208:THR:HG22	2.14	0.47
2:F:285:PHE:CE2	2:F:319:PRO:HB3	2.50	0.47
3:S:664:HIS:CE1	3:S:671:ILE:HG12	2.50	0.47
1:B:18:ARG:HD3	1:B:181:LEU:HD23	1.97	0.47
1:B:26:LEU:O	1:B:30:LYS:HG3	2.15	0.47
1:B:273:PHE:HB2	1:B:280:TYR:CE1	2.50	0.47
1:A:556:ASP:O	1:A:559:MET:HE2	2.15	0.47
2:F:71:VAL:HG12	2:F:71:VAL:O	2.14	0.47
2:F:111:GLU:HB2	2:F:121:LEU:HD11	1.96	0.47
3:S:656:PHE:CZ	3:S:660:LEU:HD11	2.50	0.47
3:T:606:VAL:HG13	3:T:610:GLU:HG3	1.97	0.47
1:B:296:ARG:HD2	3:S:664:HIS:O	2.15	0.47
1:A:425:GLN:HE22	1:B:102:ASN:CB	2.27	0.46
1:B:359:ILE:O	1:B:359:ILE:HG22	2.15	0.46
2:F:195:VAL:CG1	2:F:225:VAL:HG12	2.45	0.46
3:S:607:ASN:HB3	3:S:609:GLY:H	1.80	0.46
1:A:58:GLN:O	1:A:62:GLN:HG2	2.15	0.46
1:A:70:ILE:CG1	1:A:71:MET:N	2.78	0.46
1:B:83:CYS:HB2	2:E:106:ARG:HH22	1.80	0.46
1:B:85:VAL:HG13	2:E:75:LYS:O	2.15	0.46
1:B:345:ILE:O	1:B:349:TYR:HA	2.16	0.46
1:B:567:ASN:HD21	1:B:570:PHE:H	1.60	0.46
2:E:218:VAL:HG11	3:S:591:TRP:CZ3	2.51	0.46
3:S:606:VAL:CG1	3:S:610:GLU:HG3	2.46	0.46
3:S:612:GLU:OE1	3:S:612:GLU:HA	2.15	0.46
1:A:180:GLN:O	1:A:184:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ILE:O	1:A:215:ILE:HG13	2.15	0.46
1:B:119:ASN:ND2	1:B:542:ILE:HD11	2.30	0.46
1:B:352:PHE:HA	1:B:355:ILE:HB	1.98	0.46
2:E:144:THR:HG22	2:E:146:HIS:NE2	2.29	0.46
2:F:198:ASP:O	2:F:199:HIS:CB	2.64	0.46
2:F:390:LEU:HB3	2:F:423:TRP:CH2	2.50	0.46
3:T:606:VAL:HG12	3:T:610:GLU:HG3	1.97	0.46
1:B:117:GLN:CD	1:B:508:LYS:NZ	2.74	0.46
2:F:181:GLU:HG3	2:F:182:LEU:H	1.80	0.46
1:A:9:GLU:O	1:A:10:LYS:HB2	2.15	0.46
1:A:46:ARG:HG3	1:A:46:ARG:HH11	1.79	0.46
1:A:262:ARG:HG3	1:A:263:GLU:N	2.26	0.46
1:A:348:TYR:O	1:A:349:TYR:HB2	2.16	0.46
1:B:541:GLU:OE1	1:B:551:ARG:NH2	2.49	0.46
2:E:395:CYS:HA	2:E:421:TRP:CZ2	2.50	0.46
2:F:392:HIS:HE1	2:F:394:LYS:HB2	1.76	0.46
2:E:321:LYS:HE2	2:E:335:ASN:HD21	1.80	0.46
2:E:395:CYS:HB2	2:E:421:TRP:CE2	2.51	0.46
2:F:254:LYS:H	2:F:254:LYS:CE	2.28	0.46
3:T:674:ILE:HG12	3:T:674:ILE:O	2.15	0.46
1:A:464:ASN:HD22	1:A:464:ASN:N	2.11	0.46
1:A:182:ASP:OD2	1:A:208:SER:HB2	2.15	0.46
1:A:558:TYR:O	1:A:560:CYS:HB2	2.15	0.46
1:B:262:ARG:HG3	1:B:263:GLU:N	2.31	0.46
3:S:575:ARG:CB	3:S:575:ARG:NH1	2.77	0.46
2:F:104:SER:O	2:F:132:ASN:HA	2.15	0.46
2:F:254:LYS:HE2	2:F:254:LYS:N	2.31	0.46
1:B:64:ARG:HG2	2:E:92:LYS:NZ	2.31	0.45
1:B:275:ARG:HH11	1:B:275:ARG:CG	2.29	0.45
2:F:250:ARG:NH2	2:F:326:ILE:O	2.47	0.45
1:A:32:PHE:C	1:A:34:ARG:N	2.73	0.45
2:E:240:CYS:HB2	2:E:295:VAL:HB	1.99	0.45
2:E:279:LYS:HD3	2:E:279:LYS:N	2.31	0.45
1:A:113:TRP:CD1	1:A:582:ARG:NH2	2.85	0.45
1:B:291:PRO:HA	1:B:294:TYR:CE2	2.51	0.45
1:B:361:THR:C	1:B:362:LYS:HG2	2.42	0.45
2:F:285:PHE:CZ	2:F:319:PRO:HB3	2.51	0.45
3:S:656:PHE:CE1	3:S:660:LEU:HD11	2.51	0.45
3:S:658:LEU:HA	3:S:661:VAL:CG1	2.47	0.45
3:T:680:LYS:O	3:T:684:MET:HE3	2.16	0.45
1:A:224:THR:CG2	1:A:227:GLU:HG3	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:THR:CG2	2:E:359:TRP:CE3	3.00	0.45
1:B:120:PHE:O	1:B:541:GLU:HA	2.16	0.45
2:E:118:ILE:HD11	2:E:422:ARG:HB2	1.98	0.45
2:E:208:THR:HG21	2:E:263:SER:O	2.17	0.45
3:T:584:GLU:C	3:T:586:GLU:H	2.25	0.45
1:B:541:GLU:O	1:B:572:VAL:HA	2.17	0.45
2:E:250:ARG:NH2	2:E:327:ASP:HA	2.32	0.45
2:E:407:ASP:O	2:E:408:SER:CB	2.65	0.45
3:T:654:ARG:O	3:T:657:MET:HB3	2.16	0.45
1:A:425:GLN:HE22	1:B:102:ASN:CG	2.24	0.45
1:A:461:ALA:O	1:A:462:GLN:HB2	2.17	0.45
1:B:41:MET:HE2	1:B:41:MET:HB2	1.76	0.45
1:B:341:PHE:O	1:B:345:ILE:HG23	2.16	0.45
2:E:254:LYS:H	2:E:254:LYS:HE2	1.81	0.45
2:E:330:LYS:H	2:E:330:LYS:CD	2.20	0.45
2:F:82:LEU:CD1	2:F:101:THR:HG21	2.45	0.45
2:F:426:LEU:HD13	2:F:426:LEU:C	2.41	0.45
3:S:675:ASP:OD1	3:S:676:LYS:N	2.50	0.45
3:T:628:ALA:HB3	3:T:631:GLN:HG3	1.98	0.45
1:A:30:LYS:HE2	1:A:170:ILE:CG1	2.35	0.45
1:A:46:ARG:HA	1:A:49:ILE:HG13	1.99	0.45
1:A:121:MET:HE1	1:A:570:PHE:CE2	2.51	0.45
1:A:260:VAL:HG12	1:A:261:GLN:N	2.31	0.45
1:A:361:THR:O	1:A:362:LYS:HG2	2.17	0.45
1:A:504:GLN:HA	1:A:604:ARG:NH2	2.31	0.45
1:B:177:ALA:HA	1:B:180:GLN:OE1	2.15	0.45
1:B:342:ARG:HA	1:B:345:ILE:HG12	1.98	0.45
2:E:227:SER:HB3	2:E:240:CYS:SG	2.57	0.45
3:S:593:ARG:O	3:S:597:ILE:HG23	2.17	0.45
3:T:659:HIS:CE1	3:T:663:MET:HE2	2.52	0.45
1:A:26:LEU:O	1:A:27:ARG:C	2.60	0.45
1:B:18:ARG:O	1:B:19:VAL:C	2.59	0.45
2:F:417:ASP:O	2:F:418:ALA:HB3	2.17	0.45
3:S:613:VAL:HG23	3:S:652:LEU:HD22	1.99	0.45
3:S:674:ILE:HG12	3:S:674:ILE:O	2.16	0.45
3:T:658:LEU:HD12	3:T:658:LEU:N	2.32	0.45
1:A:63:ARG:O	1:A:64:ARG:HD3	2.16	0.45
1:B:177:ALA:O	1:B:181:LEU:HD13	2.16	0.45
1:B:447:SER:C	1:B:449:GLU:N	2.75	0.45
1:B:461:ALA:O	1:B:462:GLN:HB2	2.16	0.45
2:E:181:GLU:HG3	2:E:182:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:198:ASP:O	2:E:199:HIS:CB	2.65	0.45
2:E:294:TYR:CD1	2:E:294:TYR:C	2.94	0.45
2:F:165:THR:HG22	2:F:165:THR:O	2.17	0.45
3:T:659:HIS:CE1	3:T:663:MET:CE	3.00	0.45
1:A:116:LEU:HG	1:A:118:GLN:O	2.17	0.44
1:B:538:TYR:OH	1:B:564:PHE:HE2	2.00	0.44
2:F:306:LEU:CD1	2:F:356:MET:HE3	2.46	0.44
1:B:166:ILE:HG23	1:B:166:ILE:O	2.17	0.44
1:B:436:ALA:O	1:B:437:GLN:HB3	2.18	0.44
3:S:634:HIS:O	3:S:638:LEU:HB2	2.17	0.44
1:A:258:LYS:HB2	1:A:260:VAL:CG2	2.47	0.44
1:B:87:SER:CB	1:B:91:PHE:HB2	2.47	0.44
2:F:201:LEU:HD22	2:F:225:VAL:HG11	1.98	0.44
1:B:106:SER:HB3	2:E:157:ILE:HD11	1.99	0.44
2:F:198:ASP:OD1	2:F:198:ASP:C	2.61	0.44
2:F:294:TYR:CD1	2:F:294:TYR:C	2.95	0.44
2:F:306:LEU:HD13	2:F:363:LEU:CD1	2.48	0.44
1:A:26:LEU:O	1:A:29:LEU:HB3	2.18	0.44
1:A:333:TRP:HB2	1:A:370:PHE:HE2	1.83	0.44
1:B:83:CYS:HB3	1:B:98:LEU:HG	2.00	0.44
1:B:93:LYS:C	1:B:93:LYS:HD2	2.43	0.44
2:E:366:GLY:HA3	2:E:399:ILE:HB	1.98	0.44
2:F:356:MET:HE2	2:F:377:LEU:HD13	2.00	0.44
1:A:10:LYS:NZ	1:A:18:ARG:CZ	2.81	0.44
1:A:46:ARG:HA	1:A:49:ILE:CG1	2.48	0.44
2:E:78:HIS:O	2:E:80:GLN:HG2	2.18	0.44
1:A:283:PHE:HE1	3:T:599:GLN:OE1	2.00	0.44
1:A:350:ASP:O	1:A:352:PHE:N	2.46	0.44
1:A:425:GLN:OE1	1:B:102:ASN:ND2	2.51	0.44
1:A:531:LYS:HE2	1:A:532:ASN:HD21	1.82	0.44
1:B:101:LEU:HD13	2:E:159:ARG:HD3	1.99	0.44
1:B:473:ALA:C	1:B:474:VAL:HG23	2.42	0.44
2:F:312:ASN:HA	2:F:344:TYR:CE1	2.51	0.44
3:S:645:GLN:HE21	3:S:649:LYS:HZ2	1.65	0.44
1:B:122:VAL:HG22	1:B:543:ILE:HG22	1.99	0.44
1:B:211:ILE:O	1:B:215:ILE:HG13	2.18	0.44
2:E:367:ASN:ND2	2:E:371:LYS:HB2	2.24	0.44
2:F:197:LYS:O	2:F:197:LYS:HG2	2.18	0.44
2:F:267:ASN:O	2:F:271:THR:HG22	2.17	0.44
1:A:70:ILE:HG12	1:A:71:MET:N	2.33	0.44
1:A:86:THR:CG2	1:A:87:SER:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:VAL:CG1	1:B:264:GLN:HE21	2.30	0.44
1:A:293:THR:HG22	1:A:445:GLN:CD	2.40	0.43
1:A:464:ASN:ND2	1:A:464:ASN:N	2.60	0.43
1:B:168:ASP:HB3	1:B:235:LEU:HD13	2.00	0.43
1:A:63:ARG:C	1:A:64:ARG:HD3	2.43	0.43
1:A:354:ALA:HA	1:A:357:ARG:HH12	1.83	0.43
1:A:425:GLN:NE2	1:B:102:ASN:HB3	2.34	0.43
1:B:283:PHE:CE2	3:S:592:LEU:HD22	2.53	0.43
2:E:344:TYR:HE1	2:E:347:CYS:HB3	1.82	0.43
1:A:124:ASP:HB3	1:A:550:ARG:HH21	1.83	0.43
1:B:258:LYS:HB2	1:B:260:VAL:CG2	2.47	0.43
1:B:266:LEU:HD11	1:B:343:VAL:HG13	2.00	0.43
3:S:593:ARG:HG2	3:S:622:MET:CE	2.48	0.43
1:A:351:ASN:OD1	1:A:353:CYS:HB2	2.19	0.43
1:B:290:THR:CG2	1:B:421:ASP:OD1	2.67	0.43
1:B:550:ARG:NH1	1:B:550:ARG:HG3	2.34	0.43
3:S:577:GLN:O	3:S:578:GLU:CB	2.67	0.43
1:B:348:TYR:O	1:B:349:TYR:HB2	2.18	0.43
2:E:201:LEU:CD2	2:E:225:VAL:HG11	2.49	0.43
2:F:243:ASP:O	2:F:244:HIS:HB2	2.18	0.43
2:F:304:LEU:HD22	2:F:339:LEU:HD11	2.00	0.43
2:F:323:GLU:H	2:F:323:GLU:CD	2.26	0.43
1:A:13:ILE:O	1:A:17:LYS:HG3	2.18	0.43
3:S:661:VAL:HA	3:S:674:ILE:HD11	2.00	0.43
3:S:687:LYS:HD2	3:S:687:LYS:O	2.19	0.43
1:B:546:ASP:O	1:B:549:ASP:HB2	2.18	0.43
2:E:156:GLY:HA2	2:E:179:ILE:HG13	1.99	0.43
2:E:395:CYS:HB2	2:E:421:TRP:CZ2	2.54	0.43
1:A:33:ARG:O	1:A:37:GLU:HG3	2.18	0.43
1:A:352:PHE:HA	1:A:355:ILE:HB	2.00	0.43
1:A:580:LYS:HG3	3:T:584:GLU:OE1	2.19	0.43
1:B:65:ILE:N	1:B:65:ILE:HD12	2.33	0.43
2:E:73:SER:C	2:E:74:LEU:HD12	2.43	0.43
2:E:243:ASP:O	2:E:244:HIS:HB2	2.17	0.43
2:F:254:LYS:HG2	2:F:255:ARG:N	2.33	0.43
3:S:575:ARG:NH1	3:S:575:ARG:HB2	2.34	0.43
3:S:616:LEU:HD12	3:S:616:LEU:HA	1.75	0.43
1:A:166:ILE:O	1:A:166:ILE:HG12	2.19	0.43
1:A:359:ILE:HG22	1:A:359:ILE:O	2.19	0.43
1:B:465:THR:C	1:B:467:GLN:H	2.26	0.43
2:F:390:LEU:N	2:F:390:LEU:HD22	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ASN:ND2	1:A:569:ASP:N	2.56	0.42
1:B:464:ASN:H	1:B:464:ASN:HD22	1.67	0.42
2:F:144:THR:HG22	2:F:146:HIS:NE2	2.33	0.42
3:S:656:PHE:O	3:S:660:LEU:CD1	2.67	0.42
3:T:656:PHE:CZ	3:T:660:LEU:HD11	2.54	0.42
1:A:57:ASN:O	1:A:61:LYS:HG2	2.19	0.42
1:A:262:ARG:CD	1:A:343:VAL:HA	2.47	0.42
1:A:345:ILE:O	1:A:349:TYR:N	2.51	0.42
1:B:476:GLU:CG	1:B:597:MET:HE3	2.49	0.42
1:A:22:GLU:OE1	1:A:25:ARG:NH1	2.53	0.42
2:E:141:ASP:OD1	2:E:141:ASP:C	2.61	0.42
2:E:319:PRO:CG	2:E:329:ILE:HD13	2.45	0.42
2:E:381:ASP:HB3	2:E:382:PRO:HD2	2.00	0.42
3:T:596:THR:CG2	3:T:597:ILE:N	2.82	0.42
3:T:682:ARG:CG	3:T:682:ARG:NH1	2.80	0.42
1:A:290:THR:HG23	1:A:291:PRO:HD2	2.00	0.42
1:B:598:MET:HE3	1:B:601:GLY:HA2	2.01	0.42
2:F:102:VAL:HG11	2:F:136:CYS:HB3	2.00	0.42
2:F:108:THR:C	2:F:109:LEU:HD12	2.44	0.42
2:F:344:TYR:CE1	2:F:347:CYS:HB3	2.53	0.42
3:T:607:ASN:CB	3:T:609:GLY:H	2.32	0.42
1:A:567:ASN:HD21	1:A:570:PHE:N	2.17	0.42
1:A:584:ALA:O	1:A:623:TYR:OH	2.36	0.42
2:E:392:HIS:HE1	2:E:394:LYS:HB2	1.76	0.42
2:F:175:HIS:CE1	2:F:194:SER:OG	2.63	0.42
2:F:352:MET:HE3	2:F:352:MET:HB3	1.72	0.42
3:S:577:GLN:OE1	3:S:577:GLN:N	2.52	0.42
3:T:572:LEU:HD12	3:T:572:LEU:HA	1.68	0.42
1:B:89:LEU:HD22	2:E:72:ASN:CA	2.48	0.42
2:E:97:LEU:CD1	2:E:410:ILE:HD12	2.48	0.42
2:F:294:TYR:CE1	2:F:350:TRP:CB	3.03	0.42
2:F:366:GLY:HA3	2:F:399:ILE:HB	2.01	0.42
1:B:295:LYS:HE3	1:B:295:LYS:HB2	1.78	0.42
2:E:381:ASP:HB3	2:E:383:HIS:ND1	2.33	0.42
3:S:575:ARG:HH11	3:S:575:ARG:HB2	1.83	0.42
3:T:570:THR:C	3:T:572:LEU:H	2.27	0.42
3:T:654:ARG:O	3:T:658:LEU:CD1	2.68	0.42
1:A:113:TRP:CG	1:A:582:ARG:NH2	2.88	0.42
1:B:124:ASP:HB3	1:B:550:ARG:NH2	2.34	0.42
1:B:253:ASP:OD2	3:S:652:LEU:HA	2.20	0.42
1:B:275:ARG:NH1	1:B:275:ARG:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:ASN:HD21	1:B:570:PHE:N	2.18	0.42
2:E:185:HIS:HB2	2:E:191:LEU:HB2	2.02	0.42
2:E:205:ASN:OD1	2:E:208:THR:HG22	2.20	0.42
2:E:352:MET:HE3	2:E:352:MET:HB3	1.74	0.42
1:A:117:GLN:CD	1:A:508:LYS:HZ3	2.28	0.42
1:A:221:ASP:C	1:A:223:GLY:H	2.28	0.42
1:A:496:VAL:CG1	1:A:497:SER:N	2.83	0.42
1:A:512:LEU:HB3	3:T:565:TYR:CD1	2.54	0.42
1:B:55:ILE:HD13	1:B:55:ILE:N	2.33	0.42
2:F:363:LEU:HB2	2:F:377:LEU:HD11	2.02	0.42
3:S:625:GLY:O	3:S:627:ILE:HG23	2.20	0.42
3:T:577:GLN:OE1	3:T:577:GLN:N	2.53	0.42
3:T:675:ASP:OD1	3:T:676:LYS:N	2.52	0.42
1:A:68:VAL:HG11	2:F:109:LEU:HD23	2.02	0.42
1:B:99:LYS:O	2:E:124:TYR:HA	2.19	0.42
1:B:186:GLU:O	1:B:187:LYS:CG	2.67	0.42
2:E:195:VAL:HG13	2:E:225:VAL:CB	2.50	0.42
2:E:341:ARG:O	2:E:382:PRO:HB2	2.20	0.42
2:F:400:ARG:HA	2:F:400:ARG:HD3	1.85	0.42
1:A:41:MET:HE1	2:F:322:MET:SD	2.60	0.41
1:B:274:CYS:SG	1:B:276:ARG:HB2	2.60	0.41
1:B:417:TYR:CB	1:B:598:MET:HE1	2.49	0.41
2:E:73:SER:HB2	2:E:421:TRP:CE3	2.55	0.41
2:E:407:ASP:OD1	2:E:409:SER:HB3	2.20	0.41
3:S:645:GLN:CG	3:S:649:LYS:HZ2	2.33	0.41
3:T:658:LEU:HD12	3:T:658:LEU:H	1.85	0.41
1:A:529:VAL:HG11	1:A:609:ALA:HB2	2.03	0.41
2:E:319:PRO:O	2:E:329:ILE:HD11	2.20	0.41
3:S:600:ILE:O	3:S:611:LYS:HD2	2.19	0.41
3:T:567:HIS:HD2	3:T:583:ASP:OD1	2.03	0.41
1:A:290:THR:CG2	1:A:421:ASP:OD1	2.67	0.41
1:B:464:ASN:HD22	1:B:464:ASN:C	2.27	0.41
1:B:478:ASP:C	1:B:480:ASP:H	2.28	0.41
1:A:357:ARG:HH11	1:A:357:ARG:HB3	1.84	0.41
2:F:319:PRO:O	2:F:329:ILE:HD11	2.20	0.41
2:F:374:VAL:HG23	2:F:390:LEU:HD23	2.01	0.41
1:B:586:HIS:CG	1:B:587:SER:N	2.87	0.41
2:E:147:PRO:O	2:E:148:LEU:HD23	2.21	0.41
3:S:645:GLN:HG2	3:S:649:LYS:NZ	2.35	0.41
3:S:659:HIS:NE2	3:S:663:MET:HE1	2.35	0.41
3:T:593:ARG:HG2	3:T:622:MET:HE1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ASP:O	1:B:185:ASP:HB2	2.20	0.41
1:B:353:CYS:O	1:B:356:ALA:HB3	2.20	0.41
2:F:238:MET:HE3	2:F:305:ILE:HG12	2.02	0.41
2:F:362:MET:HE3	2:F:362:MET:HB3	1.71	0.41
1:A:358:LEU:HD21	3:T:675:ASP:HB3	2.02	0.41
1:A:618:GLU:HG2	1:A:620:PHE:CE2	2.55	0.41
1:B:465:THR:C	1:B:467:GLN:N	2.78	0.41
2:E:193:LEU:CD2	2:E:237:ILE:HD13	2.49	0.41
2:F:74:LEU:O	2:F:419:SER:HA	2.20	0.41
2:F:195:VAL:CG1	2:F:225:VAL:CG1	2.99	0.41
1:A:47:GLN:O	1:A:51:GLU:HB2	2.20	0.41
1:A:101:LEU:HD13	2:F:159:ARG:HD3	2.01	0.41
1:A:114:SER:HA	1:A:115:PRO:HD3	1.84	0.41
1:B:64:ARG:CG	2:E:92:LYS:HZ1	2.32	0.41
1:B:113:TRP:CD1	1:B:582:ARG:NH2	2.89	0.41
1:B:295:LYS:NZ	1:B:295:LYS:HB3	2.35	0.41
1:B:499:LYS:HA	1:B:499:LYS:HD3	1.90	0.41
1:A:11:GLY:HA2	1:A:12:PRO:HD3	1.90	0.41
1:A:46:ARG:HG3	1:A:46:ARG:NH1	2.36	0.41
1:A:88:ASP:C	1:A:89:LEU:HD12	2.46	0.41
1:A:88:ASP:O	1:A:89:LEU:HD12	2.21	0.41
1:A:253:ASP:OD1	3:T:654:ARG:HD2	2.20	0.41
1:A:514:ALA:HB3	1:A:524:PHE:CE2	2.56	0.41
1:A:581:ILE:HD12	1:A:581:ILE:HA	1.88	0.41
1:B:464:ASN:HD22	1:B:465:THR:HG23	1.86	0.41
2:E:72:ASN:OD1	2:E:73:SER:N	2.54	0.41
2:E:97:LEU:HD12	2:E:410:ILE:CD1	2.48	0.41
2:E:103:GLY:O	2:E:104:SER:C	2.64	0.41
2:E:144:THR:O	2:E:145:SER:HB2	2.20	0.41
2:E:198:ASP:OD1	2:E:198:ASP:C	2.62	0.41
2:E:306:LEU:CD1	2:E:356:MET:HE3	2.51	0.41
3:T:562:ASN:O	3:T:562:ASN:CG	2.64	0.41
3:T:634:HIS:O	3:T:638:LEU:HB2	2.21	0.41
3:T:638:LEU:HD23	3:T:638:LEU:HA	1.91	0.41
1:A:466:LYS:HB2	1:A:472:LEU:HD13	2.02	0.41
1:A:499:LYS:HA	1:A:499:LYS:HD3	1.86	0.41
1:B:64:ARG:HA	2:E:92:LYS:HZ3	1.85	0.41
1:B:512:LEU:HB3	3:S:565:TYR:CD1	2.56	0.41
2:E:182:LEU:HG	2:E:192:LEU:HD11	2.03	0.41
2:E:294:TYR:CD1	2:E:294:TYR:O	2.74	0.41
2:F:185:HIS:HA	2:F:186:PRO:HD3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:325:ASP:O	2:F:326:ILE:C	2.64	0.41
3:T:576:PRO:C	3:T:578:GLU:N	2.79	0.41
1:A:98:LEU:HD23	2:F:123:SER:O	2.20	0.40
1:B:260:VAL:O	1:B:342:ARG:HD3	2.21	0.40
2:E:201:LEU:HD11	2:E:239:SER:HB3	2.03	0.40
2:F:319:PRO:HG2	2:F:329:ILE:CD1	2.50	0.40
3:T:579:MET:HE2	3:T:579:MET:HB3	1.92	0.40
1:A:71:MET:HG2	2:F:166:MET:SD	2.61	0.40
1:A:183:ARG:C	1:A:185:ASP:N	2.79	0.40
1:A:462:GLN:O	1:A:463:CYS:HB2	2.21	0.40
2:E:92:LYS:NZ	2:E:92:LYS:HB2	2.36	0.40
2:E:390:LEU:HD12	2:E:423:TRP:CZ3	2.56	0.40
2:F:254:LYS:HE2	2:F:254:LYS:H	1.86	0.40
3:S:658:LEU:O	3:S:661:VAL:HG13	2.21	0.40
1:A:249:THR:O	1:A:249:THR:HG23	2.20	0.40
1:A:446:CYS:O	1:A:447:SER:C	2.65	0.40
1:B:71:MET:HB3	1:B:96:ILE:CD1	2.47	0.40
2:F:114:SER:C	2:F:116:GLY:H	2.30	0.40
2:F:141:ASP:OD1	2:F:141:ASP:C	2.65	0.40
2:F:294:TYR:CE1	2:F:350:TRP:HB3	2.56	0.40
3:T:673:SER:C	3:T:675:ASP:N	2.80	0.40
1:A:53:THR:HG21	2:F:359:TRP:CE3	2.57	0.40
1:B:441:GLU:C	1:B:443:PHE:H	2.28	0.40
2:E:74:LEU:HD13	2:E:118:ILE:HD12	2.04	0.40
2:E:98:VAL:HG13	2:E:110:TYR:O	2.21	0.40
2:E:165:THR:C	2:E:166:MET:HG2	2.46	0.40
1:A:295:LYS:HE3	1:A:295:LYS:HB2	1.75	0.40
1:A:509:LYS:CE	1:A:533:GLU:OE2	2.68	0.40
1:B:249:THR:O	1:B:249:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/643 (70%)	396 (88%)	43 (10%)	10 (2%)	5	17
1	B	451/643 (70%)	408 (90%)	36 (8%)	7 (2%)	7	24
2	E	356/362 (98%)	335 (94%)	20 (6%)	1 (0%)	36	64
2	F	357/362 (99%)	335 (94%)	20 (6%)	2 (1%)	21	48
3	S	126/191 (66%)	109 (86%)	12 (10%)	5 (4%)	2	7
3	T	126/191 (66%)	108 (86%)	13 (10%)	5 (4%)	2	7
All	All	1865/2392 (78%)	1691 (91%)	144 (8%)	30 (2%)	7	24

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S	605	ASP
3	S	607	ASN
3	T	578	GLU
3	T	605	ASP
1	A	10	LYS
1	A	251	ASN
3	S	578	GLU
3	T	562	ASN
3	T	607	ASN
1	A	208	SER
1	A	250	PRO
1	A	349	TYR
1	A	351	ASN
1	A	560	CYS
1	B	208	SER
1	B	250	PRO
1	B	251	ASN
1	B	462	GLN
3	S	577	GLN
3	S	630	ASN
3	T	580	GLU
1	A	459	CYS
1	A	462	GLN
1	B	560	CYS
2	F	285	PHE
1	A	167	ASN
2	E	199	HIS
2	F	199	HIS
1	B	497	SER
1	B	518	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	418/560 (75%)	383 (92%)	35 (8%)	10	30
1	B	420/560 (75%)	388 (92%)	32 (8%)	12	35
2	E	321/325 (99%)	303 (94%)	18 (6%)	19	48
2	F	322/325 (99%)	307 (95%)	15 (5%)	23	55
3	S	122/175 (70%)	107 (88%)	15 (12%)	4	15
3	T	122/175 (70%)	113 (93%)	9 (7%)	13	36
All	All	1725/2120 (81%)	1601 (93%)	124 (7%)	13	37

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	28	GLN
1	A	33	ARG
1	A	34	ARG
1	A	36	ASP
1	A	39	LYS
1	A	42	PHE
1	A	51	GLU
1	A	61	LYS
1	A	64	ARG
1	A	90	ASP
1	A	93	LYS
1	A	96	ILE
1	A	98	LEU
1	A	109	ILE
1	A	117	GLN
1	A	121	MET
1	A	166	ILE
1	A	252	ILE
1	A	261	GLN
1	A	262	ARG
1	A	272	LEU

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Mol	Chain	Res	Type
1	A	275	ARG
1	A	295	LYS
1	A	422	HIS
1	A	425	GLN
1	A	460	LYS
1	A	464	ASN
1	A	484	THR
1	A	529	VAL
1	A	551	ARG
1	A	561	SER
1	A	567	ASN
1	A	597	MET
1	A	604	ARG
1	B	9	GLU
1	B	13	ILE
1	B	25	ARG
1	B	51	GLU
1	B	55	ILE
1	B	62	GLN
1	B	88	ASP
1	B	90	ASP
1	B	93	LYS
1	B	96	ILE
1	B	98	LEU
1	B	116	LEU
1	B	117	GLN
1	B	121	MET
1	B	123	GLU
1	B	262	ARG
1	B	272	LEU
1	B	275	ARG
1	B	295	LYS
1	B	422	HIS
1	B	460	LYS
1	B	464	ASN
1	B	468	CYS
1	B	474	VAL
1	B	484	THR
1	B	529	VAL
1	B	542	ILE
1	B	551	ARG
1	B	567	ASN

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Mol	Chain	Res	Type
1	B	597	MET
1	B	604	ARG
1	B	614	GLN
2	E	75	LYS
2	E	181	GLU
2	E	182	LEU
2	E	201	LEU
2	E	218	VAL
2	E	254	LYS
2	E	255	ARG
2	E	258	ASN
2	E	299	ARG
2	E	328	LYS
2	E	330	LYS
2	E	348	ASP
2	E	357	ASP
2	E	362	MET
2	E	384	LYS
2	E	388	THR
2	E	394	LYS
2	E	425	ARG
2	F	75	LYS
2	F	182	LEU
2	F	201	LEU
2	F	218	VAL
2	F	250	ARG
2	F	254	LYS
2	F	255	ARG
2	F	258	ASN
2	F	330	LYS
2	F	348	ASP
2	F	362	MET
2	F	384	LYS
2	F	388	THR
2	F	394	LYS
2	F	426	LEU
3	S	561	HIS
3	S	572	LEU
3	S	574	LEU
3	S	575	ARG
3	S	577	GLN
3	S	579	MET

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Mol	Chain	Res	Type
3	S	583	ASP
3	S	584	GLU
3	S	586	GLU
3	S	590	GLU
3	S	597	ILE
3	S	616	LEU
3	S	638	LEU
3	S	661	VAL
3	S	671	ILE
3	T	572	LEU
3	T	579	MET
3	T	583	ASP
3	T	590	GLU
3	T	597	ILE
3	T	616	LEU
3	T	638	LEU
3	T	661	VAL
3	T	671	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	94	GLN
1	A	117	GLN
1	A	264	GLN
1	A	366	GLN
1	A	416	ASN
1	A	422	HIS
1	A	425	GLN
1	A	429	ASN
1	A	445	GLN
1	A	464	ASN
1	A	504	GLN
1	A	532	ASN
1	A	545	GLN
1	A	567	ASN
1	A	603	HIS
1	B	43	ASN
1	B	47	GLN
1	B	50	GLN
1	B	57	ASN

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Mol	Chain	Res	Type
1	B	58	GLN
1	B	62	GLN
1	B	66	GLN
1	B	94	GLN
1	B	102	ASN
1	B	180	GLN
1	B	264	GLN
1	B	366	GLN
1	B	418	GLN
1	B	422	HIS
1	B	429	ASN
1	B	464	ASN
1	B	500	ASN
1	B	504	GLN
1	B	530	GLN
1	B	532	ASN
1	B	545	GLN
1	B	567	ASN
1	B	568	ASN
1	B	600	ASN
1	B	603	HIS
2	E	86	GLN
2	E	175	HIS
2	E	269	ASN
2	E	291	HIS
2	E	346	GLN
2	E	360	GLN
2	E	367	ASN
2	F	86	GLN
2	F	90	HIS
2	F	175	HIS
2	F	269	ASN
2	F	291	HIS
2	F	335	ASN
2	F	346	GLN
2	F	360	GLN
2	F	367	ASN
3	S	562	ASN
3	S	567	HIS
3	S	630	ASN
3	S	631	GLN
3	S	634	HIS

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Mol	Chain	Res	Type
3	S	642	ASN
3	S	645	GLN
3	S	659	HIS
3	S	664	HIS
3	T	631	GLN
3	T	645	GLN
3	T	659	HIS
3	T	664	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
5	CJD	B	708	-	32,34,34	1.74	9 (28%)	32,50,50	1.33	6 (18%)
5	CJD	A	708	-	32,34,34	1.71	8 (25%)	32,50,50	1.27	4 (12%)

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
5	CJD	B	708	-	-	1/14/35/35	0/4/4/4
5	CJD	A	708	-	-	2/14/35/35	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	708	CJD	C18-C13	4.73	1.52	1.44
5	B	708	CJD	C18-C13	4.14	1.51	1.44
5	A	708	CJD	C6-C1	3.36	1.43	1.40
5	B	708	CJD	O21-C14	3.23	1.42	1.36
5	B	708	CJD	C2-C1	3.20	1.44	1.39
5	A	708	CJD	C2-C1	3.00	1.44	1.39
5	B	708	CJD	C2-C3	2.92	1.43	1.38
5	A	708	CJD	C5-C4	2.87	1.45	1.40
5	A	708	CJD	O21-C14	2.80	1.41	1.36
5	B	708	CJD	C6-C1	2.79	1.43	1.40
5	B	708	CJD	C5-C6	2.68	1.45	1.39
5	B	708	CJD	C3-C4	2.57	1.43	1.39
5	A	708	CJD	C15-C14	2.54	1.49	1.41
5	B	708	CJD	C5-C4	2.48	1.45	1.40
5	B	708	CJD	C15-C14	2.34	1.48	1.41
5	A	708	CJD	C5-C8	2.26	1.52	1.47
5	A	708	CJD	C5-C6	2.01	1.44	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	708	CJD	C11-C10-N9	3.17	113.30	110.03
5	A	708	CJD	C5-C6-C1	-3.00	120.13	123.01
5	B	708	CJD	C5-C6-C1	-2.99	120.14	123.01
5	A	708	CJD	C11-C10-N9	2.86	112.97	110.03
5	A	708	CJD	O19-C18-C13	-2.32	121.70	124.56
5	B	708	CJD	O19-C18-C13	-2.24	121.80	124.56
5	B	708	CJD	O23-C8-C5	-2.23	119.58	124.19
5	B	708	CJD	C29-C26-C27	-2.14	85.21	99.39
5	A	708	CJD	C29-C26-C27	-2.11	85.39	99.39
5	B	708	CJD	C2-C3-C4	-2.07	119.86	123.16

There are no chirality outliers.

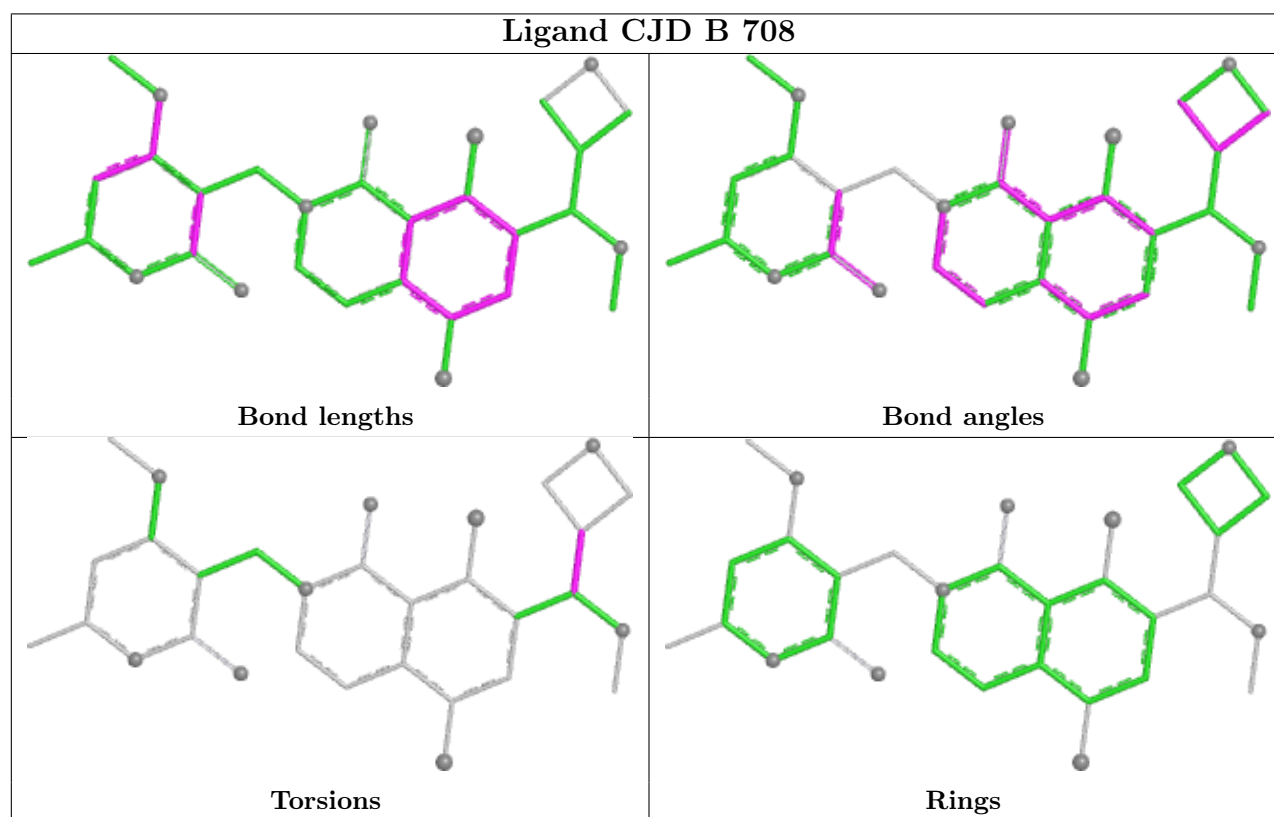
All (3) torsion outliers are listed below:

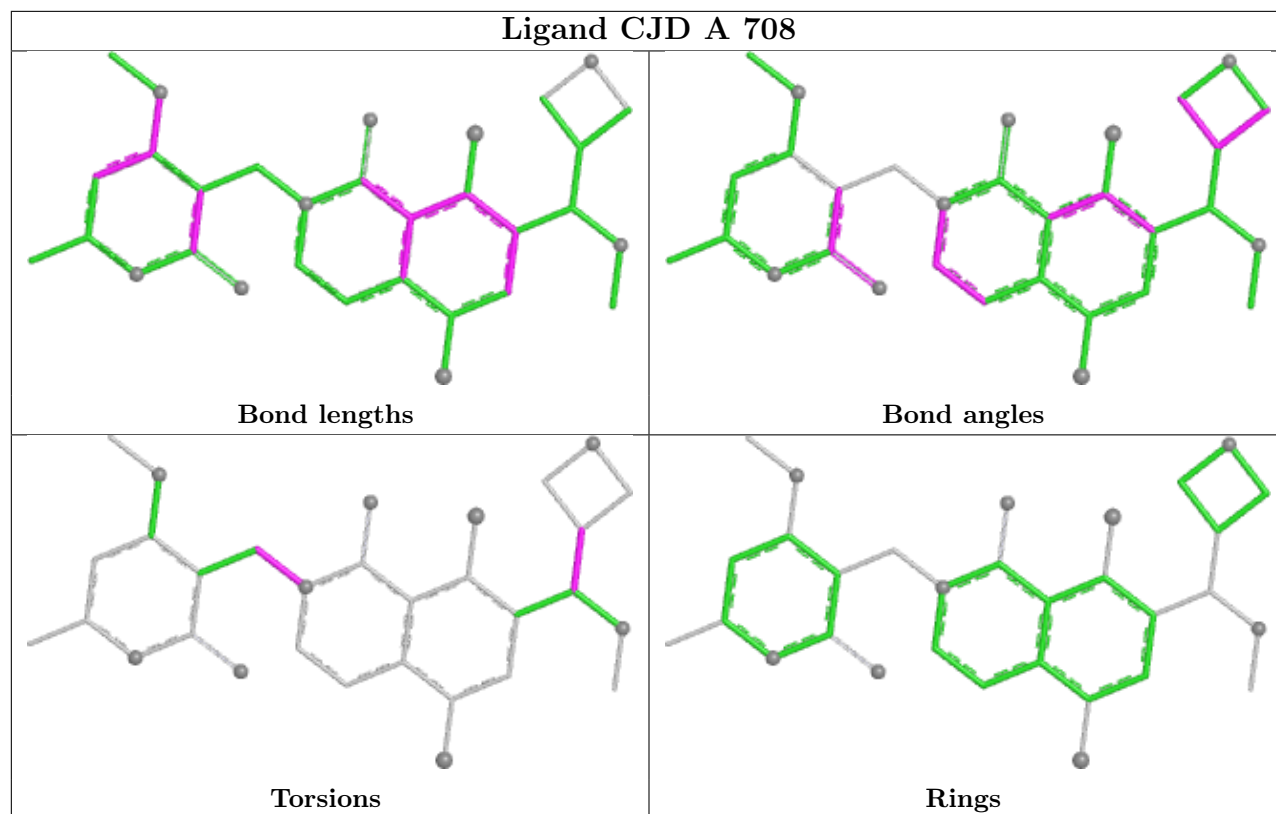
Mol	Chain	Res	Type	Atoms
5	A	708	CJD	C1-C25-C26-C29
5	B	708	CJD	C1-C25-C26-C29
5	A	708	CJD	C13-C12-N9-C8

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	463/643 (72%)	0.04	4 (0%) 81 74	43, 74, 104, 121	0
1	B	465/643 (72%)	0.07	8 (1%) 69 60	42, 74, 106, 121	0
2	E	358/362 (98%)	-0.15	2 (0%) 85 80	42, 63, 87, 122	0
2	F	359/362 (99%)	-0.20	0 100 100	45, 64, 87, 122	0
3	S	128/191 (67%)	0.10	0 100 100	51, 79, 114, 120	0
3	T	128/191 (67%)	0.19	2 (1%) 70 61	47, 76, 113, 124	0
All	All	1901/2392 (79%)	-0.02	16 (0%) 82 75	42, 69, 104, 124	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	PRO	4.0
1	A	630	ALA	3.1
1	B	630	ALA	2.9
1	B	207	PRO	2.9
3	T	653	CYS	2.6
3	T	688	LEU	2.5
1	B	250	PRO	2.4
1	B	249	THR	2.4
2	E	383	HIS	2.4
1	B	289	ALA	2.4
1	A	249	THR	2.3
1	A	364	CYS	2.3
1	B	293	THR	2.2
2	E	143	ASN	2.1
1	B	368	TYR	2.1
1	B	367	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

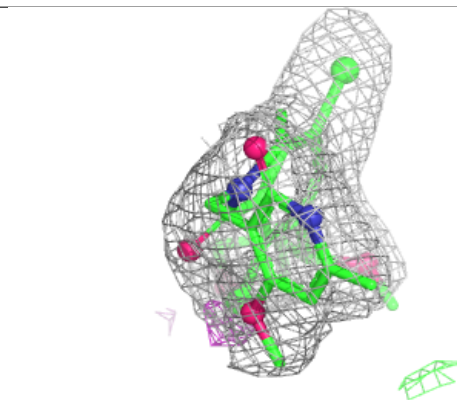
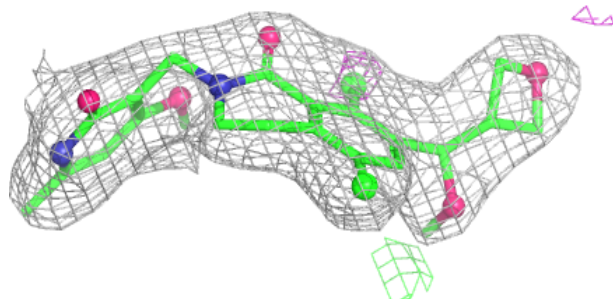
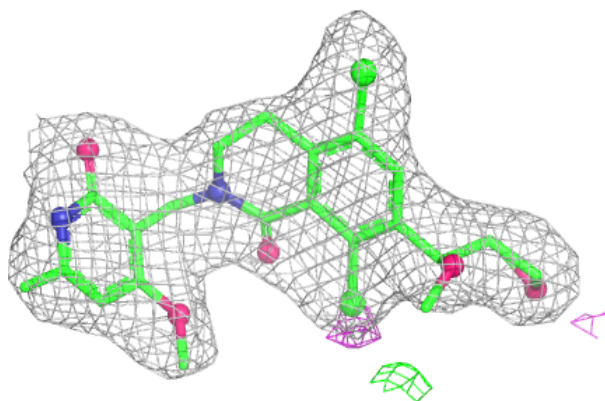
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CJD	B	708	31/31	0.94	0.09	42,56,63,66	0
5	CJD	A	708	31/31	0.95	0.08	43,53,61,65	0
4	ZN	B	705	1/1	0.98	0.06	79,79,79,79	1
4	ZN	B	701	1/1	0.98	0.08	78,78,78,78	1
4	ZN	B	702	1/1	0.98	0.04	71,71,71,71	1
4	ZN	A	706	1/1	0.99	0.03	58,58,58,58	1
4	ZN	A	707	1/1	0.99	0.03	63,63,63,63	1
4	ZN	A	701	1/1	0.99	0.04	75,75,75,75	1
4	ZN	A	702	1/1	0.99	0.04	65,65,65,65	1
4	ZN	B	703	1/1	0.99	0.06	72,72,72,72	1
4	ZN	B	704	1/1	0.99	0.04	54,54,54,54	1
4	ZN	A	703	1/1	0.99	0.03	77,77,77,77	1
4	ZN	B	706	1/1	0.99	0.06	72,72,72,72	1
4	ZN	A	704	1/1	0.99	0.04	74,74,74,74	1
4	ZN	A	705	1/1	0.99	0.07	65,65,65,65	1
4	ZN	B	707	1/1	1.00	0.04	60,60,60,60	1

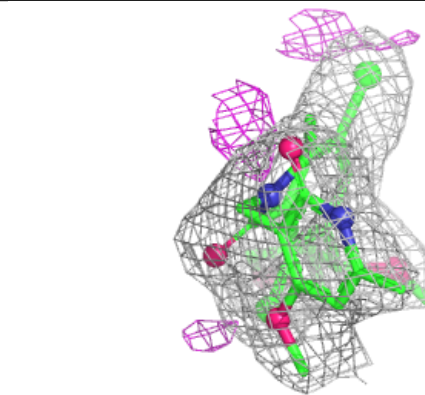
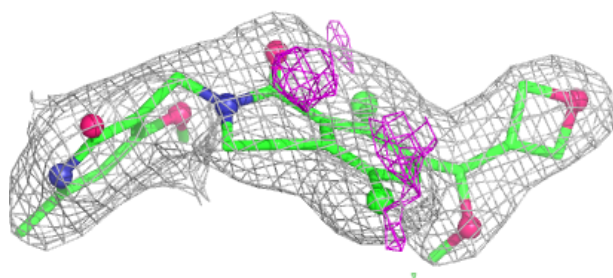
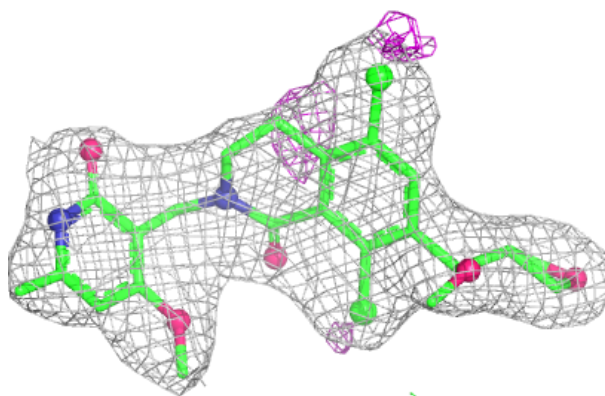
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CJD B 708:

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

**Electron density around CJD A 708:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.