



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:20 AM UTC

PDB ID : 9J7F / pdb_00009j7f
Title : Crystal structure of Keap1_compound_1
Authors : Xu, K.
Deposited on : 2024-08-18
Resolution : 2.99 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

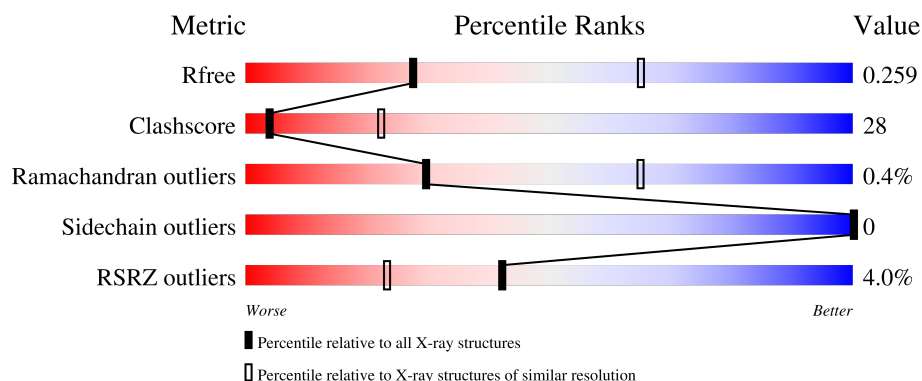
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	288	11% 67% 33%
1	B	288	67% 32% .
1	C	288	2% 60% 39% ..
1	D	288	11% 44% 52% .

2 Entry composition [i](#)

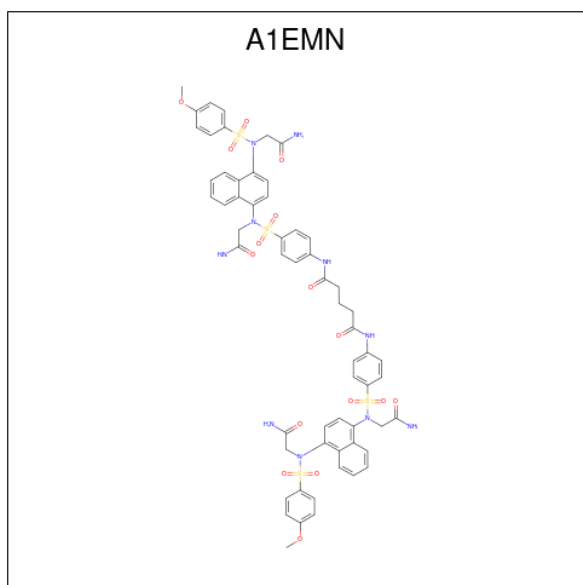
There are 2 unique types of molecules in this entry. The entry contains 9099 atoms, of which 116 are hydrogens and 0 are deuteriums.

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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	1	0
			2228	1385	405	423	15			
1	B	286	Total	C	N	O	S	0	0	0
			2201	1368	398	420	15			
1	C	286	Total	C	N	O	S	0	1	0
			2212	1374	402	421	15			
1	D	280	Total	C	N	O	S	0	1	0
			2164	1347	391	411	15			

- Molecule 2 is {N}, {N}'-bis[4-[(2-azanyl-2-oxidanylidene-ethyl)-[4-[(2-azanyl-2-oxidanylidene-ethyl)-(4-methoxyphenyl)sulfonyl-amino]naphthalen-1-yl]sulfamoyl]phenyl]pentanediamide (CCD ID: A1EMN) (formula: C₅₉H₅₈N₁₀O₁₆S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O S	0	0
			147	59	58	10	16 4		

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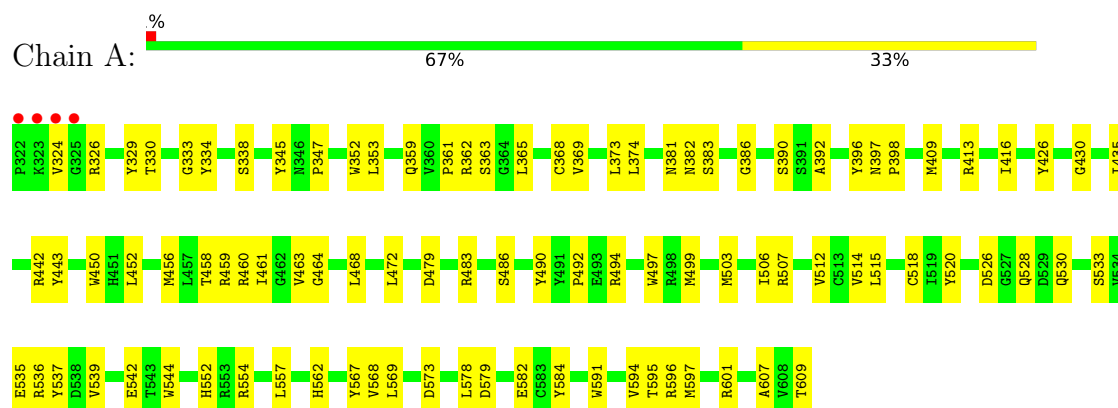
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total	C	H	N	O	S	0	0
			147	59	58	10	16	4		

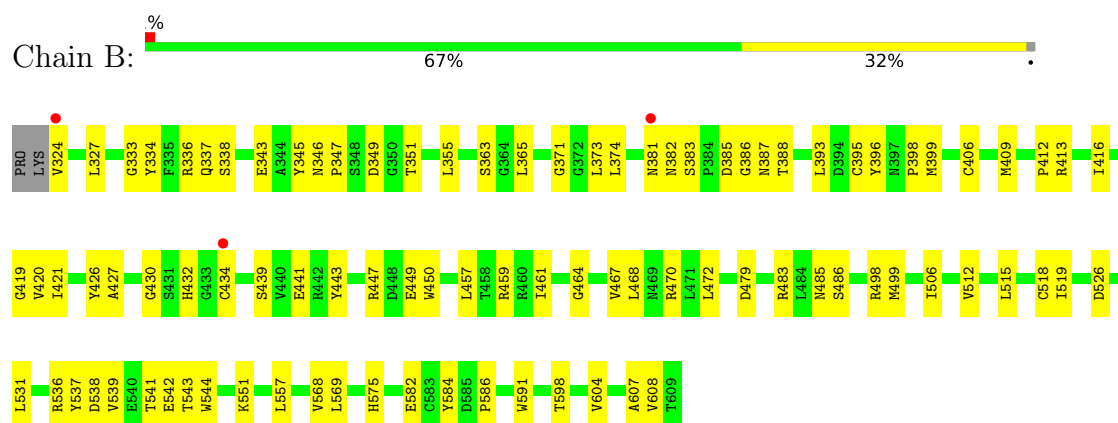
3 Residue-property plots

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.

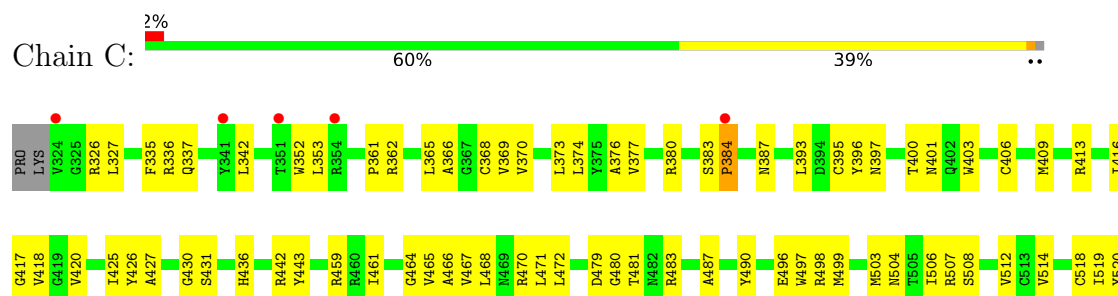
• Molecule 1: Kelch-like ECH-associated protein 1



• Molecule 1: Kelch-like ECH-associated protein 1

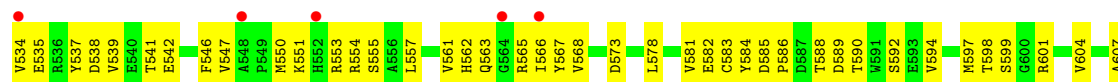
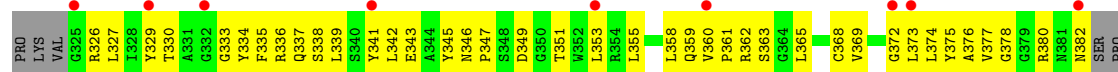
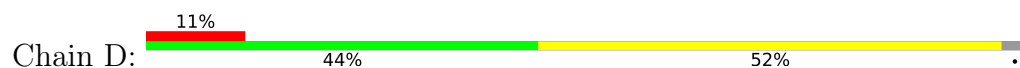


• Molecule 1: Kelch-like ECH-associated protein 1





● Molecule 1: Kelch-like ECH-associated protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.97Å 74.17Å 122.77Å 90.00° 101.22° 90.00°	Depositor
Resolution (Å)	48.70 – 2.99 48.70 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.70-2.99) 91.8 (48.70-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.199 , 0.252 0.206 , 0.259	Depositor DCC
R_{free} test set	1990 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	66.2	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9099	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1EMN

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	0.28	0/2282	0.53	0/3104
1	B	0.29	0/2254	0.53	0/3068
1	C	0.27	0/2265	0.54	1/3082 (0.0%)
1	D	0.30	0/2218	0.55	0/3016
All	All	0.29	0/9019	0.54	1/12270 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	597	MET	CB-CA-C	-5.32	109.46	115.79

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	2228	0	2125	88	0
1	B	2201	0	2093	90	0
1	C	2212	0	2104	131	0
1	D	2164	0	2063	192	0
2	A	89	58	0	4	0
2	D	89	58	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8983	116	8385	488	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 28.

All (488) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:VAL:HG22	1:D:393:LEU:HD13	1.24	1.19
1:D:415:ARG:CZ	2:D:801:A1EMN:O85	1.91	1.17
1:D:327:LEU:HD22	1:D:346:ASN:HA	1.20	1.17
1:D:415:ARG:NH2	2:D:801:A1EMN:O85	1.77	1.17
1:D:457:LEU:HD12	1:D:499:MET:HG2	1.28	1.12
1:A:362[B]:ARG:HH12	1:A:392:ALA:HB3	1.09	1.08
1:D:428:VAL:HA	1:D:440:VAL:HG22	1.34	1.06
1:D:375:TYR:HB3	1:D:393:LEU:HD11	1.38	1.04
1:D:563:GLN:NE2	1:D:567:TYR:HE1	1.57	1.01
1:D:466:ALA:HB1	1:D:514:VAL:HG13	1.43	1.01
1:D:416:ILE:HD11	1:D:427:ALA:HB1	1.40	0.98
1:D:563:GLN:HE22	1:D:567:TYR:HE1	1.08	0.95
1:C:352:TRP:HE1	1:C:595:THR:HG21	1.30	0.94
1:A:435:ILE:CD1	1:B:542:GLU:HB3	1.97	0.93
1:D:493:GLU:HB2	1:D:494:ARG:NH1	1.86	0.91
1:C:503:MET:HB3	1:C:535:GLU:OE2	1.70	0.90
1:D:573:ASP:HB3	1:D:578:LEU:HD21	1.51	0.90
1:C:595:THR:HG22	1:C:596:ARG:H	1.36	0.90
1:D:554:ARG:HD3	1:D:557:LEU:HD21	1.52	0.89
1:A:362[B]:ARG:NH1	1:A:392:ALA:HB3	1.86	0.88
1:A:435:ILE:HD13	1:B:542:GLU:HB3	1.53	0.88
1:C:369:VAL:HG22	1:C:374:LEU:HA	1.55	0.88
1:D:562:HIS:O	1:D:563:GLN:NE2	2.07	0.87
1:B:385:ASP:O	1:D:482:ASN:ND2	2.07	0.87
1:A:362[B]:ARG:HH12	1:A:392:ALA:CB	1.88	0.86
1:D:334:TYR:CE1	1:D:337:GLN:HA	2.10	0.86
1:A:362[B]:ARG:NH1	1:A:390:SER:OG	2.09	0.86
1:D:486:SER:OG	1:D:499:MET:HE1	1.75	0.85
1:D:483:ARG:HB3	1:D:506:ILE:HG21	1.56	0.84
1:C:496:GLU:OE2	1:C:498:ARG:NH1	2.11	0.83
1:D:459:ARG:O	1:D:479:ASP:HA	1.80	0.82
1:B:557:LEU:HD23	1:B:557:LEU:H	1.45	0.82
1:C:397:ASN:HB3	1:C:400:THR:CG2	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:503:MET:HB3	1:D:535:GLU:OE1	1.80	0.81
1:C:352:TRP:HE1	1:C:595:THR:CG2	1.94	0.81
1:D:339:LEU:HD12	1:D:601:ARG:HD3	1.63	0.80
1:D:491:TYR:HB3	1:D:494:ARG:HE	1.46	0.79
1:B:468:LEU:HD23	1:B:539:VAL:HG11	1.64	0.79
1:C:520:TYR:OH	1:C:536:ARG:NH1	2.15	0.79
1:D:561:VAL:HG22	1:D:566:ILE:HA	1.65	0.78
1:C:504:ASN:ND2	1:C:535:GLU:OE1	2.18	0.77
1:D:522:ALA:HB2	1:D:534:VAL:HG13	1.66	0.77
1:C:557:LEU:H	1:C:557:LEU:HD23	1.49	0.76
1:C:538:ASP:HB3	1:C:541:THR:CG2	2.15	0.76
1:D:562:HIS:O	1:D:563:GLN:CD	2.29	0.76
1:D:563:GLN:NE2	1:D:567:TYR:CE1	2.48	0.76
1:C:526:ASP:HB3	1:C:531:LEU:HD11	1.67	0.75
1:A:459:ARG:NH1	1:A:479:ASP:O	2.19	0.74
1:D:568:VAL:O	1:D:581:VAL:HG13	1.86	0.74
1:D:491:TYR:HB3	1:D:494:ARG:NE	2.02	0.74
1:D:428:VAL:HA	1:D:440:VAL:CG2	2.17	0.74
1:D:585:ASP:HB3	1:D:588:THR:OG1	1.87	0.74
1:A:362[B]:ARG:HE	1:A:381:ASN:HB3	1.53	0.74
1:C:426:TYR:CZ	1:C:442:ARG:HD3	2.23	0.74
1:A:362[B]:ARG:HG2	1:A:381:ASN:HA	1.69	0.73
1:D:326:ARG:O	1:D:327:LEU:HD23	1.89	0.73
1:A:369:VAL:HG23	1:A:607:ALA:HB1	1.70	0.72
1:D:427:ALA:O	1:D:440:VAL:HG13	1.89	0.72
1:B:413:ARG:HH22	1:B:439:SER:HB3	1.53	0.72
1:D:428:VAL:HG13	1:D:440:VAL:HG21	1.70	0.71
1:C:538:ASP:OD1	1:C:541:THR:HG22	1.89	0.71
1:C:534:VAL:HB	1:C:547:VAL:CG2	2.21	0.71
1:B:413:ARG:HH22	1:B:439:SER:CB	2.04	0.71
1:D:506:ILE:HD12	1:D:506:ILE:H	1.54	0.71
1:C:373:LEU:HD23	1:C:395:CYS:SG	2.30	0.71
1:A:507:ARG:HH22	1:A:533:SER:HB2	1.56	0.71
1:C:352:TRP:NE1	1:C:595:THR:HG21	2.02	0.71
1:D:421:ILE:HG12	1:D:467:VAL:HG11	1.73	0.71
1:D:439:SER:OG	1:D:452:LEU:HD21	1.90	0.70
1:C:425:ILE:HD12	1:C:443:TYR:HD2	1.56	0.70
1:C:380[B]:ARG:NH1	1:C:387:ASN:O	2.19	0.70
1:A:503:MET:HE1	1:A:507:ARG:HB2	1.73	0.69
1:A:362[B]:ARG:NE	1:A:381:ASN:HB3	2.07	0.69
1:D:457:LEU:CD1	1:D:499:MET:HG2	2.16	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ARG:HH11	1:A:494:ARG:HG3	1.57	0.69
1:A:426:TYR:CZ	1:A:442:ARG:HD3	2.28	0.69
1:A:507:ARG:NH2	1:A:533:SER:HB2	2.08	0.69
1:C:557:LEU:HD12	1:C:568:VAL:HG13	1.76	0.68
1:B:434:CYS:HB3	1:D:434:CYS:SG	2.32	0.68
1:D:327:LEU:CD2	1:D:346:ASN:HA	2.13	0.68
1:A:557:LEU:HD23	1:A:557:LEU:H	1.59	0.68
1:D:493:GLU:HB2	1:D:494:ARG:HH11	1.58	0.68
1:C:464:GLY:HA3	1:C:512:VAL:CG2	2.24	0.68
1:D:563:GLN:HE21	1:D:565:ARG:HB2	1.59	0.68
1:B:536:ARG:HG2	1:B:537:TYR:N	2.09	0.68
1:B:338:SER:H	1:B:382:ASN:ND2	1.91	0.68
1:B:346:ASN:HB3	1:B:349:ASP:OD1	1.94	0.68
1:D:369:VAL:HG13	1:D:607:ALA:HB1	1.76	0.68
1:D:507:ARG:HE	1:D:531:LEU:HD13	1.59	0.67
1:D:565:ARG:HB3	1:D:583:CYS:SG	2.34	0.67
1:B:365:LEU:H	1:B:365:LEU:HD23	1.58	0.67
1:C:520:TYR:CE2	1:C:536:ARG:HD3	2.30	0.67
1:D:430:GLY:O	1:D:461:ILE:HG22	1.95	0.67
1:C:530:GLN:O	1:C:553:ARG:HD2	1.94	0.66
1:D:456:MET:HE1	1:D:460:ARG:HB2	1.76	0.66
1:A:486:SER:HB2	1:A:499:MET:HE1	1.77	0.66
1:D:522:ALA:HB2	1:D:534:VAL:CG1	2.26	0.66
1:A:468:LEU:HD13	1:A:514:VAL:HG21	1.78	0.65
1:B:355:LEU:HD22	1:B:396:TYR:OH	1.96	0.65
1:D:372:GLY:C	1:D:373:LEU:HD23	2.22	0.65
1:B:447:ARG:O	1:B:449:GLU:HG3	1.97	0.65
1:C:506:ILE:H	1:C:506:ILE:HD12	1.59	0.65
1:D:355:LEU:HD22	1:D:396:TYR:OH	1.96	0.65
1:D:415:ARG:CZ	2:D:801:A1EMN:C83	2.72	0.65
1:A:483:ARG:HB3	1:A:506:ILE:HG21	1.78	0.65
1:D:338:SER:OG	1:D:361:PRO:HB2	1.96	0.65
1:A:579:ASP:OD1	1:A:596:ARG:HD3	1.96	0.65
1:C:464:GLY:HA3	1:C:512:VAL:HG21	1.79	0.65
1:D:523:GLY:HA2	1:D:531:LEU:HB2	1.79	0.64
1:D:565:ARG:HH12	1:D:585:ASP:CG	2.05	0.64
1:B:464:GLY:HA3	1:B:512:VAL:HG21	1.79	0.64
1:D:562:HIS:C	1:D:563:GLN:CD	2.65	0.64
1:D:507:ARG:NE	1:D:531:LEU:HD13	2.11	0.64
1:B:537:TYR:HB2	1:B:544:TRP:CZ3	2.32	0.64
1:D:506:ILE:HD12	1:D:506:ILE:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380[B]:ARG:HH12	1:C:387:ASN:C	2.03	0.63
1:B:464:GLY:HA3	1:B:512:VAL:CG2	2.28	0.63
1:D:553:ARG:HH11	1:D:553:ARG:HG2	1.63	0.63
1:B:457:LEU:HD12	1:B:499:MET:HG2	1.80	0.63
1:C:579:ASP:O	1:C:597:MET:HG3	1.99	0.63
1:D:597:MET:HE2	1:D:601:ARG:HH21	1.64	0.63
1:A:329:TYR:CE1	1:A:609:THR:HG22	2.33	0.62
1:D:534:VAL:O	1:D:547:VAL:HG22	1.99	0.62
1:D:394:ASP:OD2	1:D:405:PRO:HA	1.99	0.62
1:D:483:ARG:HB3	1:D:506:ILE:CG2	2.27	0.62
1:D:365:LEU:H	1:D:365:LEU:HD23	1.62	0.62
1:A:362[B]:ARG:HG2	1:A:381:ASN:CA	2.28	0.62
1:A:507:ARG:NH1	1:A:535:GLU:OE2	2.32	0.62
1:B:416:ILE:HD11	1:B:427:ALA:HB1	1.82	0.62
1:C:595:THR:HG22	1:C:596:ARG:N	2.12	0.61
1:A:365:LEU:HD23	1:A:365:LEU:H	1.64	0.61
1:C:534:VAL:HB	1:C:547:VAL:HG23	1.81	0.61
1:D:380:ARG:HE	1:D:388:THR:HG23	1.65	0.61
1:C:470:ARG:O	1:C:471:LEU:HD23	2.01	0.61
1:C:397:ASN:CG	1:C:400:THR:HG22	2.26	0.61
1:C:538:ASP:HB3	1:C:541:THR:HG22	1.82	0.61
1:C:487:ALA:O	1:C:499:MET:HG3	2.00	0.60
1:D:330:THR:O	1:D:342:LEU:HA	2.02	0.60
1:D:524:GLY:C	1:D:555:SER:HB2	2.26	0.60
1:B:575:HIS:CD2	1:D:336:ARG:HD2	2.36	0.60
1:D:346:ASN:HB3	1:D:349:ASP:OD1	2.00	0.60
1:D:554:ARG:CD	1:D:557:LEU:HD21	2.27	0.60
1:A:584:TYR:HB2	1:A:591:TRP:CZ3	2.36	0.60
1:C:395:CYS:HB2	1:C:406:CYS:SG	2.41	0.60
1:D:490:TYR:HB2	1:D:497:TRP:CZ2	2.37	0.60
1:D:524:GLY:O	1:D:555:SER:HB2	2.01	0.60
1:A:597:MET:HE1	1:A:601:ARG:HD2	1.84	0.60
1:D:368:CYS:SG	1:D:425:ILE:HD13	2.42	0.60
1:D:483:ARG:NH2	1:D:527:GLY:HA2	2.16	0.60
1:D:551:LYS:HE2	1:D:551:LYS:HA	1.84	0.60
1:A:345:TYR:CE1	1:A:595:THR:HG21	2.37	0.59
1:A:362[B]:ARG:HG2	1:A:381:ASN:HB3	1.83	0.59
1:C:370:VAL:CG1	1:C:420:VAL:HG11	2.32	0.59
1:C:369:VAL:HG22	1:C:374:LEU:CA	2.30	0.59
1:D:534:VAL:HB	1:D:547:VAL:CG2	2.31	0.59
1:D:414:ASN:HB3	1:D:431:SER:OG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ARG:HG3	1:A:494:ARG:NH1	2.18	0.59
1:B:434:CYS:CB	1:D:434:CYS:SG	2.90	0.59
1:B:519:ILE:HB	1:B:537:TYR:HB3	1.85	0.59
1:D:464:GLY:HA3	1:D:512:VAL:CG2	2.32	0.59
1:C:409:MET:SD	1:C:413:ARG:HD2	2.42	0.59
1:C:466:ALA:HB3	1:C:519:ILE:HD12	1.84	0.59
1:D:522:ALA:CB	1:D:534:VAL:HG13	2.33	0.59
1:B:537:TYR:OH	1:B:542:GLU:HG3	2.03	0.58
1:A:430:GLY:C	1:A:461:ILE:HG22	2.29	0.58
1:D:599:SER:HB3	1:D:601:ARG:NH1	2.19	0.58
1:B:412:PRO:HD2	1:B:432:HIS:CD2	2.39	0.58
1:C:465:VAL:CG1	1:C:472:LEU:HD11	2.33	0.58
1:B:324:VAL:HG22	1:B:324:VAL:O	2.02	0.58
1:D:441:GLU:HB3	1:D:452:LEU:HD12	1.86	0.58
1:A:452:LEU:HD13	1:B:485:ASN:HD21	1.69	0.57
1:C:562:HIS:HB3	1:C:567:TYR:CE1	2.39	0.57
1:D:330:THR:HG22	1:D:343:GLU:O	2.04	0.57
1:D:361:PRO:HG3	1:D:382:ASN:HD22	1.69	0.57
1:A:368:CYS:O	1:A:374:LEU:HD12	2.05	0.57
1:B:383:SER:HB3	1:B:385:ASP:H	1.69	0.57
1:C:585:ASP:HB3	1:C:588:THR:OG1	2.05	0.57
1:A:579:ASP:CG	1:A:596:ARG:HD3	2.30	0.57
1:D:327:LEU:HD22	1:D:346:ASN:CA	2.14	0.57
1:A:443:TYR:HB2	1:A:450:TRP:CE2	2.40	0.56
1:C:397:ASN:HB3	1:C:400:THR:HG22	1.88	0.56
1:C:514:VAL:HB	1:C:519:ILE:HD13	1.88	0.56
1:D:343:GLU:OE2	1:D:598:THR:HG21	2.06	0.56
1:D:568:VAL:HG23	1:D:582:GLU:H	1.69	0.56
1:A:443:TYR:HB2	1:A:450:TRP:CD2	2.41	0.56
2:A:701:A1EMN:O19	2:A:701:A1EMN:N44	2.38	0.56
1:B:468:LEU:CD2	1:B:539:VAL:HG11	2.35	0.56
1:D:584:TYR:HA	1:D:590:THR:O	2.05	0.56
1:D:464:GLY:HA3	1:D:512:VAL:HG21	1.88	0.56
1:A:594:VAL:HG23	1:A:595:THR:HG22	1.88	0.56
1:D:479:ASP:OD1	1:D:482:ASN:HB2	2.06	0.56
1:D:532:ASN:HA	1:D:550:MET:HE3	1.88	0.56
1:D:568:VAL:HG22	1:D:582:GLU:O	2.06	0.56
1:A:584:TYR:HB2	1:A:591:TRP:CH2	2.41	0.55
1:C:383:SER:HB3	1:C:384:PRO:HD2	1.89	0.55
1:C:416:ILE:HD11	1:C:427:ALA:HB1	1.88	0.55
1:D:436:HIS:CE1	1:D:461:ILE:HD13	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:554:ARG:HB2	1:D:557:LEU:HD11	1.89	0.55
1:C:426:TYR:OH	1:C:442:ARG:HD3	2.07	0.55
1:D:561:VAL:CG2	1:D:566:ILE:HG12	2.36	0.55
1:A:483:ARG:HB3	1:A:506:ILE:CG2	2.36	0.55
1:D:523:GLY:HA3	1:D:557:LEU:HD11	1.89	0.55
1:B:470:ARG:HB3	1:B:470:ARG:NH2	2.22	0.55
1:B:537:TYR:OH	1:B:542:GLU:CG	2.55	0.55
1:D:465:VAL:HG13	1:D:472:LEU:HD21	1.88	0.55
1:D:415:ARG:NE	2:D:801:A1EMN:O85	2.37	0.54
1:D:483:ARG:CZ	1:D:527:GLY:HA2	2.37	0.54
1:A:490:TYR:CE2	1:A:492:PRO:HA	2.43	0.54
1:C:538:ASP:O	1:C:542:GLU:N	2.41	0.54
1:A:426:TYR:OH	1:A:442:ARG:HD3	2.07	0.54
1:C:377:VAL:HG22	1:C:393:LEU:HD12	1.90	0.54
1:C:503:MET:CE	1:C:507:ARG:HD2	2.38	0.54
1:D:362:ARG:NH1	1:D:392:ALA:HB3	2.23	0.54
1:B:386:GLY:O	1:B:388:THR:HG23	2.08	0.54
1:C:365:LEU:HD12	1:C:376:ALA:HB1	1.89	0.54
1:A:490:TYR:HB2	1:A:497:TRP:CH2	2.42	0.54
1:C:352:TRP:CZ2	1:C:597:MET:HA	2.43	0.54
1:B:541:THR:OG1	1:B:543:THR:HG22	2.07	0.54
1:C:369:VAL:HG23	1:C:374:LEU:HD12	1.89	0.54
1:B:526:ASP:HB3	1:B:531:LEU:HD21	1.90	0.54
1:C:335:PHE:O	1:C:336:ARG:HB2	2.07	0.54
1:D:584:TYR:OH	1:D:589:ASP:HA	2.08	0.54
1:A:362[B]:ARG:HG2	1:A:381:ASN:CB	2.38	0.54
1:C:377:VAL:HG22	1:C:393:LEU:CD1	2.38	0.54
1:A:568:VAL:C	1:A:569:LEU:HD12	2.32	0.54
1:D:537:TYR:OH	1:D:542:GLU:HG2	2.08	0.54
1:C:520:TYR:CZ	1:C:536:ARG:HD3	2.43	0.53
1:A:435:ILE:HD11	1:B:542:GLU:HB3	1.87	0.53
1:B:443:TYR:HB2	1:B:450:TRP:CE2	2.43	0.53
1:B:486:SER:HB2	1:B:499:MET:HE1	1.91	0.53
1:B:343:GLU:OE2	1:B:598:THR:HG21	2.09	0.53
1:B:536:ARG:HG2	1:B:537:TYR:H	1.72	0.53
1:C:596:ARG:HG2	1:C:596:ARG:HH21	1.74	0.53
1:B:537:TYR:OH	1:B:542:GLU:CD	2.52	0.53
1:D:342:LEU:C	1:D:342:LEU:HD23	2.34	0.53
1:D:436:HIS:ND1	1:D:461:ILE:HD13	2.24	0.52
1:D:581:VAL:O	1:D:594:VAL:HG12	2.09	0.52
1:B:374:LEU:CD1	1:B:607:ALA:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:GLY:O	1:C:461:ILE:HG22	2.09	0.52
1:C:326:ARG:HA	1:C:609:THR:OXT	2.10	0.52
1:C:596:ARG:HG2	1:C:596:ARG:NH2	2.23	0.52
1:D:421:ILE:HG12	1:D:467:VAL:CG1	2.39	0.52
1:D:465:VAL:CG1	1:D:472:LEU:HD21	2.39	0.52
1:D:479:ASP:OD1	1:D:482:ASN:N	2.38	0.52
1:B:399:MET:N	1:B:399:MET:HE2	2.25	0.52
1:C:365:LEU:HD23	1:C:365:LEU:H	1.74	0.52
1:A:472:LEU:HB3	1:A:490:TYR:HB3	1.92	0.52
1:D:334:TYR:HE1	1:D:337:GLN:OE1	1.93	0.52
1:B:538:ASP:O	1:B:542:GLU:N	2.42	0.52
1:B:483:ARG:HB3	1:B:506:ILE:HG21	1.92	0.52
1:C:397:ASN:HB3	1:C:400:THR:HG23	1.92	0.52
1:C:370:VAL:HG12	1:C:420:VAL:HG11	1.92	0.52
1:D:396:TYR:HE1	1:D:401:ASN:OD1	1.93	0.52
1:D:561:VAL:HG22	1:D:566:ILE:CA	2.36	0.52
1:C:470:ARG:HH11	1:C:470:ARG:HB3	1.74	0.51
1:C:518:CYS:HB3	1:C:537:TYR:O	2.10	0.51
1:C:366:ALA:HB3	1:C:418:VAL:CG2	2.40	0.51
1:D:424:HIS:HD2	1:D:442:ARG:HE	1.58	0.51
1:B:443:TYR:HB2	1:B:450:TRP:CD2	2.45	0.51
1:D:457:LEU:N	1:D:488:GLU:OE1	2.34	0.51
1:D:468:LEU:CD2	1:D:539:VAL:HG21	2.40	0.51
1:D:515:LEU:HD21	1:D:586:PRO:HG3	1.93	0.51
1:D:372:GLY:O	1:D:373:LEU:HD23	2.11	0.51
1:A:352:TRP:C	1:A:353:LEU:HD12	2.36	0.51
1:D:430:GLY:C	1:D:461:ILE:HG22	2.35	0.51
1:D:568:VAL:CG2	1:D:582:GLU:H	2.24	0.51
1:D:358:LEU:HD22	1:D:360:VAL:H	1.76	0.51
2:A:701:A1EMN:O17	1:C:602:SER:OG	2.28	0.51
1:A:338:SER:HB2	1:A:382:ASN:HB2	1.93	0.50
1:A:459:ARG:HD3	1:B:543:THR:HG21	1.93	0.50
1:D:339:LEU:HD12	1:D:601:ARG:CD	2.39	0.50
1:D:353:LEU:O	1:D:355:LEU:HD12	2.11	0.50
1:B:381:ASN:OD1	1:B:382:ASN:N	2.45	0.50
1:B:518:CYS:SG	1:B:536:ARG:HD3	2.51	0.50
1:C:569:LEU:N	1:C:569:LEU:HD12	2.26	0.50
1:D:397:ASN:O	1:D:401:ASN:N	2.44	0.50
1:C:565:ARG:HG2	1:C:584:TYR:O	2.11	0.50
1:D:338:SER:OG	1:D:361:PRO:C	2.55	0.50
1:C:369:VAL:HG13	1:C:373:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:HB3	1:A:520:TYR:CE1	2.47	0.50
1:D:510:ALA:CB	1:D:523:GLY:O	2.60	0.50
1:A:396:TYR:CE2	1:A:398:PRO:HA	2.47	0.50
1:D:467:VAL:O	1:D:514:VAL:HG11	2.12	0.49
1:D:554:ARG:HD3	1:D:557:LEU:CD2	2.33	0.49
1:D:584:TYR:OH	1:D:589:ASP:OD1	2.30	0.49
1:B:537:TYR:OH	1:B:542:GLU:OE2	2.26	0.49
1:C:335:PHE:C	1:C:337:GLN:H	2.20	0.49
1:C:483:ARG:HB3	1:C:506:ILE:HG21	1.94	0.49
1:C:366:ALA:HB3	1:C:418:VAL:HG23	1.93	0.49
1:C:431:SER:HB3	1:C:461:ILE:HG21	1.95	0.49
1:D:510:ALA:HA	1:D:523:GLY:O	2.12	0.49
1:D:336:ARG:HD3	1:D:336:ARG:N	2.28	0.49
1:D:490:TYR:CE2	1:D:492:PRO:HA	2.47	0.49
1:A:362[B]:ARG:CG	1:A:381:ASN:HB3	2.43	0.49
1:B:337:GLN:HB2	1:B:382:ASN:HD22	1.78	0.49
1:B:395:CYS:HB2	1:B:406:CYS:SG	2.53	0.49
1:D:490:TYR:HB2	1:D:497:TRP:CE2	2.48	0.49
1:C:490:TYR:HB2	1:C:497:TRP:CH2	2.48	0.49
1:D:376:ALA:O	1:D:393:LEU:HD12	2.12	0.49
1:A:569:LEU:HD12	1:A:569:LEU:N	2.28	0.49
1:B:371:GLY:O	1:B:373:LEU:HD13	2.13	0.49
1:C:436:HIS:NE2	1:C:480:GLY:HA2	2.28	0.49
1:D:374:LEU:HD13	1:D:607:ALA:HB3	1.94	0.48
1:D:421:ILE:CG1	1:D:467:VAL:HG11	2.41	0.48
1:B:398:PRO:C	1:B:399:MET:HE2	2.38	0.48
1:B:459:ARG:O	1:B:479:ASP:HA	2.13	0.48
1:D:468:LEU:HD22	1:D:539:VAL:HG21	1.95	0.48
1:A:537:TYR:HE2	1:A:539:VAL:HG12	1.78	0.48
1:C:397:ASN:CB	1:C:400:THR:HG22	2.43	0.48
1:D:330:THR:O	1:D:330:THR:HG23	2.13	0.48
1:D:415:ARG:NE	2:D:801:A1EMN:C83	2.76	0.48
1:A:326:ARG:HG2	1:A:326:ARG:HH11	1.79	0.48
1:C:380[B]:ARG:NH1	1:C:387:ASN:C	2.68	0.48
1:A:506:ILE:O	1:A:526:ASP:HA	2.14	0.48
1:A:568:VAL:CG2	1:A:582:GLU:HB2	2.44	0.48
1:C:342:LEU:HD22	1:C:403:TRP:CZ2	2.48	0.48
1:C:538:ASP:HB3	1:C:541:THR:HG23	1.92	0.48
2:A:701:A1EMN:N44	1:C:508:SER:OG	2.47	0.47
1:C:436:HIS:O	1:C:459:ARG:HB3	2.13	0.47
1:C:585:ASP:CG	1:C:588:THR:HG23	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ARG:HH22	1:B:439:SER:HB2	1.79	0.47
1:C:369:VAL:HG23	1:C:374:LEU:CD1	2.45	0.47
1:B:349:ASP:OD2	1:B:351:THR:OG1	2.33	0.47
1:B:430:GLY:O	1:B:461:ILE:HG22	2.13	0.47
1:C:568:VAL:O	1:C:581:VAL:HA	2.13	0.47
1:B:381:ASN:O	1:B:387:ASN:HA	2.14	0.47
1:A:361:PRO:HG2	1:A:382:ASN:HB3	1.95	0.47
1:B:327:LEU:O	1:B:608:VAL:HG23	2.14	0.47
1:C:425:ILE:HD12	1:C:443:TYR:CD2	2.42	0.47
1:D:446:GLU:OE2	1:D:447:ARG:HG2	2.15	0.47
1:A:329:TYR:HE1	1:A:609:THR:HG22	1.76	0.47
1:D:365:LEU:HD12	1:D:376:ALA:HB1	1.96	0.47
1:A:518:CYS:SG	1:A:536:ARG:HD2	2.54	0.47
1:A:584:TYR:HB2	1:A:591:TRP:CE3	2.50	0.47
1:A:490:TYR:HB2	1:A:497:TRP:CZ3	2.50	0.47
1:D:506:ILE:H	1:D:506:ILE:CD1	2.24	0.47
1:C:558:GLY:HA3	1:C:606:VAL:HG21	1.96	0.46
1:D:327:LEU:HD21	1:D:346:ASN:CG	2.39	0.46
1:A:537:TYR:HB2	1:A:544:TRP:CE2	2.50	0.46
1:A:345:TYR:CE2	1:A:347:PRO:HA	2.49	0.46
1:B:470:ARG:CZ	1:B:470:ARG:CB	2.93	0.46
1:C:538:ASP:OD1	1:C:540:GLU:HB2	2.15	0.46
1:D:456:MET:HE1	1:D:460:ARG:HD2	1.96	0.46
1:B:468:LEU:HD23	1:B:539:VAL:CG1	2.41	0.46
1:B:537:TYR:HH	1:B:542:GLU:CD	2.21	0.46
1:C:380[B]:ARG:HG2	1:C:380[B]:ARG:HH11	1.80	0.46
1:D:561:VAL:HG22	1:D:566:ILE:HG12	1.97	0.46
1:C:565:ARG:HG2	1:C:585:ASP:HA	1.98	0.46
1:D:345:TYR:HA	1:D:351:THR:O	2.16	0.46
1:A:573:ASP:HB3	1:A:578:LEU:HD21	1.98	0.46
1:B:568:VAL:CG2	1:B:582:GLU:HB2	2.46	0.46
1:C:584:TYR:HB2	1:C:591:TRP:CH2	2.50	0.46
1:C:479:ASP:OD1	1:C:479:ASP:C	2.58	0.46
1:D:465:VAL:HG13	1:D:472:LEU:CD2	2.45	0.46
1:A:413:ARG:HB2	1:A:416:ILE:HD12	1.97	0.45
1:C:397:ASN:CB	1:C:400:THR:CG2	2.91	0.45
1:D:522:ALA:CA	1:D:534:VAL:HG13	2.46	0.45
1:A:562:HIS:HB3	1:A:567:TYR:CE1	2.51	0.45
1:D:339:LEU:O	1:D:361:PRO:HA	2.16	0.45
1:B:506:ILE:O	1:B:526:ASP:HA	2.16	0.45
1:B:551:LYS:HG2	1:B:582:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:TYR:HB2	1:B:591:TRP:CE2	2.52	0.45
1:D:447:ARG:HH11	1:D:449:GLU:CD	2.24	0.45
1:A:333:GLY:O	1:A:363:SER:HB3	2.16	0.45
1:D:358:LEU:HD22	1:D:360:VAL:O	2.17	0.45
1:D:436:HIS:O	1:D:459:ARG:HD3	2.16	0.45
1:A:347:PRO:HG2	1:A:562:HIS:CD2	2.51	0.45
1:B:383:SER:CB	1:B:385:ASP:H	2.30	0.45
1:D:390:SER:O	1:D:412:PRO:HA	2.17	0.45
1:D:491:TYR:HB3	1:D:494:ARG:CZ	2.47	0.45
1:B:345:TYR:CE2	1:B:347:PRO:HA	2.52	0.45
1:C:361:PRO:O	1:C:362:ARG:HG2	2.17	0.45
1:D:341:TYR:HD1	1:D:601:ARG:NH1	2.15	0.45
1:C:417:GLY:HA3	1:C:465:VAL:HG23	2.00	0.44
1:B:541:THR:CB	1:B:543:THR:HG22	2.47	0.44
1:C:374:LEU:CD1	1:C:607:ALA:HB3	2.48	0.44
1:D:531:LEU:O	1:D:553:ARG:HA	2.17	0.44
1:D:585:ASP:HB3	1:D:590:THR:HG1	1.82	0.44
1:A:464:GLY:HA3	1:A:512:VAL:CG2	2.47	0.44
1:A:542:GLU:CG	1:A:542:GLU:O	2.65	0.44
1:B:498:ARG:NE	1:C:481:THR:HG21	2.32	0.44
1:D:341:TYR:HD1	1:D:601:ARG:HH12	1.64	0.44
1:D:505:THR:OG1	1:D:507:ARG:NH1	2.50	0.44
1:D:505:THR:HG23	1:D:546:PHE:HZ	1.82	0.44
1:D:565:ARG:NH1	1:D:585:ASP:CG	2.75	0.44
1:D:588:THR:OG1	1:D:590:THR:HG23	2.18	0.44
1:D:424:HIS:CD2	1:D:442:ARG:HE	2.35	0.44
1:D:523:GLY:HA3	1:D:557:LEU:CD1	2.47	0.44
1:A:456:MET:HE1	1:A:460:ARG:HB2	2.00	0.44
1:A:383:SER:OG	1:A:386:GLY:O	2.32	0.44
1:A:458:THR:HG22	1:A:459:ARG:O	2.17	0.44
1:C:470:ARG:C	1:C:471:LEU:HD23	2.43	0.44
1:B:515:LEU:HD21	1:B:586:PRO:HG3	2.00	0.43
1:D:428:VAL:CA	1:D:440:VAL:HG22	2.25	0.43
1:D:582:GLU:HA	1:D:592:SER:O	2.18	0.43
1:B:421:ILE:HD11	1:B:472:LEU:HB2	1.99	0.43
1:B:584:TYR:HB2	1:B:591:TRP:CD2	2.53	0.43
1:C:490:TYR:HB2	1:C:497:TRP:CZ2	2.53	0.43
1:D:343:GLU:OE1	1:D:601:ARG:NH2	2.50	0.43
1:D:523:GLY:C	1:D:531:LEU:HD12	2.43	0.43
1:D:567:TYR:CE2	1:D:594:VAL:HG11	2.53	0.43
1:C:327:LEU:O	1:C:608:VAL:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:ARG:O	1:C:479:ASP:HA	2.18	0.43
1:C:470:ARG:HB3	1:C:470:ARG:NH1	2.34	0.43
1:D:494:ARG:O	1:D:495:ASN:HB3	2.18	0.43
1:D:588:THR:CB	1:D:590:THR:HG23	2.48	0.43
1:B:569:LEU:N	1:B:569:LEU:HD12	2.34	0.43
1:B:575:HIS:NE2	1:D:336:ARG:HD2	2.33	0.43
1:C:468:LEU:HD13	1:C:514:VAL:HG21	2.00	0.43
1:C:499:MET:HE3	1:C:499:MET:HB2	1.92	0.43
1:B:333:GLY:HA3	1:B:604:VAL:HG12	2.00	0.43
1:C:562:HIS:O	1:C:563:GLN:C	2.61	0.43
1:A:460:ARG:HB3	1:A:463:VAL:HB	2.00	0.43
1:A:528:GLN:OE1	1:C:336:ARG:NH2	2.52	0.43
1:A:552:HIS:HB2	1:A:554:ARG:HH21	1.82	0.43
1:C:503:MET:CE	1:C:521:ALA:CB	2.96	0.43
1:D:598:THR:HB	1:D:601:ARG:HH22	1.83	0.43
1:A:409:MET:HB2	1:A:409:MET:HE3	1.76	0.43
1:D:345:TYR:CE2	1:D:347:PRO:HA	2.53	0.43
1:B:568:VAL:C	1:B:569:LEU:HD12	2.43	0.43
1:C:595:THR:CG2	1:C:596:ARG:H	2.18	0.43
1:B:393:LEU:HD22	1:B:450:TRP:CZ2	2.54	0.42
1:B:483:ARG:HB3	1:B:506:ILE:CG2	2.49	0.42
1:C:430:GLY:C	1:C:461:ILE:HG22	2.43	0.42
1:C:538:ASP:CB	1:C:541:THR:HG22	2.49	0.42
1:C:369:VAL:CG2	1:C:374:LEU:HA	2.36	0.42
1:D:524:GLY:CA	1:D:531:LEU:HD12	2.49	0.42
1:B:336:ARG:NH2	1:D:529:ASP:OD1	2.52	0.42
1:B:420:VAL:O	1:B:467:VAL:HG21	2.18	0.42
1:C:584:TYR:HB2	1:C:591:TRP:CZ2	2.55	0.42
1:D:436:HIS:CE1	1:D:461:ILE:CD1	3.02	0.42
1:C:467:VAL:HG22	1:C:472:LEU:CD1	2.49	0.42
1:C:557:LEU:HD12	1:C:568:VAL:CG1	2.47	0.42
1:A:326:ARG:HG2	1:A:326:ARG:NH1	2.34	0.42
1:A:373:LEU:HD23	1:A:373:LEU:HA	1.94	0.42
1:A:594:VAL:O	1:A:595:THR:HB	2.20	0.42
1:B:413:ARG:HH21	1:B:441:GLU:HG3	1.85	0.42
1:C:503:MET:CE	1:C:521:ALA:HB3	2.48	0.42
1:C:503:MET:HE1	1:C:507:ARG:HD2	2.01	0.42
1:C:598:THR:HG22	1:C:598:THR:O	2.20	0.42
1:C:368:CYS:O	1:C:374:LEU:HD12	2.20	0.41
1:A:530:GLN:HE21	1:A:530:GLN:HB2	1.68	0.41
1:D:335:PHE:O	1:D:337:GLN:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:ASN:O	1:D:430:GLY:HA2	2.20	0.41
1:D:538:ASP:HB3	1:D:541:THR:OG1	2.20	0.41
1:A:330:THR:O	1:A:330:THR:HG23	2.19	0.41
1:D:333:GLY:O	1:D:363:SER:HB3	2.19	0.41
1:D:337:GLN:O	1:D:339:LEU:HD23	2.19	0.41
1:D:428:VAL:HG22	1:D:440:VAL:HG11	2.01	0.41
1:D:584:TYR:CZ	1:D:589:ASP:HA	2.55	0.41
1:D:507:ARG:NH2	1:D:533:SER:OG	2.54	0.41
1:C:370:VAL:HG11	1:C:420:VAL:HG11	2.01	0.41
1:C:383:SER:CB	1:C:384:PRO:HD2	2.50	0.41
1:C:568:VAL:C	1:C:569:LEU:HD12	2.46	0.41
1:D:358:LEU:HD23	1:D:359:GLN:N	2.36	0.41
1:D:598:THR:O	1:D:598:THR:HG22	2.21	0.41
1:B:518:CYS:HB3	1:B:536:ARG:CG	2.50	0.41
1:D:329:TYR:CD1	1:D:329:TYR:N	2.88	0.41
1:D:362:ARG:HD2	1:D:378:GLY:O	2.20	0.41
1:A:359:GLN:H	1:A:359:GLN:HG2	1.75	0.41
1:C:548:ALA:O	1:C:591:TRP:NE1	2.54	0.41
1:C:565:ARG:HE	1:C:565:ARG:HB2	1.70	0.41
1:D:368:CYS:O	1:D:374:LEU:HD12	2.20	0.41
1:A:362[B]:ARG:CZ	1:A:390:SER:OG	2.68	0.41
1:B:334:TYR:HB2	1:B:363:SER:HB3	2.02	0.41
1:B:393:LEU:HD22	1:B:450:TRP:HZ2	1.85	0.41
1:B:419:GLY:HA3	1:B:472:LEU:HD11	2.03	0.41
1:B:551:LYS:HE2	1:B:591:TRP:HB2	2.02	0.41
1:C:353:LEU:HD12	1:C:353:LEU:N	2.35	0.41
1:C:436:HIS:CD2	1:C:480:GLY:HA2	2.56	0.41
1:A:373:LEU:CD2	1:A:397:ASN:HA	2.51	0.41
1:C:326:ARG:HA	1:C:609:THR:C	2.46	0.41
1:C:396:TYR:CZ	1:C:401:ASN:HA	2.56	0.41
1:C:566:ILE:HB	1:C:584:TYR:HB3	2.03	0.41
1:D:347:PRO:HG2	1:D:562:HIS:CE1	2.56	0.41
1:A:435:ILE:CD1	1:B:542:GLU:CB	2.85	0.40
1:C:417:GLY:HA3	1:C:465:VAL:CG2	2.51	0.40
1:D:330:THR:OG1	1:D:604:VAL:HG11	2.21	0.40
1:D:428:VAL:HG13	1:D:440:VAL:CG2	2.45	0.40
1:B:409:MET:HE3	1:B:409:MET:HB2	1.92	0.40
1:B:584:TYR:HB2	1:B:591:TRP:CE3	2.56	0.40
1:C:396:TYR:CE1	1:C:401:ASN:HA	2.56	0.40
1:D:380:ARG:NE	1:D:388:THR:HG23	2.34	0.40
1:A:334:TYR:HB3	2:A:701:A1EMN:O59	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:534:VAL:HB	1:C:547:VAL:HG22	2.00	0.40
1:D:504:ASN:HD22	1:D:504:ASN:N	2.18	0.40
1:B:426:TYR:HA	1:B:441:GLU:O	2.22	0.40
1:C:520:TYR:HH	1:C:536:ARG:HH11	1.61	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	287/288 (100%)	277 (96%)	9 (3%)	1 (0%)	36	70
1	B	284/288 (99%)	271 (95%)	13 (5%)	0	100	100
1	C	285/288 (99%)	269 (94%)	15 (5%)	1 (0%)	30	65
1	D	277/288 (96%)	264 (95%)	11 (4%)	2 (1%)	18	53
All	All	1133/1152 (98%)	1081 (95%)	48 (4%)	4 (0%)	30	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	481	THR
1	D	523	GLY
1	C	384	PRO
1	A	324	VAL

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	235/234 (100%)	235 (100%)	0	100	100
1	B	232/234 (99%)	232 (100%)	0	100	100
1	C	233/234 (100%)	233 (100%)	0	100	100
1	D	228/234 (97%)	228 (100%)	0	100	100
All	All	928/936 (99%)	928 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	382	ASN
1	A	517	ASN
1	A	530	GLN
1	C	432	HIS
1	C	517	ASN
1	D	382	ASN
1	D	402	GLN
1	D	424	HIS
1	D	432	HIS
1	D	436	HIS
1	D	563	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	A1EMN	D	801	-	92,96,96	2.59	29 (31%)	137,141,141	3.10	45 (32%)
2	A1EMN	A	701	-	92,96,96	2.80	31 (33%)	137,141,141	3.17	39 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1EMN	D	801	-	-	30/98/98/98	0/8/8/8
2	A1EMN	A	701	-	-	29/98/98/98	0/8/8/8

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	A1EMN	S13-N12	8.68	1.77	1.65
2	A	701	A1EMN	S14-N11	8.60	1.77	1.65
2	D	801	A1EMN	S13-N12	8.12	1.76	1.65
2	A	701	A1EMN	S71-N70	7.21	1.75	1.65
2	A	701	A1EMN	C72-S71	7.18	1.86	1.76
2	D	801	A1EMN	S14-N11	6.98	1.75	1.65
2	A	701	A1EMN	S56-N57	6.97	1.75	1.65
2	D	801	A1EMN	C72-S71	6.91	1.85	1.76
2	A	701	A1EMN	C15-S14	6.71	1.85	1.76
2	D	801	A1EMN	C15-S14	6.58	1.85	1.76
2	D	801	A1EMN	C53-S56	5.81	1.84	1.76
2	A	701	A1EMN	C34-N33	5.57	1.47	1.35
2	A	701	A1EMN	C53-S56	5.52	1.83	1.76
2	D	801	A1EMN	C34-N33	5.19	1.46	1.35
2	A	701	A1EMN	C39-N40	5.01	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	A1EMN	S56-N57	4.95	1.72	1.65
2	A	701	A1EMN	C16-S13	4.92	1.83	1.76
2	D	801	A1EMN	S71-N70	4.84	1.72	1.65
2	A	701	A1EMN	C87-N88	4.36	1.46	1.32
2	D	801	A1EMN	C83-N84	4.29	1.46	1.32
2	D	801	A1EMN	O58-S56	4.11	1.47	1.43
2	D	801	A1EMN	C47-N48	4.09	1.46	1.32
2	A	701	A1EMN	C83-N84	4.09	1.46	1.32
2	D	801	A1EMN	C87-N88	4.08	1.46	1.32
2	D	801	A1EMN	C16-S13	4.05	1.81	1.76
2	A	701	A1EMN	C47-N48	4.01	1.45	1.32
2	A	701	A1EMN	O58-S56	4.01	1.47	1.43
2	D	801	A1EMN	C39-N40	4.00	1.44	1.35
2	A	701	A1EMN	C28-N33	3.92	1.49	1.41
2	A	701	A1EMN	O74-S71	3.80	1.47	1.43
2	D	801	A1EMN	O74-S71	3.77	1.47	1.43
2	D	801	A1EMN	O17-S13	3.76	1.47	1.43
2	D	801	A1EMN	C43-N44	3.75	1.44	1.32
2	D	801	A1EMN	C28-N33	3.67	1.49	1.41
2	A	701	A1EMN	O17-S13	3.55	1.47	1.43
2	A	701	A1EMN	C43-N44	3.51	1.44	1.32
2	D	801	A1EMN	O59-S56	3.45	1.47	1.43
2	D	801	A1EMN	O18-S13	3.37	1.47	1.43
2	A	701	A1EMN	O59-S56	3.31	1.47	1.43
2	A	701	A1EMN	C62-C61	-3.27	1.37	1.43
2	A	701	A1EMN	O18-S13	3.06	1.46	1.43
2	D	801	A1EMN	C05-C04	-2.93	1.37	1.43
2	A	701	A1EMN	O20-S14	2.91	1.46	1.43
2	D	801	A1EMN	O19-S14	2.87	1.46	1.43
2	A	701	A1EMN	O73-S71	2.82	1.46	1.43
2	A	701	A1EMN	O19-S14	2.75	1.46	1.43
2	A	701	A1EMN	C05-C04	-2.74	1.38	1.43
2	D	801	A1EMN	O73-S71	2.74	1.46	1.43
2	D	801	A1EMN	C62-C61	-2.69	1.38	1.43
2	D	801	A1EMN	O36-C34	-2.53	1.18	1.23
2	A	701	A1EMN	C65-C64	2.52	1.42	1.38
2	D	801	A1EMN	O50-C39	-2.45	1.18	1.23
2	A	701	A1EMN	C41-N40	2.44	1.46	1.41
2	D	801	A1EMN	C08-C09	2.33	1.42	1.38
2	D	801	A1EMN	O20-S14	2.30	1.46	1.43
2	A	701	A1EMN	O36-C34	-2.18	1.18	1.23
2	D	801	A1EMN	C65-C64	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	A1EMN	C38-C39	2.09	1.55	1.51
2	A	701	A1EMN	O50-C39	-2.06	1.19	1.23
2	A	701	A1EMN	O80-C77	2.03	1.41	1.37

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	A1EMN	O19-S14-O20	-12.20	100.55	119.59
2	A	701	A1EMN	O19-S14-O20	-11.85	101.09	119.59
2	A	701	A1EMN	O17-S13-O18	-11.75	101.26	119.59
2	A	701	A1EMN	O59-S56-O58	-11.60	101.48	119.59
2	D	801	A1EMN	O59-S56-O58	-11.52	101.61	119.59
2	A	701	A1EMN	O74-S71-O73	-11.41	101.78	119.59
2	D	801	A1EMN	O17-S13-O18	-11.30	101.96	119.59
2	D	801	A1EMN	O74-S71-O73	-11.27	102.00	119.59
2	A	701	A1EMN	O58-S56-N57	10.01	118.34	106.69
2	A	701	A1EMN	O19-S14-N11	8.37	116.44	106.69
2	A	701	A1EMN	C86-N57-C60	8.01	127.07	117.38
2	D	801	A1EMN	O59-S56-N57	7.58	115.52	106.69
2	D	801	A1EMN	C82-N70-C63	7.37	126.30	117.38
2	A	701	A1EMN	C42-N11-S14	7.01	131.68	117.47
2	A	701	A1EMN	C42-N11-C10	-6.48	109.54	117.38
2	D	801	A1EMN	C86-N57-C60	6.43	125.16	117.38
2	A	701	A1EMN	O59-S56-N57	6.39	114.13	106.69
2	A	701	A1EMN	O17-S13-N12	6.07	113.76	106.69
2	D	801	A1EMN	O58-S56-N57	5.96	113.62	106.69
2	D	801	A1EMN	C15-S14-N11	5.93	114.72	106.97
2	A	701	A1EMN	C53-S56-N57	-5.88	99.29	106.97
2	A	701	A1EMN	C41-N40-C39	-5.65	117.52	127.52
2	D	801	A1EMN	C43-C42-N11	5.44	123.99	112.44
2	D	801	A1EMN	O74-S71-N70	5.26	112.81	106.69
2	D	801	A1EMN	O58-S56-C53	5.16	114.52	108.10
2	D	801	A1EMN	C53-S56-N57	-5.12	100.28	106.97
2	A	701	A1EMN	C72-S71-N70	5.09	113.62	106.97
2	A	701	A1EMN	O59-S56-C53	5.08	114.42	108.10
2	D	801	A1EMN	O19-S14-N11	4.72	112.18	106.69
2	A	701	A1EMN	C43-C42-N11	4.71	122.45	112.44
2	D	801	A1EMN	O18-S13-N12	4.70	112.16	106.69
2	D	801	A1EMN	C41-N40-C39	-4.66	119.27	127.52
2	D	801	A1EMN	C42-C43-N44	4.65	124.99	115.61
2	D	801	A1EMN	O17-S13-N12	4.53	111.96	106.69
2	D	801	A1EMN	O74-S71-C72	4.32	113.47	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	A1EMN	C16-S13-N12	4.31	112.60	106.97
2	A	701	A1EMN	C16-S13-N12	4.18	112.43	106.97
2	A	701	A1EMN	C28-N33-C34	-3.95	120.53	127.52
2	A	701	A1EMN	O18-S13-N12	3.89	111.22	106.69
2	D	801	A1EMN	O19-S14-C15	3.89	112.94	108.10
2	A	701	A1EMN	O20-S14-N11	3.86	111.18	106.69
2	A	701	A1EMN	C46-N12-C07	3.81	121.99	117.38
2	D	801	A1EMN	O73-S71-N70	3.78	111.09	106.69
2	D	801	A1EMN	O73-S71-C72	3.77	112.78	108.10
2	D	801	A1EMN	C09-C10-N11	3.63	124.02	119.75
2	A	701	A1EMN	C38-C39-N40	3.63	120.91	114.59
2	A	701	A1EMN	O74-S71-N70	3.62	110.90	106.69
2	A	701	A1EMN	C15-S14-N11	3.49	111.53	106.97
2	A	701	A1EMN	C42-C43-N44	3.48	122.62	115.61
2	A	701	A1EMN	C35-C34-N33	3.43	120.56	114.59
2	D	801	A1EMN	C83-C82-N70	3.36	119.57	112.44
2	D	801	A1EMN	O18-S13-C16	3.34	112.25	108.10
2	D	801	A1EMN	C42-N11-S14	3.31	124.18	117.47
2	D	801	A1EMN	C46-C47-N48	3.16	121.98	115.61
2	A	701	A1EMN	C69-C62-C63	-3.12	117.38	122.81
2	A	701	A1EMN	C82-N70-C63	3.09	121.11	117.38
2	D	801	A1EMN	C28-N33-C34	-3.06	122.11	127.52
2	D	801	A1EMN	O59-S56-C53	3.06	111.90	108.10
2	D	801	A1EMN	C35-C34-N33	3.05	119.90	114.59
2	D	801	A1EMN	C46-N12-C07	2.90	120.88	117.38
2	D	801	A1EMN	O50-C39-N40	-2.83	118.57	123.64
2	D	801	A1EMN	C64-C63-N70	-2.80	116.47	119.75
2	A	701	A1EMN	O73-S71-N70	2.74	109.88	106.69
2	D	801	A1EMN	C81-O80-C77	-2.70	111.70	117.50
2	D	801	A1EMN	C26-C16-S13	-2.68	117.07	119.73
2	A	701	A1EMN	C66-C61-C60	-2.61	118.28	122.81
2	A	701	A1EMN	O73-S71-C72	2.59	111.33	108.10
2	D	801	A1EMN	C66-C61-C60	-2.56	118.36	122.81
2	A	701	A1EMN	O50-C39-N40	-2.54	119.08	123.64
2	D	801	A1EMN	C42-N11-C10	2.54	120.45	117.38
2	A	701	A1EMN	C63-C62-C61	2.43	121.84	119.33
2	A	701	A1EMN	C32-O31-C23	-2.40	112.36	117.50
2	D	801	A1EMN	O17-S13-C16	-2.32	105.21	108.10
2	D	801	A1EMN	O45-C43-C42	-2.30	116.72	120.77
2	D	801	A1EMN	C69-C62-C63	-2.27	118.86	122.81
2	D	801	A1EMN	C65-C60-N57	-2.20	117.17	119.75
2	A	701	A1EMN	C66-C61-C62	2.14	121.08	118.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	A1EMN	C30-C16-S13	2.14	121.86	119.73
2	D	801	A1EMN	O20-S14-N11	2.08	109.11	106.69
2	D	801	A1EMN	C37-C35-C34	-2.06	107.47	113.19
2	A	701	A1EMN	C82-N70-S71	2.06	121.65	117.47
2	A	701	A1EMN	O45-C43-C42	-2.05	117.15	120.77
2	A	701	A1EMN	C06-C05-C10	-2.05	119.25	122.81
2	A	701	A1EMN	O36-C34-C35	-2.00	118.39	122.02

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	A1EMN	C43-C42-N11-C10
2	A	701	A1EMN	C43-C42-N11-S14
2	A	701	A1EMN	N57-C86-C87-N88
2	A	701	A1EMN	N57-C86-C87-O89
2	D	801	A1EMN	C83-C82-N70-C63
2	D	801	A1EMN	C83-C82-N70-S71
2	A	701	A1EMN	C24-C23-O31-C32
2	A	701	A1EMN	C22-C23-O31-C32
2	A	701	A1EMN	C76-C77-O80-C81
2	D	801	A1EMN	C24-C23-O31-C32
2	D	801	A1EMN	C22-C23-O31-C32
2	A	701	A1EMN	C78-C77-O80-C81
2	D	801	A1EMN	C76-C77-O80-C81
2	D	801	A1EMN	C78-C77-O80-C81
2	D	801	A1EMN	C51-C41-N40-C39
2	D	801	A1EMN	C55-C41-N40-C39
2	D	801	A1EMN	N12-C46-C47-O49
2	A	701	A1EMN	C46-N12-S13-O17
2	A	701	A1EMN	C42-N11-S14-O20
2	A	701	A1EMN	C42-N11-S14-O19
2	A	701	A1EMN	C82-N70-S71-O73
2	A	701	A1EMN	C82-N70-S71-O74
2	D	801	A1EMN	C46-N12-S13-O17
2	D	801	A1EMN	C42-N11-S14-O20
2	A	701	A1EMN	C47-C46-N12-C07
2	D	801	A1EMN	N12-C46-C47-N48
2	A	701	A1EMN	C46-N12-S13-O18
2	A	701	A1EMN	C82-N70-S71-C72
2	A	701	A1EMN	C55-C41-N40-C39
2	D	801	A1EMN	C79-C72-S71-O73

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Mol	Chain	Res	Type	Atoms
2	D	801	A1EMN	C75-C72-S71-O73
2	A	701	A1EMN	C63-N70-S71-O74
2	A	701	A1EMN	C51-C41-N40-C39
2	D	801	A1EMN	C46-N12-S13-O18
2	D	801	A1EMN	C82-N70-S71-O74
2	A	701	A1EMN	C87-C86-N57-C60
2	A	701	A1EMN	C21-C15-S14-O19
2	A	701	A1EMN	C25-C15-S14-O19
2	D	801	A1EMN	C86-N57-S56-O59
2	A	701	A1EMN	C07-N12-S13-O17
2	A	701	A1EMN	C46-N12-S13-C16
2	A	701	A1EMN	C42-N11-S14-C15
2	D	801	A1EMN	C46-N12-S13-C16
2	D	801	A1EMN	C42-N11-S14-C15
2	D	801	A1EMN	C42-N11-S14-O19
2	D	801	A1EMN	N70-C82-C83-O85
2	D	801	A1EMN	N57-C86-C87-N88
2	D	801	A1EMN	N57-C86-C87-O89
2	D	801	A1EMN	C79-C72-S71-N70
2	D	801	A1EMN	N70-C82-C83-N84
2	D	801	A1EMN	C75-C72-S71-N70
2	D	801	A1EMN	C25-C15-S14-O19
2	A	701	A1EMN	C10-N11-S14-O20
2	A	701	A1EMN	C35-C37-C38-C39
2	D	801	A1EMN	C86-N57-S56-C53
2	D	801	A1EMN	C21-C15-S14-O19
2	A	701	A1EMN	C34-C35-C37-C38
2	D	801	A1EMN	C87-C86-N57-C60
2	A	701	A1EMN	C83-C82-N70-S71

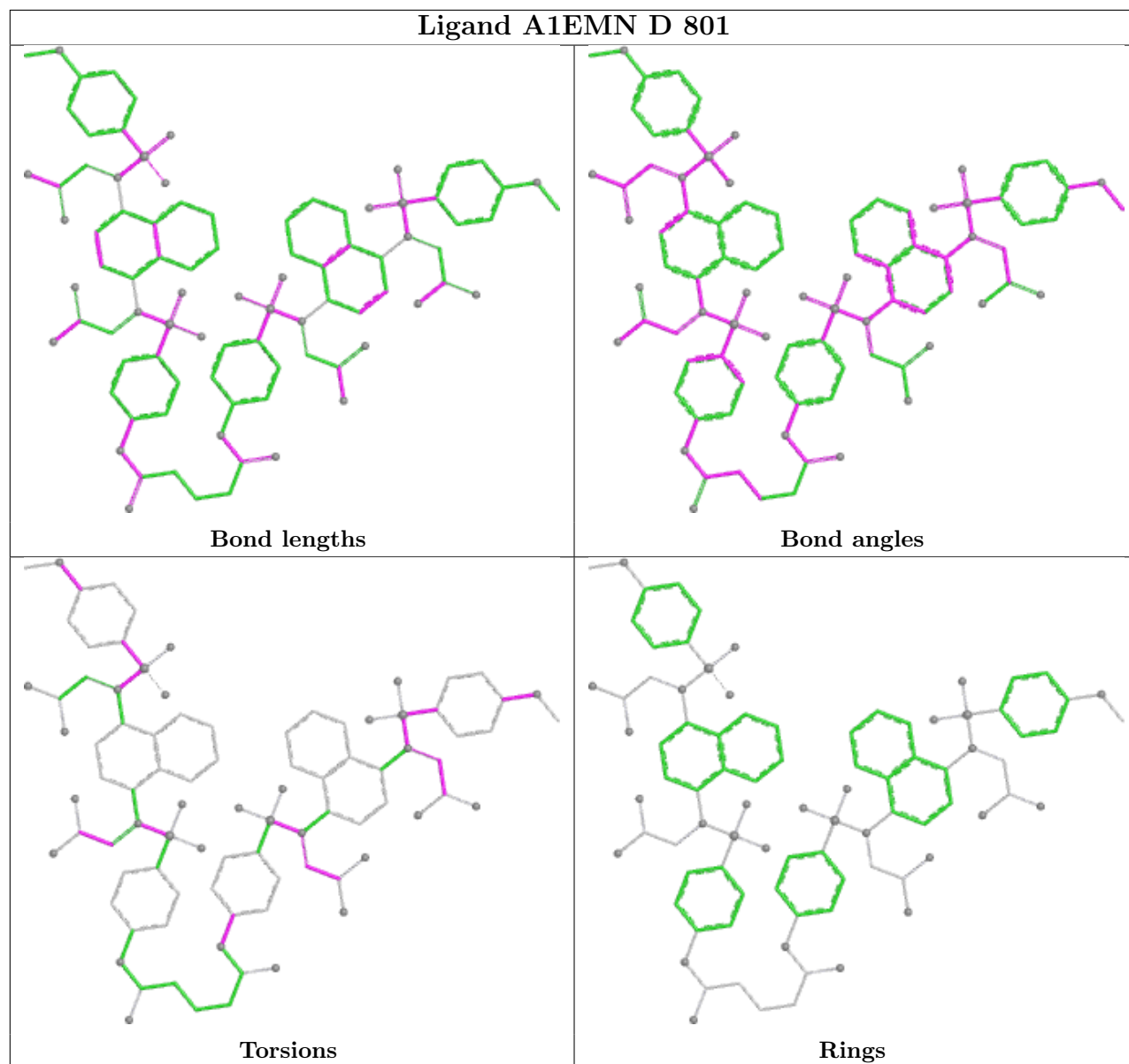
There are no ring outliers.

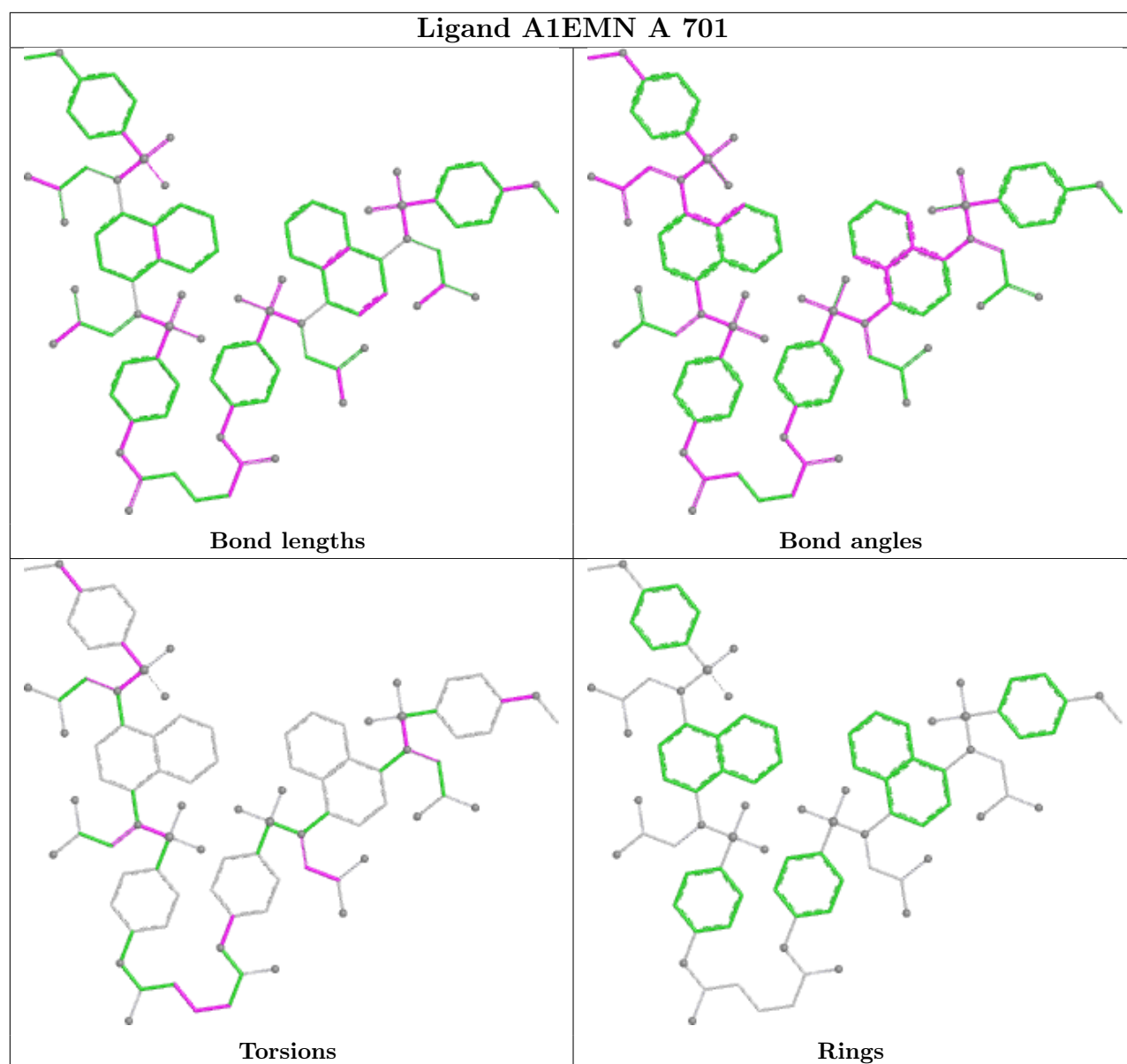
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	A1EMN	5	0
2	A	701	A1EMN	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 [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	288/288 (100%)	-0.12	4 (1%) 73 51	27, 58, 89, 126	1 (0%)
1	B	286/288 (99%)	-0.04	3 (1%) 79 59	47, 66, 93, 136	0
1	C	286/288 (99%)	0.31	7 (2%) 59 36	34, 78, 102, 125	1 (0%)
1	D	280/288 (97%)	1.14	32 (11%) 10 6	70, 112, 135, 146	1 (0%)
All	All	1140/1152 (98%)	0.32	46 (4%) 42 23	27, 73, 125, 146	3 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	382	ASN	4.6
1	C	324	VAL	4.2
1	D	388	THR	3.8
1	A	322	PRO	3.8
1	D	332	GLY	3.4
1	D	372	GLY	3.3
1	D	373	LEU	3.2
1	D	341	TYR	3.0
1	B	324	VAL	3.0
1	D	548	ALA	2.9
1	D	552	HIS	2.9
1	D	443	TYR	2.8
1	D	523	GLY	2.8
1	B	434	CYS	2.7
1	D	533	SER	2.7
1	C	384	PRO	2.6
1	D	431	SER	2.6
1	D	506	ILE	2.6
1	D	360	VAL	2.5
1	D	494	ARG	2.4
1	B	381	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	353	LEU	2.4
1	D	425	ILE	2.4
1	D	435	ILE	2.4
1	D	564	GLY	2.4
1	C	341	TYR	2.4
1	D	329	TYR	2.4
1	D	534	VAL	2.3
1	D	400	THR	2.3
1	D	520	TYR	2.2
1	D	505	THR	2.2
1	D	325	GLY	2.2
1	C	551	LYS	2.2
1	D	476	GLY	2.2
1	A	325	GLY	2.1
1	C	354	ARG	2.1
1	D	566	ILE	2.1
1	C	542	GLU	2.1
1	A	324	VAL	2.1
1	C	351	THR	2.1
1	D	437	HIS	2.0
1	D	608	VAL	2.0
1	A	323	LYS	2.0
1	D	434	CYS	2.0
1	D	518	CYS	2.0
1	D	457	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

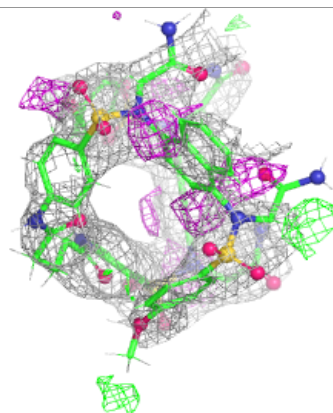
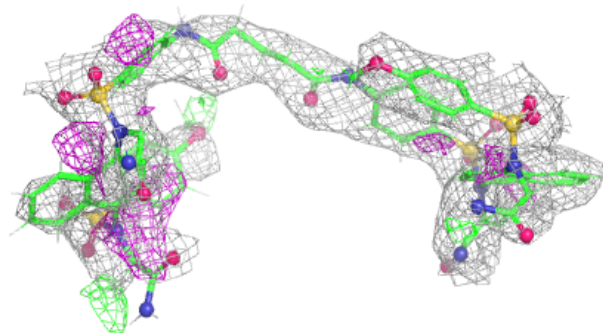
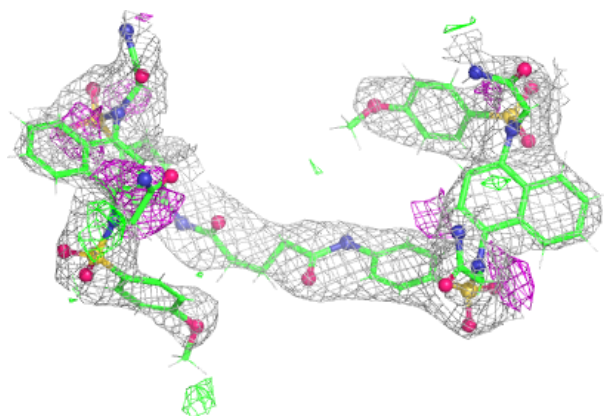
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1EMN	D	801	89/89	0.89	0.17	58,113,162,179	0
2	A1EMN	A	701	89/89	0.94	0.12	56,90,118,140	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.

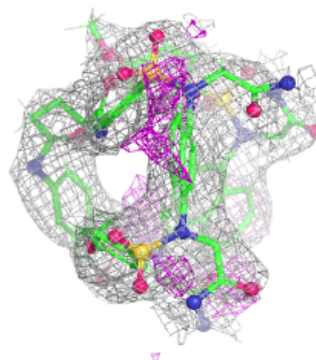
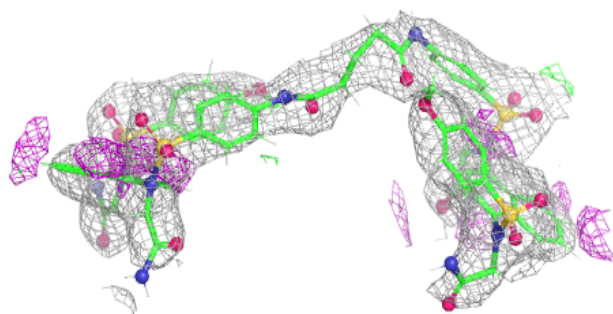
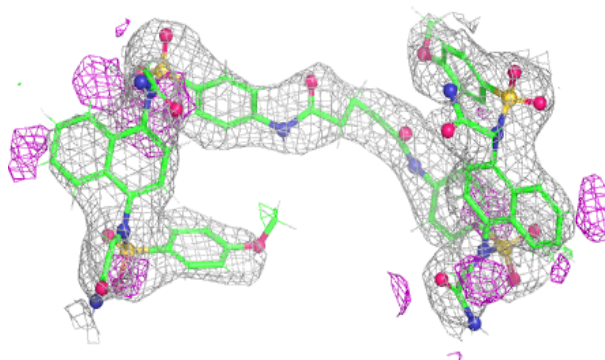
Electron density around A1EMN D 801:

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 A1EMN A 701:

$2mF_o - DF_c$ (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.