



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:37 PM UTC

PDB ID : 8F6S / pdb_00008f6s
Title : LSD1-CoREST in complex with T105
Authors : Caroli, J.; Mattevi, A.
Deposited on : 2022-11-17
Resolution : 2.91 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

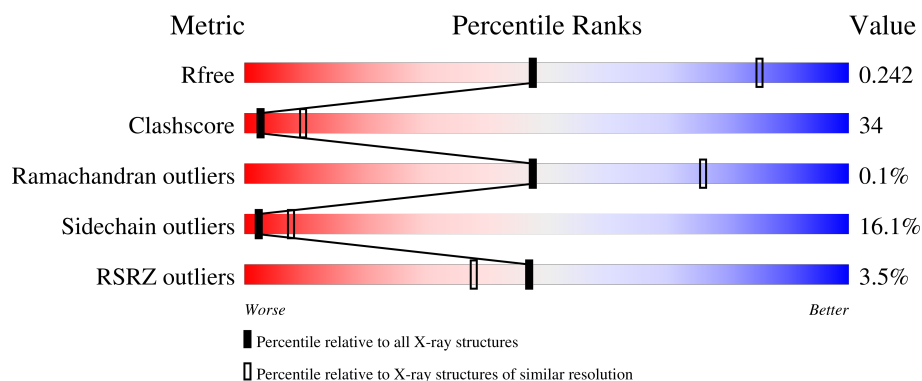
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	871	2% 44% 25% 6% 24%
2	B	144	10% 42% 34% 15% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6381 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 Lysine-specific histone demethylase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	665	5210	3319	905	966	20	0	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP O60341
A	-17	SER	-	expression tag	UNP O60341
A	-16	SER	-	expression tag	UNP O60341
A	-15	HIS	-	expression tag	UNP O60341
A	-14	HIS	-	expression tag	UNP O60341
A	-13	HIS	-	expression tag	UNP O60341
A	-12	HIS	-	expression tag	UNP O60341
A	-11	HIS	-	expression tag	UNP O60341
A	-10	HIS	-	expression tag	UNP O60341
A	-9	SER	-	expression tag	UNP O60341
A	-8	SER	-	expression tag	UNP O60341
A	-7	GLY	-	expression tag	UNP O60341
A	-6	LEU	-	expression tag	UNP O60341
A	-5	VAL	-	expression tag	UNP O60341
A	-4	PRO	-	expression tag	UNP O60341
A	-3	ARG	-	expression tag	UNP O60341
A	-2	GLY	-	expression tag	UNP O60341
A	-1	SER	-	expression tag	UNP O60341
A	0	HIS	-	expression tag	UNP O60341

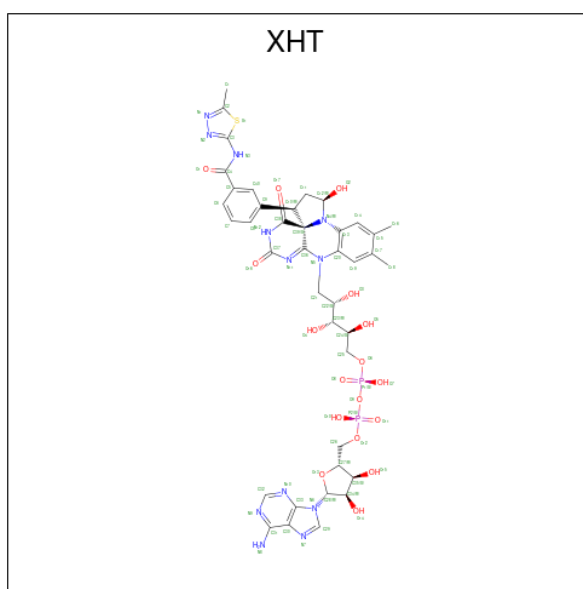
- Molecule 2 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	133	1076	676	194	203	3	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

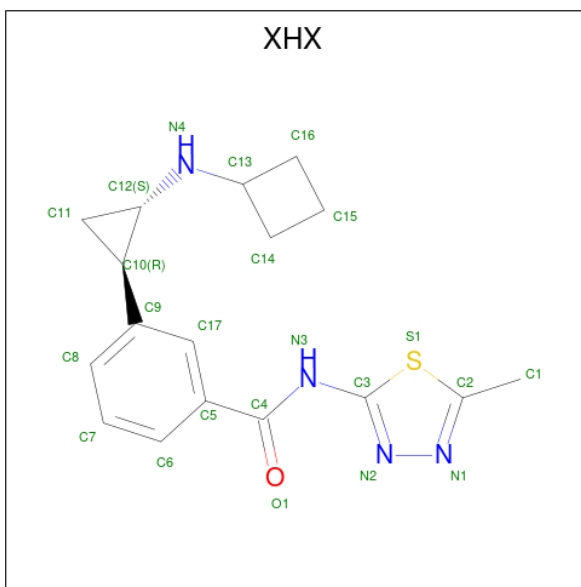
Chain	Residue	Modelled	Actual	Comment	Reference
B	297	GLY	-	expression tag	UNP Q9UKL0
B	298	PRO	-	expression tag	UNP Q9UKL0
B	299	LEU	-	expression tag	UNP Q9UKL0
B	300	GLY	-	expression tag	UNP Q9UKL0
B	301	SER	-	expression tag	UNP Q9UKL0
B	302	PRO	-	expression tag	UNP Q9UKL0
B	303	GLU	-	expression tag	UNP Q9UKL0
B	304	PHE	-	expression tag	UNP Q9UKL0

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methyl (2S,3R,4S)-2,3,4-trihydroxy-5-[(1R,3R,3aS,13R)-1-hydroxy-10,11-dimethyl-3-{3-[(5-methyl-1,3,4-thiadiazol-2-yl)carbamoyl]phenyl}-4,6-dioxo-2,3,5,6-tetrahydro-1H-benzo[g]pyrrolo[2,1-e]pteridin-8(4H)-yl]pentyl dihydrogen diphosphate (non-preferred name) (CCD ID: XHT) (formula: C₄₀H₄₆N₁₂O₁₇P₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	S	0	0
			72	40	12	17	2	1		

- Molecule 4 is 3-[(1R,2S)-2-(cyclobutylamino)cyclopropyl]-N-(5-methyl-1,3,4-thiadiazol-2-yl)benzamide (CCD ID: XHX) (formula: C₁₇H₂₀N₄OS) (labeled as "Ligand of Interest" by depositor).

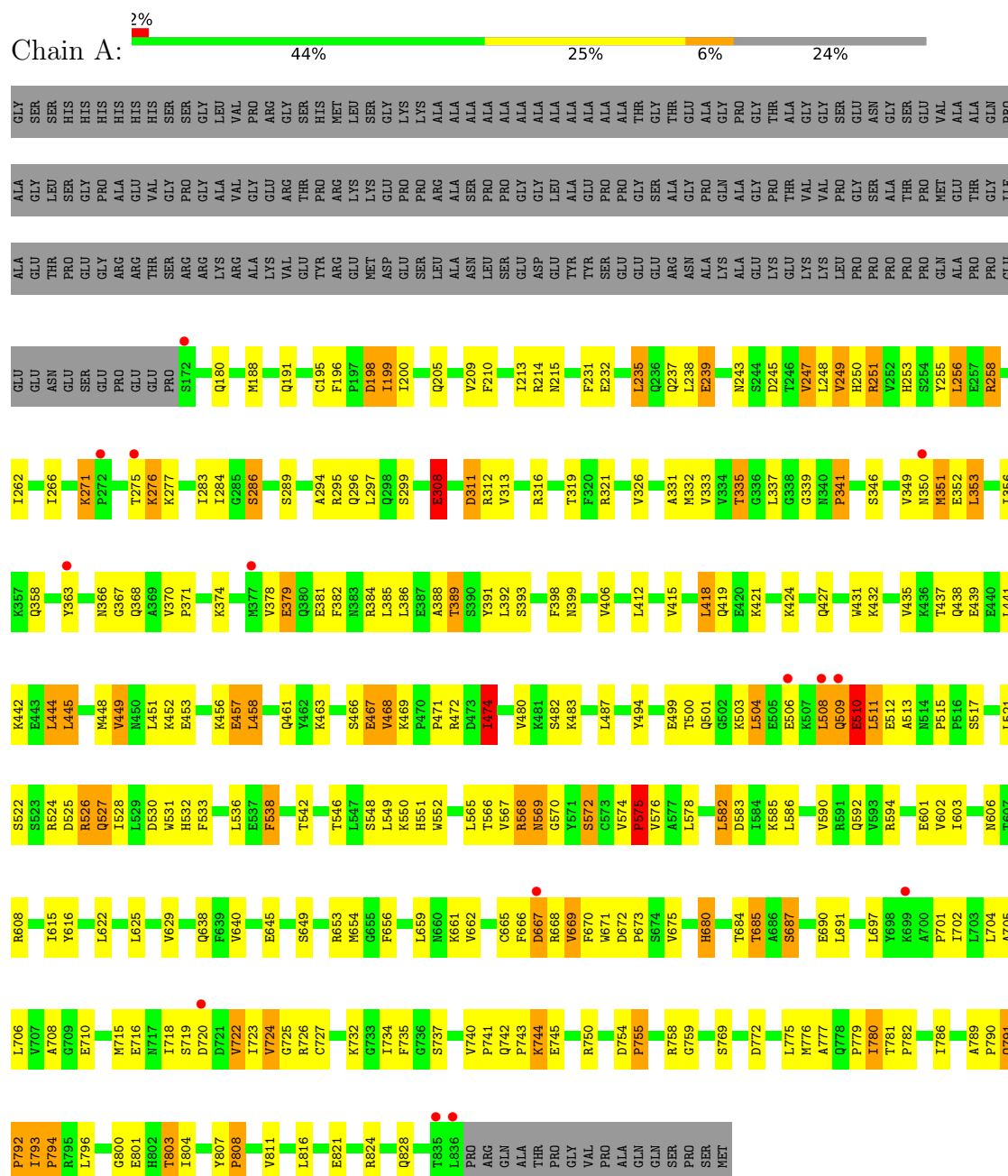


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	23	17	4	1	1	0	0

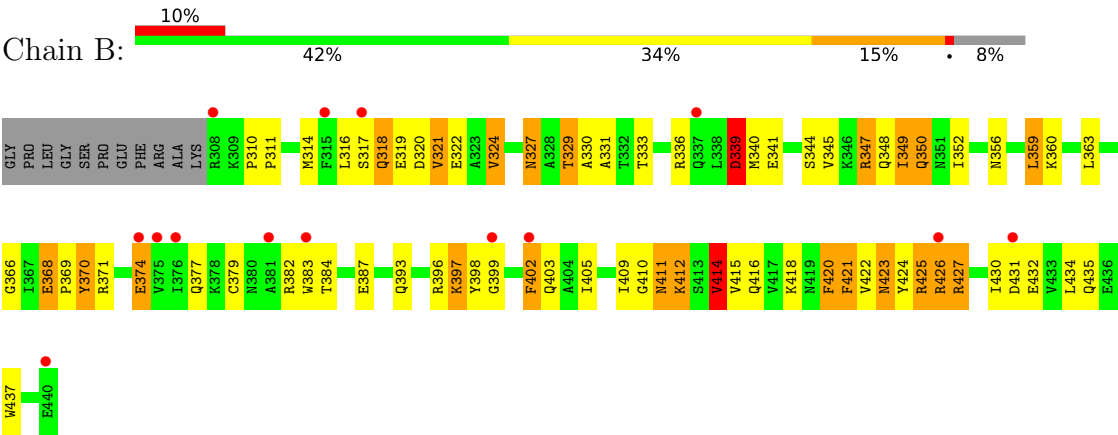
3 Residue-property plots

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: Lysine-specific histone demethylase 1A



● Molecule 2: REST corepressor 1



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.02Å 179.59Å 232.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.68 – 2.91 45.68 – 2.91	Depositor EDS
% Data completeness (in resolution range)	98.2 (45.68-2.91) 98.3 (45.68-2.91)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.214 , 0.244 0.225 , 0.242	Depositor DCC
R_{free} test set	2000 reflections (3.63%)	wwPDB-VP
Wilson B-factor (Å ²)	93.1	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6381	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: XHT, XHX

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	1.00	8/5323 (0.2%)	1.16	14/7221 (0.2%)
2	B	0.87	0/1091	1.35	5/1471 (0.3%)
All	All	0.98	8/6414 (0.1%)	1.20	19/8692 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	808	PRO	C-O	-5.84	1.16	1.23
1	A	575	PRO	C-O	-5.65	1.16	1.24
1	A	779	PRO	C-O	-5.58	1.16	1.23
1	A	794	PRO	C-O	-5.38	1.17	1.23
1	A	341	PRO	C-O	-5.30	1.17	1.24
1	A	755	PRO	C-O	-5.30	1.17	1.24
1	A	782	PRO	C-O	-5.11	1.17	1.23
1	A	792	PRO	C-O	-5.11	1.17	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	510	GLU	CB-CA-C	-8.79	97.08	110.88
2	B	387	GLU	CB-CG-CD	7.88	126.00	112.60
1	A	499	GLU	N-CA-C	-7.51	102.24	111.40
2	B	414	VAL	CA-C-N	-6.79	111.87	120.56
2	B	414	VAL	C-N-CA	-6.79	111.87	120.56
1	A	513	ALA	CA-C-N	-6.58	115.38	123.21
1	A	513	ALA	C-N-CA	-6.58	115.38	123.21
1	A	389	THR	CA-CB-OG1	-6.27	100.20	109.60
1	A	800	GLY	CA-C-O	-6.26	117.94	122.45
1	A	503	LYS	CB-CA-C	-5.90	101.62	110.88
1	A	741	PRO	CB-CA-C	-5.70	102.73	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	PRO	CB-CA-C	-5.62	103.71	113.20
1	A	527	GLN	N-CA-C	-5.39	105.49	111.36
1	A	515	PRO	N-CA-C	-5.36	104.16	110.70
1	A	474	ILE	CA-C-O	-5.35	115.39	120.95
1	A	803	THR	CA-CB-OG1	-5.26	101.72	109.60
1	A	308	GLU	N-CA-CB	-5.19	101.96	110.68
2	B	318	GLN	N-CA-C	-5.17	105.54	111.07
2	B	339	ASP	N-CA-C	-5.15	105.74	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5210	0	5244	327	0
2	B	1076	0	1091	153	0
3	A	72	0	0	4	0
4	A	23	0	0	1	0
All	All	6381	0	6335	429	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 34.

All (429) 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:B:402:PHE:HB3	2:B:418:LYS:CE	1.53	1.35
2:B:317:SER:HB3	2:B:320:ASP:OD1	1.14	1.29
1:A:435:VAL:CG1	2:B:349:ILE:CD1	2.10	1.28
2:B:424:TYR:CE2	2:B:427:ARG:NH1	2.02	1.28
1:A:720:ASP:O	1:A:724:VAL:HG23	1.28	1.25
1:A:435:VAL:HG12	2:B:349:ILE:CD1	1.67	1.20
1:A:437:THR:HG22	1:A:508:LEU:HD21	1.23	1.19
2:B:317:SER:CB	2:B:320:ASP:OD1	1.92	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:PHE:O	1:A:701:PRO:HG2	1.45	1.16
2:B:402:PHE:CB	2:B:418:LYS:HE3	1.77	1.15
1:A:720:ASP:O	1:A:724:VAL:CG2	1.96	1.13
2:B:424:TYR:O	2:B:430:ILE:HD11	1.48	1.12
1:A:435:VAL:CG1	2:B:349:ILE:HD11	1.75	1.12
1:A:437:THR:CG2	1:A:508:LEU:HD21	1.79	1.11
1:A:231:PHE:HE1	1:A:249:VAL:HG12	0.95	1.10
1:A:435:VAL:HG13	2:B:349:ILE:HD11	1.17	1.09
1:A:231:PHE:CE1	1:A:249:VAL:HG12	1.86	1.09
1:A:442:LYS:HB2	2:B:356:ASN:OD1	1.50	1.08
1:A:654:MET:HE1	1:A:776:MET:CG	1.83	1.08
1:A:437:THR:CG2	1:A:508:LEU:CD2	2.32	1.08
1:A:435:VAL:HG13	2:B:349:ILE:CD1	1.81	1.06
2:B:424:TYR:CD2	2:B:427:ARG:NH1	2.21	1.05
1:A:719:SER:HB3	1:A:722:VAL:HG23	1.37	1.04
1:A:456:LYS:HA	2:B:370:TYR:CE2	1.91	1.04
1:A:732:LYS:HG3	1:A:740:VAL:HG11	1.38	1.03
1:A:732:LYS:CG	1:A:740:VAL:HG11	1.87	1.02
1:A:793:ILE:HD12	1:A:793:ILE:H	1.27	0.99
1:A:437:THR:HG22	1:A:508:LEU:CD2	1.95	0.97
2:B:318:GLN:NE2	2:B:322:GLU:OE2	1.98	0.96
2:B:424:TYR:HE2	2:B:427:ARG:HH12	1.00	0.96
1:A:437:THR:HG21	1:A:508:LEU:HD23	1.47	0.96
1:A:231:PHE:HE1	1:A:249:VAL:CG1	1.79	0.96
2:B:402:PHE:CB	2:B:418:LYS:CE	2.41	0.95
1:A:393:SER:HB2	1:A:549:LEU:HD22	1.50	0.94
1:A:435:VAL:CG1	2:B:349:ILE:HD13	1.97	0.93
1:A:346:SER:HA	1:A:351:MET:HE2	1.49	0.93
2:B:402:PHE:HB3	2:B:418:LYS:HE3	0.91	0.91
1:A:435:VAL:HG12	2:B:349:ILE:HD12	1.50	0.91
1:A:666:PHE:O	1:A:701:PRO:CG	2.19	0.91
1:A:456:LYS:HA	2:B:370:TYR:CD2	2.07	0.90
1:A:245:ASP:OD1	1:A:247:VAL:HG23	1.72	0.89
1:A:379:GLU:HG2	1:A:532:HIS:CE1	2.08	0.89
1:A:379:GLU:CG	1:A:532:HIS:CE1	2.56	0.89
1:A:286:SER:OG	1:A:313:VAL:HG12	1.70	0.88
1:A:308:GLU:HB3	1:A:586:LEU:HA	1.53	0.88
2:B:311:PRO:HG2	2:B:314:MET:HG3	1.56	0.86
1:A:654:MET:HE1	1:A:776:MET:HG3	1.55	0.86
1:A:456:LYS:HA	2:B:370:TYR:HE2	1.41	0.85
1:A:666:PHE:CE1	1:A:743:PRO:HA	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LYS:CG	2:B:370:TYR:HE2	1.90	0.85
1:A:346:SER:HA	1:A:351:MET:CE	2.05	0.85
1:A:346:SER:HB3	1:A:351:MET:CE	2.07	0.84
1:A:198:ASP:OD1	1:A:198:ASP:N	2.08	0.84
1:A:379:GLU:CG	1:A:532:HIS:HE1	1.91	0.83
1:A:437:THR:HG21	1:A:508:LEU:CD2	2.01	0.82
2:B:402:PHE:HB3	2:B:418:LYS:NZ	1.95	0.82
1:A:654:MET:HE1	1:A:776:MET:HG2	1.61	0.81
1:A:346:SER:HB3	1:A:351:MET:HE3	1.61	0.81
2:B:424:TYR:HE2	2:B:427:ARG:NH1	1.52	0.81
2:B:322:GLU:OE1	2:B:322:GLU:N	2.14	0.80
2:B:350:GLN:HA	2:B:350:GLN:NE2	1.96	0.80
1:A:666:PHE:CE1	1:A:743:PRO:CA	2.65	0.80
2:B:424:TYR:O	2:B:430:ILE:CD1	2.30	0.79
1:A:442:LYS:CB	2:B:356:ASN:OD1	2.30	0.79
2:B:348:GLN:HE21	2:B:348:GLN:HA	1.47	0.79
1:A:732:LYS:HG2	1:A:740:VAL:HG11	1.65	0.78
1:A:198:ASP:CG	1:A:251:ARG:HH22	1.91	0.78
1:A:724:VAL:O	1:A:727:CYS:HB2	1.84	0.78
1:A:312:ARG:HH11	1:A:312:ARG:HG3	1.46	0.78
1:A:421:LYS:NZ	2:B:320:ASP:OD2	2.16	0.78
1:A:319:THR:HB	1:A:572:SER:HB3	1.66	0.77
1:A:666:PHE:HE1	1:A:743:PRO:CA	1.98	0.77
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.67	0.77
1:A:666:PHE:CD1	1:A:743:PRO:HA	2.19	0.77
1:A:379:GLU:HG3	1:A:532:HIS:CE1	2.19	0.76
2:B:382:ARG:O	2:B:412:LYS:NZ	2.19	0.76
2:B:359:LEU:HD23	2:B:359:LEU:N	2.01	0.75
1:A:654:MET:CE	1:A:776:MET:CG	2.63	0.75
2:B:425:ARG:HA	2:B:430:ILE:HD12	1.69	0.75
2:B:416:GLN:OE1	2:B:416:GLN:N	2.15	0.74
1:A:509:GLN:HA	1:A:509:GLN:NE2	2.02	0.74
2:B:383:TRP:CZ3	2:B:420:PHE:CD1	2.76	0.74
1:A:504:LEU:N	1:A:504:LEU:HD23	2.02	0.73
2:B:424:TYR:HA	2:B:427:ARG:HD3	1.69	0.73
2:B:383:TRP:CH2	2:B:420:PHE:CD1	2.75	0.73
1:A:319:THR:CB	1:A:572:SER:HB3	2.17	0.73
2:B:424:TYR:HD2	2:B:427:ARG:HH11	1.36	0.73
2:B:377:GLN:NE2	2:B:410:GLY:O	2.20	0.73
1:A:456:LYS:CG	2:B:370:TYR:CE2	2.72	0.73
1:A:311:ASP:OD1	1:A:311:ASP:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:SER:CA	1:A:351:MET:CE	2.67	0.72
2:B:318:GLN:O	2:B:321:VAL:HG23	1.90	0.72
1:A:346:SER:CB	1:A:351:MET:HE3	2.20	0.71
1:A:754:ASP:OD1	1:A:755:PRO:HD2	1.89	0.71
1:A:793:ILE:HD12	1:A:793:ILE:N	2.03	0.71
1:A:312:ARG:HG3	1:A:312:ARG:NH1	2.04	0.71
1:A:654:MET:CE	1:A:776:MET:HG2	2.20	0.71
1:A:346:SER:CB	1:A:351:MET:CE	2.69	0.71
2:B:421:PHE:HD1	2:B:421:PHE:H	1.39	0.71
1:A:456:LYS:CA	2:B:370:TYR:HE2	2.02	0.71
1:A:691:LEU:CD2	1:A:727:CYS:SG	2.79	0.70
1:A:526:ARG:HH11	1:A:526:ARG:CG	2.05	0.70
1:A:286:SER:HB3	1:A:308:GLU:OE2	1.92	0.70
1:A:458:LEU:HB3	1:A:487:LEU:HD12	1.74	0.70
1:A:209:VAL:HG12	1:A:213:ILE:HD11	1.73	0.69
1:A:439:GLU:CG	2:B:352:ILE:CD1	2.70	0.69
2:B:426:ARG:HH21	2:B:427:ARG:HD2	1.57	0.69
1:A:456:LYS:HG3	2:B:370:TYR:CE2	2.27	0.69
1:A:569:ASN:OD1	1:A:569:ASN:N	2.18	0.69
1:A:271:LYS:HG3	1:A:271:LYS:O	1.92	0.69
1:A:583:ASP:OD2	1:A:585:LYS:NZ	2.26	0.69
1:A:437:THR:CG2	1:A:508:LEU:HD23	2.10	0.68
1:A:418:LEU:HD13	2:B:324:VAL:HG11	1.74	0.68
1:A:793:ILE:HG22	1:A:794:PRO:CD	2.24	0.68
2:B:348:GLN:HA	2:B:348:GLN:NE2	2.07	0.68
1:A:793:ILE:HG22	1:A:794:PRO:HD2	1.76	0.68
1:A:439:GLU:HG2	2:B:352:ILE:CD1	2.23	0.68
1:A:574:VAL:HB	1:A:575:PRO:HD3	1.75	0.68
1:A:438:GLN:HG2	1:A:508:LEU:HD11	1.77	0.67
2:B:319:GLU:HG2	2:B:319:GLU:O	1.93	0.67
1:A:384:ARG:HB3	2:B:314:MET:HE3	1.75	0.67
2:B:383:TRP:CZ3	2:B:420:PHE:CE1	2.82	0.67
2:B:402:PHE:HB2	2:B:414:VAL:CG1	2.25	0.66
3:A:901:XHT:O17	3:A:901:XHT:O2	2.13	0.66
1:A:521:LEU:HD22	1:A:525:ASP:HB3	1.78	0.66
2:B:377:GLN:CG	2:B:410:GLY:O	2.42	0.66
1:A:720:ASP:C	1:A:724:VAL:HG23	2.15	0.66
2:B:424:TYR:HD2	2:B:427:ARG:NH1	1.90	0.66
1:A:821:GLU:HA	1:A:821:GLU:OE1	1.95	0.66
1:A:352:GLU:HB3	1:A:568:ARG:HB2	1.79	0.65
2:B:425:ARG:HG3	2:B:425:ARG:HH11	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:SER:HB3	1:A:722:VAL:CG2	2.22	0.65
1:A:442:LYS:N	2:B:356:ASN:HD21	1.95	0.65
2:B:382:ARG:O	2:B:412:LYS:CE	2.46	0.64
2:B:424:TYR:HA	2:B:427:ARG:CD	2.26	0.64
1:A:435:VAL:HG12	2:B:349:ILE:HD13	1.67	0.64
1:A:456:LYS:CB	2:B:370:TYR:HE2	2.10	0.64
1:A:456:LYS:CA	2:B:370:TYR:CE2	2.73	0.64
1:A:691:LEU:HD23	1:A:727:CYS:SG	2.37	0.64
1:A:732:LYS:HG2	1:A:740:VAL:CG1	2.27	0.64
1:A:393:SER:HB2	1:A:549:LEU:CD2	2.26	0.63
1:A:720:ASP:O	1:A:724:VAL:HG22	1.96	0.63
2:B:424:TYR:HA	2:B:427:ARG:CG	2.28	0.63
1:A:399:ASN:C	1:A:406:VAL:HG23	2.23	0.63
2:B:336:ARG:HA	2:B:339:ASP:HB2	1.80	0.63
2:B:397:LYS:O	2:B:397:LYS:HG3	1.96	0.63
1:A:448:MET:CE	2:B:363:LEU:HD13	2.29	0.63
1:A:453:GLU:OE1	1:A:453:GLU:HA	1.98	0.63
1:A:718:ILE:HG22	1:A:723:ILE:HG13	1.81	0.63
1:A:424:LYS:HE3	2:B:339:ASP:OD1	1.99	0.62
1:A:198:ASP:OD2	1:A:251:ARG:NH2	2.32	0.62
1:A:235:LEU:O	1:A:235:LEU:HD12	2.00	0.62
1:A:510:GLU:OE1	1:A:510:GLU:HA	2.00	0.61
1:A:526:ARG:HH11	1:A:526:ARG:HG2	1.65	0.61
1:A:530:ASP:OD2	1:A:685:THR:HA	2.01	0.61
1:A:379:GLU:HG2	1:A:532:HIS:HE1	1.54	0.61
1:A:594:ARG:HG2	1:A:640:VAL:HB	1.82	0.61
1:A:258:ARG:NH1	1:A:258:ARG:HG2	2.15	0.61
1:A:444:LEU:HD23	1:A:444:LEU:C	2.26	0.61
2:B:425:ARG:HH11	2:B:425:ARG:CG	2.12	0.61
1:A:199:ILE:N	1:A:199:ILE:HD13	2.16	0.60
1:A:399:ASN:O	1:A:406:VAL:HG23	2.01	0.60
1:A:286:SER:OG	1:A:286:SER:O	2.14	0.60
1:A:295:ARG:HD3	1:A:578:LEU:O	2.01	0.60
1:A:793:ILE:H	1:A:793:ILE:CD1	2.04	0.60
1:A:740:VAL:O	1:A:740:VAL:HG13	2.01	0.60
1:A:456:LYS:HG3	2:B:370:TYR:OH	2.01	0.60
1:A:744:LYS:HG3	1:A:745:GLU:HG2	1.84	0.60
1:A:645:GLU:OE1	1:A:649:SER:OG	2.16	0.60
2:B:348:GLN:HE21	2:B:348:GLN:CA	2.09	0.60
2:B:431:ASP:O	2:B:435:GLN:HG3	2.01	0.60
1:A:468:VAL:HG12	1:A:468:VAL:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:ILE:HG23	1:A:804:ILE:O	2.02	0.59
1:A:382:PHE:CZ	1:A:386:LEU:HD11	2.36	0.59
1:A:574:VAL:HB	1:A:575:PRO:CD	2.32	0.59
1:A:732:LYS:CG	1:A:740:VAL:CG1	2.74	0.59
1:A:346:SER:HB3	1:A:351:MET:HE1	1.85	0.59
1:A:319:THR:OG1	1:A:572:SER:HB3	2.02	0.59
2:B:377:GLN:CD	2:B:410:GLY:O	2.45	0.59
1:A:509:GLN:HA	1:A:509:GLN:HE21	1.68	0.59
1:A:669:VAL:HG12	1:A:669:VAL:O	2.02	0.59
1:A:385:LEU:O	1:A:388:ALA:HB3	2.03	0.59
1:A:316:ARG:NH1	1:A:801:GLU:OE2	2.35	0.59
1:A:439:GLU:HG3	2:B:352:ILE:CD1	2.33	0.59
2:B:424:TYR:HA	2:B:427:ARG:HG3	1.84	0.59
1:A:691:LEU:N	1:A:691:LEU:HD12	2.18	0.59
2:B:396:ARG:O	2:B:396:ARG:NH1	2.33	0.59
1:A:452:LYS:HE3	2:B:366:GLY:O	2.03	0.58
1:A:256:LEU:HB3	1:A:262:ILE:HG12	1.85	0.58
2:B:399:GLY:HA3	2:B:437:TRP:CD2	2.38	0.58
1:A:418:LEU:CD1	2:B:324:VAL:HG11	2.32	0.58
1:A:452:LYS:CE	2:B:366:GLY:O	2.52	0.58
2:B:402:PHE:HB3	2:B:418:LYS:HZ1	1.69	0.58
1:A:742:GLN:OE1	1:A:742:GLN:HA	2.03	0.57
2:B:370:TYR:N	2:B:370:TYR:CD1	2.71	0.57
1:A:744:LYS:HD2	1:A:744:LYS:O	2.04	0.57
1:A:457:GLU:O	1:A:461:GLN:HG3	2.04	0.57
1:A:371:PRO:HG2	1:A:374:LYS:CG	2.35	0.57
2:B:402:PHE:HB2	2:B:414:VAL:HG13	1.86	0.56
1:A:789:ALA:HB1	1:A:790:PRO:HD2	1.86	0.56
2:B:350:GLN:HA	2:B:350:GLN:HE21	1.71	0.56
1:A:680:HIS:C	1:A:680:HIS:CD2	2.84	0.56
1:A:370:VAL:HG21	1:A:528:ILE:CD1	2.36	0.55
2:B:370:TYR:N	2:B:370:TYR:HD1	2.03	0.55
1:A:592:GLN:NE2	1:A:638:GLN:HE21	2.03	0.55
1:A:238:LEU:HD22	1:A:243:ASN:HB3	1.87	0.55
1:A:424:LYS:CE	2:B:339:ASP:OD1	2.54	0.55
1:A:235:LEU:HD11	1:A:243:ASN:HB2	1.89	0.55
1:A:331:ALA:HA	3:A:901:XHT:N4	2.21	0.55
1:A:258:ARG:HG2	1:A:258:ARG:HH11	1.70	0.55
1:A:666:PHE:CE1	1:A:743:PRO:HB3	2.42	0.55
2:B:383:TRP:HA	2:B:412:LYS:HE2	1.89	0.55
1:A:603:ILE:HG13	1:A:615:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:THR:O	1:A:335:THR:OG1	2.16	0.54
2:B:383:TRP:CE3	2:B:420:PHE:CE1	2.96	0.54
1:A:444:LEU:HD23	1:A:445:LEU:HD23	1.88	0.54
2:B:420:PHE:CD2	2:B:420:PHE:C	2.85	0.54
1:A:363:TYR:CE1	1:A:734:ILE:HG23	2.43	0.54
2:B:318:GLN:O	2:B:322:GLU:OE1	2.26	0.54
1:A:258:ARG:HH11	1:A:258:ARG:CG	2.20	0.54
1:A:356:ILE:HG21	3:A:901:XHT:C1	2.38	0.54
1:A:791:GLN:OE1	1:A:792:PRO:HD2	2.07	0.54
1:A:793:ILE:HG23	1:A:828:GLN:NE2	2.23	0.54
1:A:442:LYS:HA	2:B:356:ASN:OD1	2.07	0.54
1:A:199:ILE:N	1:A:199:ILE:CD1	2.72	0.53
1:A:444:LEU:HD13	1:A:500:THR:HG22	1.91	0.53
1:A:601:GLU:HA	1:A:616:TYR:O	2.09	0.53
1:A:188:MET:CE	1:A:200:ILE:HB	2.38	0.53
1:A:474:ILE:N	1:A:474:ILE:CD1	2.71	0.53
2:B:347:ARG:NH1	2:B:347:ARG:HG3	2.23	0.53
1:A:188:MET:HE1	1:A:200:ILE:HB	1.91	0.53
1:A:294:ALA:HB1	1:A:582:LEU:HD13	1.91	0.53
2:B:374:GLU:OE2	2:B:374:GLU:HA	2.04	0.53
2:B:383:TRP:CZ2	2:B:420:PHE:HD1	2.26	0.53
1:A:412:LEU:HD13	1:A:533:PHE:CE1	2.43	0.53
1:A:511:LEU:N	1:A:511:LEU:CD2	2.71	0.53
1:A:439:GLU:HG2	2:B:352:ILE:HD13	1.90	0.52
1:A:474:ILE:N	1:A:474:ILE:HD12	2.24	0.52
1:A:625:LEU:HD22	1:A:629:VAL:HG11	1.91	0.52
1:A:671:TRP:O	1:A:673:PRO:HD3	2.09	0.52
1:A:456:LYS:HG3	2:B:370:TYR:CZ	2.45	0.52
1:A:602:VAL:HG22	1:A:616:TYR:HB2	1.90	0.52
1:A:653:ARG:HG3	1:A:653:ARG:HH11	1.75	0.52
1:A:255:TYR:CD2	1:A:256:LEU:HD13	2.45	0.52
1:A:439:GLU:HG2	2:B:352:ILE:HD11	1.91	0.52
1:A:511:LEU:N	1:A:511:LEU:HD23	2.24	0.52
2:B:347:ARG:HH11	2:B:347:ARG:CG	2.23	0.52
1:A:653:ARG:HE	1:A:772:ASP:CG	2.18	0.52
2:B:421:PHE:CD1	2:B:421:PHE:N	2.78	0.52
1:A:284:ILE:HG12	1:A:590:VAL:HG21	1.90	0.52
1:A:442:LYS:CA	2:B:356:ASN:OD1	2.58	0.52
1:A:509:GLN:NE2	1:A:509:GLN:CA	2.73	0.51
1:A:653:ARG:HG3	1:A:653:ARG:NH1	2.24	0.51
2:B:359:LEU:N	2:B:359:LEU:CD2	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:VAL:O	1:A:213:ILE:HG13	2.11	0.51
1:A:687:SER:O	1:A:687:SER:OG	2.25	0.51
2:B:402:PHE:CB	2:B:418:LYS:NZ	2.69	0.51
2:B:383:TRP:CH2	2:B:420:PHE:HD1	2.26	0.51
1:A:461:GLN:OE1	1:A:483:LYS:HE3	2.10	0.51
1:A:467:GLU:OE2	1:A:467:GLU:HA	2.11	0.51
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.93	0.51
1:A:449:VAL:HG23	2:B:363:LEU:HG	1.92	0.51
1:A:654:MET:CE	1:A:776:MET:SD	2.99	0.51
2:B:425:ARG:CG	2:B:425:ARG:NH1	2.72	0.51
1:A:239:GLU:CD	1:A:239:GLU:H	2.19	0.51
1:A:378:VAL:HG11	1:A:528:ILE:HG21	1.93	0.51
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.45	0.51
1:A:530:ASP:OD2	1:A:685:THR:OG1	2.15	0.51
2:B:369:PRO:HB2	2:B:370:TYR:CD1	2.46	0.51
1:A:321:ARG:NH2	1:A:569:ASN:O	2.44	0.50
1:A:205:GLN:O	1:A:209:VAL:HG23	2.11	0.50
1:A:574:VAL:CB	1:A:575:PRO:CD	2.89	0.50
1:A:574:VAL:CB	1:A:575:PRO:HD3	2.41	0.50
2:B:424:TYR:HD2	2:B:427:ARG:HD3	1.77	0.50
1:A:214:ARG:NH1	1:A:215:ASN:OD1	2.44	0.50
1:A:245:ASP:OD1	1:A:247:VAL:CG2	2.54	0.50
2:B:317:SER:HB2	2:B:320:ASP:OD1	2.00	0.50
2:B:424:TYR:CA	2:B:427:ARG:HG3	2.41	0.50
1:A:341:PRO:HG3	1:A:816:LEU:HD21	1.94	0.50
1:A:666:PHE:HE1	1:A:743:PRO:N	2.09	0.50
1:A:438:GLN:OE1	1:A:508:LEU:CD1	2.61	0.49
1:A:716:GLU:HG2	1:A:750:ARG:HG2	1.93	0.49
1:A:744:LYS:C	1:A:744:LYS:CD	2.85	0.49
1:A:382:PHE:CE1	1:A:386:LEU:HD11	2.47	0.49
2:B:330:ALA:O	2:B:333:THR:HB	2.12	0.49
2:B:347:ARG:NH1	2:B:347:ARG:CG	2.75	0.49
1:A:656:PHE:CE2	1:A:759:GLY:HA3	2.47	0.49
1:A:666:PHE:CE1	1:A:743:PRO:CB	2.95	0.49
1:A:437:THR:CB	1:A:508:LEU:HD21	2.39	0.49
1:A:444:LEU:CD1	1:A:500:THR:HG22	2.43	0.49
1:A:458:LEU:HD13	1:A:487:LEU:HB2	1.94	0.49
1:A:667:ASP:OD1	1:A:667:ASP:N	2.43	0.49
1:A:180:GLN:HA	1:A:339:GLY:HA2	1.94	0.48
1:A:232:GLU:CD	1:A:232:GLU:H	2.21	0.48
1:A:363:TYR:CD1	1:A:734:ILE:HG23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:MET:HB3	1:A:448:MET:HE3	1.63	0.48
1:A:266:ILE:HD11	1:A:578:LEU:HD23	1.94	0.48
1:A:378:VAL:HG11	1:A:528:ILE:CG2	2.42	0.48
1:A:337:LEU:HD23	1:A:337:LEU:N	2.28	0.48
1:A:793:ILE:N	1:A:793:ILE:CD1	2.73	0.48
1:A:239:GLU:CD	1:A:239:GLU:N	2.72	0.48
1:A:474:ILE:HG22	2:B:393:GLN:OE1	2.14	0.48
2:B:430:ILE:HG22	2:B:434:LEU:CD1	2.44	0.48
1:A:352:GLU:HB3	1:A:568:ARG:CB	2.42	0.48
1:A:379:GLU:HG3	1:A:532:HIS:HE1	1.68	0.47
1:A:775:LEU:HD23	1:A:775:LEU:HA	1.64	0.47
1:A:793:ILE:CG2	1:A:794:PRO:CD	2.91	0.47
1:A:370:VAL:HG21	1:A:528:ILE:HD11	1.96	0.47
1:A:253:HIS:ND1	1:A:253:HIS:C	2.73	0.47
1:A:538:PHE:HB2	1:A:708:ALA:HB2	1.96	0.47
1:A:358:GLN:OE1	1:A:358:GLN:N	2.47	0.47
1:A:392:LEU:HD11	2:B:316:LEU:HD13	1.97	0.47
2:B:402:PHE:CB	2:B:418:LYS:HZ1	2.28	0.47
1:A:521:LEU:CD2	1:A:525:ASP:HB3	2.44	0.47
1:A:567:VAL:HG11	1:A:570:GLY:O	2.15	0.46
2:B:418:LYS:HD3	2:B:418:LYS:HA	1.78	0.46
1:A:296:GLN:O	1:A:299:SER:HB3	2.14	0.46
1:A:438:GLN:OE1	1:A:508:LEU:HD12	2.15	0.46
1:A:438:GLN:HB3	2:B:352:ILE:CG2	2.45	0.46
2:B:359:LEU:HD23	2:B:359:LEU:H	1.76	0.46
2:B:424:TYR:CD2	2:B:427:ARG:HD3	2.50	0.46
1:A:452:LYS:HE2	2:B:366:GLY:O	2.15	0.46
1:A:807:TYR:N	1:A:808:PRO:CD	2.78	0.46
1:A:742:GLN:HG3	1:A:743:PRO:HD2	1.97	0.46
1:A:289:SER:OG	3:A:901:XHT:O7	2.28	0.46
4:A:902:XHX:C15	4:A:902:XHX:C12	2.91	0.46
2:B:426:ARG:NH2	2:B:427:ARG:HD2	2.30	0.46
1:A:531:TRP:O	1:A:531:TRP:CE3	2.69	0.45
2:B:369:PRO:HB2	2:B:370:TYR:HD1	1.81	0.45
2:B:317:SER:O	2:B:321:VAL:HG22	2.16	0.45
1:A:370:VAL:HG21	1:A:528:ILE:HD13	1.98	0.45
1:A:448:MET:HE2	2:B:363:LEU:HD13	1.97	0.45
1:A:670:PHE:O	1:A:670:PHE:CD1	2.70	0.45
1:A:691:LEU:HD21	1:A:727:CYS:SG	2.56	0.45
2:B:430:ILE:HG22	2:B:434:LEU:HD11	1.98	0.45
1:A:353:LEU:HD12	1:A:353:LEU:HA	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLN:O	1:A:431:TRP:HD1	1.99	0.45
1:A:444:LEU:CD1	1:A:500:THR:CG2	2.94	0.45
1:A:526:ARG:CG	1:A:526:ARG:NH1	2.72	0.45
2:B:402:PHE:CA	2:B:418:LYS:CE	2.94	0.45
1:A:781:THR:HA	1:A:794:PRO:HA	1.99	0.45
1:A:419:GLN:NE2	2:B:314:MET:HA	2.32	0.45
1:A:213:ILE:CD1	1:A:248:LEU:HD23	2.47	0.45
1:A:238:LEU:HD13	1:A:249:VAL:HG21	1.99	0.45
1:A:538:PHE:CD1	1:A:706:LEU:HD23	2.51	0.45
2:B:397:LYS:HG2	2:B:398:TYR:CE2	2.52	0.45
1:A:392:LEU:CD1	2:B:316:LEU:HD13	2.47	0.44
1:A:391:TYR:CZ	2:B:310:PRO:HD3	2.52	0.44
1:A:524:ARG:HA	1:A:527:GLN:NE2	2.33	0.44
1:A:424:LYS:HD3	2:B:339:ASP:OD1	2.17	0.44
2:B:423:ASN:OD1	2:B:423:ASN:N	2.49	0.44
1:A:384:ARG:HB3	2:B:314:MET:CE	2.46	0.44
1:A:566:THR:HG21	1:A:697:LEU:HD22	2.00	0.44
1:A:606:ASN:HD21	1:A:608:ARG:HE	1.65	0.44
1:A:744:LYS:HD2	1:A:744:LYS:C	2.42	0.44
2:B:336:ARG:O	2:B:340:MET:HG3	2.18	0.44
1:A:438:GLN:HB3	2:B:352:ILE:HG21	1.99	0.44
1:A:524:ARG:HA	1:A:527:GLN:HE21	1.81	0.44
1:A:548:SER:O	1:A:552:TRP:HB3	2.17	0.43
1:A:308:GLU:HG2	1:A:586:LEU:CD2	2.48	0.43
1:A:542:THR:OG1	1:A:546:THR:OG1	2.27	0.43
1:A:777:ALA:HB2	1:A:803:THR:HB	2.01	0.43
1:A:690:GLU:OE2	1:A:726:ARG:NH1	2.50	0.43
2:B:399:GLY:HA3	2:B:437:TRP:CE3	2.53	0.43
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.83	0.43
1:A:456:LYS:HA	2:B:370:TYR:HD2	1.72	0.43
1:A:671:TRP:HA	1:A:735:PHE:CE1	2.53	0.43
1:A:439:GLU:CG	2:B:352:ILE:HD11	2.46	0.43
2:B:368:GLU:HB2	2:B:369:PRO:HD3	2.00	0.43
1:A:780:ILE:HB	1:A:796:LEU:HB3	2.00	0.43
1:A:231:PHE:CZ	1:A:250:HIS:HB2	2.53	0.43
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.80	0.43
1:A:319:THR:HB	1:A:572:SER:CB	2.43	0.43
1:A:672:ASP:HB3	1:A:675:VAL:HG22	2.01	0.43
1:A:321:ARG:HG2	1:A:326:VAL:HG22	2.01	0.43
1:A:370:VAL:CG2	1:A:528:ILE:HD11	2.49	0.43
1:A:191:GLN:HG2	1:A:255:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:CYS:HA	1:A:702:ILE:HG12	2.01	0.43
1:A:715:MET:O	1:A:723:ILE:HD11	2.18	0.43
2:B:383:TRP:CE3	2:B:420:PHE:HE1	2.35	0.42
1:A:333:VAL:HA	1:A:565:LEU:O	2.19	0.42
1:A:432:LYS:HA	1:A:435:VAL:HG22	2.00	0.42
1:A:276:LYS:HD2	1:A:277:LYS:N	2.34	0.42
1:A:538:PHE:HD1	1:A:659:LEU:HD22	1.83	0.42
1:A:732:LYS:HG2	1:A:737:SER:HA	2.02	0.42
2:B:341:GLU:O	2:B:341:GLU:HG3	2.16	0.42
2:B:349:ILE:HD12	2:B:349:ILE:HA	1.78	0.42
2:B:383:TRP:CE3	2:B:420:PHE:CD1	3.08	0.42
2:B:383:TRP:CZ2	2:B:420:PHE:CD1	3.06	0.42
1:A:471:PRO:O	1:A:471:PRO:HG2	2.19	0.42
1:A:522:SER:HG	1:A:525:ASP:H	1.62	0.42
2:B:350:GLN:NE2	2:B:350:GLN:CA	2.73	0.42
1:A:283:ILE:HG12	1:A:622:LEU:HB3	2.01	0.42
1:A:371:PRO:HG2	1:A:374:LYS:HG2	2.02	0.42
1:A:438:GLN:HG2	1:A:508:LEU:CD1	2.49	0.42
1:A:258:ARG:HD3	1:A:258:ARG:HA	1.35	0.42
2:B:324:VAL:HG23	2:B:331:ALA:HB2	2.00	0.42
2:B:425:ARG:HD3	2:B:430:ILE:HD12	2.01	0.42
1:A:385:LEU:O	1:A:389:THR:HG23	2.20	0.41
2:B:420:PHE:C	2:B:420:PHE:HD2	2.26	0.41
1:A:239:GLU:N	1:A:239:GLU:OE2	2.49	0.41
1:A:550:LYS:HG2	1:A:551:HIS:CE1	2.54	0.41
1:A:527:GLN:HE21	1:A:527:GLN:HB2	1.63	0.41
1:A:653:ARG:HH11	1:A:653:ARG:CG	2.33	0.41
1:A:198:ASP:OD2	1:A:251:ARG:NH1	2.53	0.41
1:A:210:PHE:CD2	1:A:210:PHE:C	2.98	0.41
1:A:662:VAL:HB	1:A:705:ALA:HB3	2.02	0.41
1:A:720:ASP:C	1:A:724:VAL:CG2	2.85	0.41
1:A:438:GLN:CG	1:A:508:LEU:HD11	2.47	0.41
1:A:510:GLU:HB2	1:A:511:LEU:HD23	2.03	0.41
1:A:715:MET:HE1	1:A:726:ARG:NH1	2.34	0.41
1:A:793:ILE:CG2	1:A:828:GLN:CG	2.99	0.41
1:A:691:LEU:HA	1:A:706:LEU:O	2.20	0.41
1:A:332:MET:HG3	1:A:661:LYS:NZ	2.36	0.41
1:A:458:LEU:HD23	1:A:458:LEU:HA	1.65	0.41
1:A:538:PHE:CD1	1:A:538:PHE:O	2.74	0.41
1:A:710:GLU:H	1:A:710:GLU:HG2	1.67	0.41
1:A:828:GLN:O	1:A:828:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:GLU:N	2:B:369:PRO:CD	2.84	0.41
1:A:238:LEU:HD23	1:A:239:GLU:N	2.36	0.40
2:B:324:VAL:O	2:B:324:VAL:CG2	2.69	0.40
1:A:531:TRP:CE3	1:A:531:TRP:C	3.00	0.40
1:A:734:ILE:O	1:A:734:ILE:CG2	2.69	0.40
1:A:366:ASN:OD1	1:A:367:GLY:N	2.54	0.40
1:A:594:ARG:HA	1:A:640:VAL:O	2.21	0.40
1:A:725:GLY:C	1:A:727:CYS:N	2.79	0.40
2:B:327:ASN:OD1	2:B:329:THR:N	2.55	0.40
1:A:195:CYS:HB2	1:A:196:PHE:CD1	2.57	0.40
1:A:572:SER:O	1:A:576:VAL:HG23	2.21	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	663/871 (76%)	628 (95%)	35 (5%)	0	100	100
2	B	131/144 (91%)	119 (91%)	11 (8%)	1 (1%)	16	43
All	All	794/1015 (78%)	747 (94%)	46 (6%)	1 (0%)	48	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	411	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	565/715 (79%)	490 (87%)	75 (13%)	4	12
2	B	117/125 (94%)	82 (70%)	35 (30%)	0	1
All	All	682/840 (81%)	572 (84%)	110 (16%)	2	8

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	199	ILE
1	A	235	LEU
1	A	237	GLN
1	A	239	GLU
1	A	247	VAL
1	A	249	VAL
1	A	251	ARG
1	A	256	LEU
1	A	258	ARG
1	A	271	LYS
1	A	275	THR
1	A	276	LYS
1	A	286	SER
1	A	308	GLU
1	A	311	ASP
1	A	335	THR
1	A	349	VAL
1	A	350	ASN
1	A	351	MET
1	A	353	LEU
1	A	368	GLN
1	A	379	GLU
1	A	381	GLU
1	A	415	VAL
1	A	418	LEU
1	A	444	LEU
1	A	445	LEU
1	A	449	VAL
1	A	457	GLU
1	A	458	LEU
1	A	463	LYS
1	A	466	SER

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Mol	Chain	Res	Type
1	A	467	GLU
1	A	468	VAL
1	A	469	LYS
1	A	472	ARG
1	A	474	ILE
1	A	480	VAL
1	A	482	SER
1	A	501	GLN
1	A	504	LEU
1	A	506	GLU
1	A	508	LEU
1	A	509	GLN
1	A	510	GLU
1	A	511	LEU
1	A	512	GLU
1	A	517	SER
1	A	526	ARG
1	A	536	LEU
1	A	538	PHE
1	A	568	ARG
1	A	569	ASN
1	A	572	SER
1	A	575	PRO
1	A	582	LEU
1	A	667	ASP
1	A	668	ARG
1	A	669	VAL
1	A	680	HIS
1	A	684	THR
1	A	685	THR
1	A	687	SER
1	A	722	VAL
1	A	724	VAL
1	A	744	LYS
1	A	758	ARG
1	A	769	SER
1	A	780	ILE
1	A	786	ILE
1	A	791	GLN
1	A	793	ILE
1	A	811	VAL
1	A	824	ARG

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Mol	Chain	Res	Type
2	B	321	VAL
2	B	324	VAL
2	B	327	ASN
2	B	329	THR
2	B	339	ASP
2	B	344	SER
2	B	345	VAL
2	B	347	ARG
2	B	349	ILE
2	B	350	GLN
2	B	359	LEU
2	B	360	LYS
2	B	368	GLU
2	B	370	TYR
2	B	371	ARG
2	B	374	GLU
2	B	379	CYS
2	B	384	THR
2	B	397	LYS
2	B	402	PHE
2	B	403	GLN
2	B	405	ILE
2	B	409	ILE
2	B	411	ASN
2	B	412	LYS
2	B	414	VAL
2	B	415	VAL
2	B	420	PHE
2	B	421	PHE
2	B	422	VAL
2	B	423	ASN
2	B	425	ARG
2	B	426	ARG
2	B	427	ARG
2	B	432	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	A	237	GLN
1	A	298	GLN

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Mol	Chain	Res	Type
1	A	422	HIS
1	A	459	HIS
1	A	509	GLN
1	A	514	ASN
1	A	527	GLN
1	A	532	HIS
1	A	551	HIS
1	A	633	GLN
1	A	638	GLN
2	B	348	GLN
2	B	350	GLN
2	B	429	ASN
2	B	435	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	XHX	A	902	-	25,26,26	1.31	3 (12%)	28,37,37	0.97	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	XHT	A	901	-	77,80,80	1.44	14 (18%)	106,124,124	1.18	8 (7%)

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
4	XHX	A	902	-	-	2/12/27/27	0/4/4/4
3	XHT	A	901	-	-	16/46/114/114	0/8/9/9

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	XHT	P2-O9	-3.67	1.55	1.59
3	A	901	XHT	C37-N11	-3.23	1.29	1.36
3	A	901	XHT	O3-C22	-3.04	1.37	1.43
3	A	901	XHT	C3-N3	-3.03	1.33	1.38
3	A	901	XHT	C3-S1	-3.00	1.68	1.73
3	A	901	XHT	C13-N4	-2.96	1.36	1.41
3	A	901	XHT	C38-N12	-2.94	1.32	1.37
3	A	901	XHT	P1-O9	-2.94	1.56	1.59
4	A	902	XHX	C3-N3	-2.92	1.33	1.38
4	A	902	XHX	C12-N4	-2.87	1.42	1.47
4	A	902	XHX	C3-S1	-2.60	1.69	1.73
3	A	901	XHT	C36-N5	-2.48	1.32	1.38
3	A	901	XHT	O4-C23	-2.30	1.37	1.43
3	A	901	XHT	O16-C37	-2.15	1.20	1.24
3	A	901	XHT	C21-C22	-2.13	1.49	1.52
3	A	901	XHT	P2-O10	-2.05	1.45	1.55
3	A	901	XHT	C20-C13	-2.03	1.37	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	XHT	C13-N4-C12	-5.03	112.37	123.92
3	A	901	XHT	C38-C39-C36	-3.77	106.72	113.40
3	A	901	XHT	C39-N4-C12	-3.76	105.72	109.50
3	A	901	XHT	C38-N12-C37	-3.17	120.64	125.42
4	A	902	XHX	C3-S1-C2	-2.96	86.22	88.39
3	A	901	XHT	C35-C34-C28	-2.63	96.49	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	XHT	O16-C37-N11	-2.10	118.31	121.80
3	A	901	XHT	C3-S1-C2	-2.03	86.91	88.39
3	A	901	XHT	O10-P2-O11	2.02	121.84	112.44

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	XHT	N2-C3-N3-C4
3	A	901	XHT	S1-C3-N3-C4
3	A	901	XHT	C21-C22-C23-C24
3	A	901	XHT	C21-C22-C23-O4
3	A	901	XHT	O3-C22-C23-C24
3	A	901	XHT	O3-C22-C23-O4
3	A	901	XHT	C26-O12-P2-O11
3	A	901	XHT	C25-O6-P1-O8
3	A	901	XHT	C25-O6-P1-O9
4	A	902	XHX	N2-C3-N3-C4
4	A	902	XHX	S1-C3-N3-C4
3	A	901	XHT	P1-O9-P2-O11
3	A	901	XHT	O5-C24-C25-O6
3	A	901	XHT	P2-O9-P1-O6
3	A	901	XHT	C25-O6-P1-O7
3	A	901	XHT	P1-O9-P2-O10
3	A	901	XHT	P2-O9-P1-O8
3	A	901	XHT	O12-C26-C27-O13

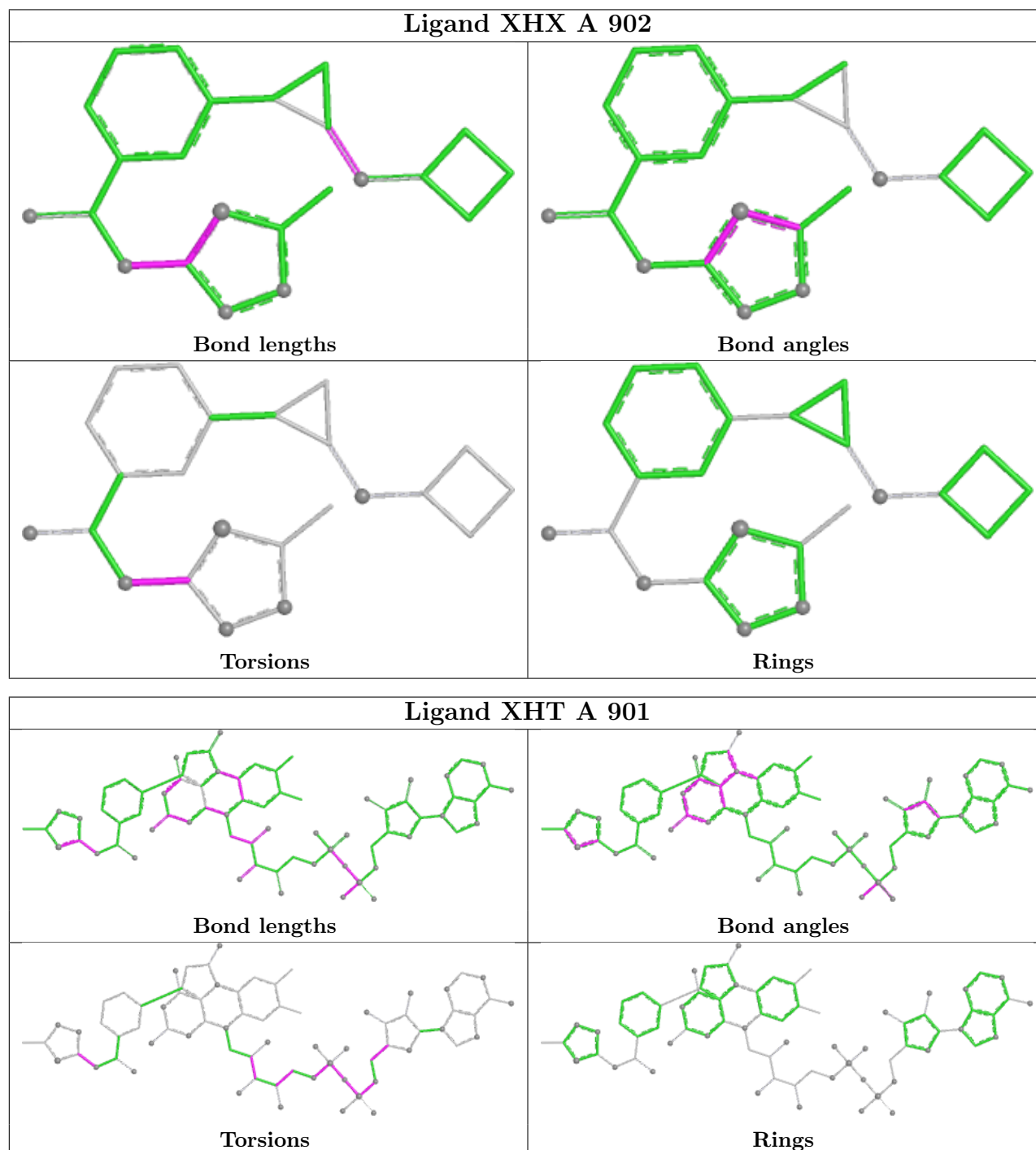
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	XHX	1	0
3	A	901	XHT	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	665/871 (76%)	0.28	14 (2%) 63 54	59, 90, 124, 138	0
2	B	133/144 (92%)	0.89	14 (10%) 11 10	86, 121, 142, 155	0
All	All	798/1015 (78%)	0.38	28 (3%) 47 38	59, 97, 130, 155	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	836	LEU	6.4
2	B	402	PHE	4.7
2	B	374	GLU	3.9
1	A	835	THR	3.7
1	A	667	ASP	3.7
1	A	275	THR	3.3
2	B	376	ILE	3.1
2	B	317	SER	2.8
2	B	308	ARG	2.7
1	A	272	PRO	2.7
2	B	375	VAL	2.7
2	B	399	GLY	2.7
1	A	699	LYS	2.7
1	A	377	MET	2.5
1	A	350	ASN	2.5
1	A	363	TYR	2.4
2	B	431	ASP	2.4
2	B	381	ALA	2.4
2	B	440	GLU	2.4
1	A	506	GLU	2.3
2	B	426	ARG	2.3
1	A	509	GLN	2.3
2	B	337	GLN	2.2
2	B	383	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	172	SER	2.1
2	B	315	PHE	2.1
1	A	720	ASP	2.1
1	A	508	LEU	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](#)

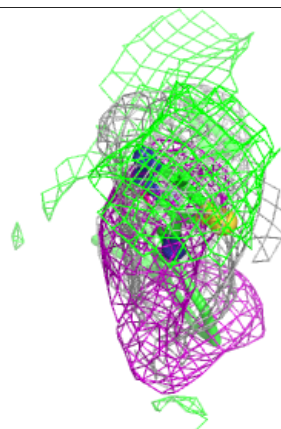
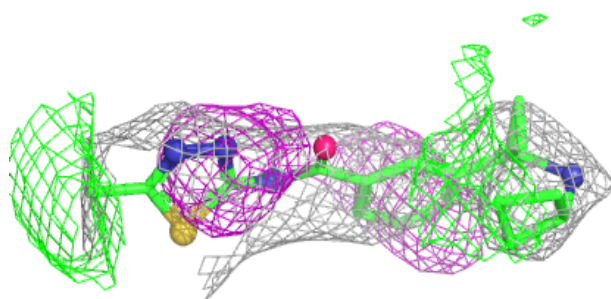
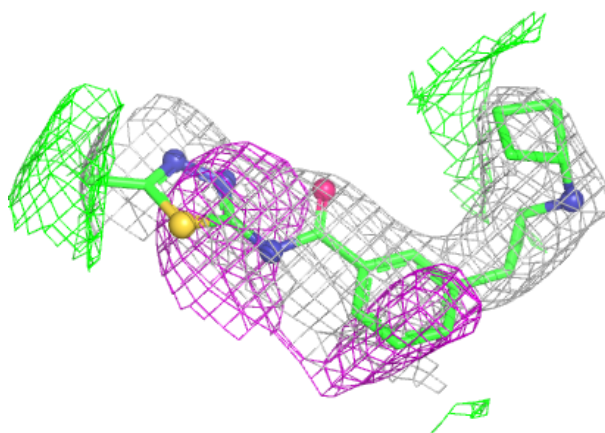
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	XHX	A	902	23/23	0.79	0.26	93,107,135,147	0
3	XHT	A	901	72/72	0.94	0.12	56,75,109,124	0

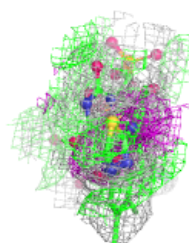
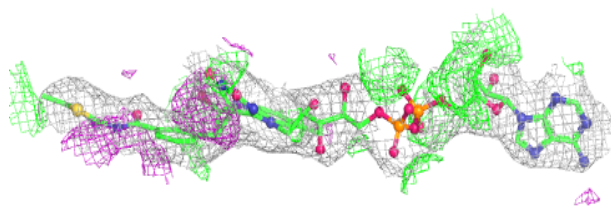
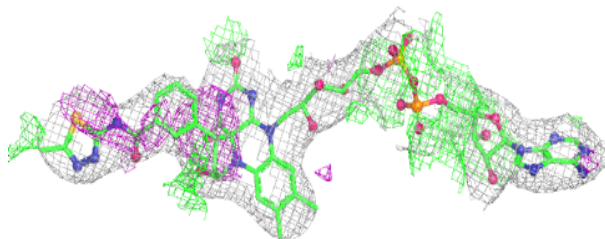
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XHX A 902:

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

**Electron density around XHT A 901:**

$2mF_o-DF_c$ (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.