Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 07:46 AM EDT

PDB ID	:	3Q7J
Title	:	Engineered Thermoplasma Acidophilum F3 factor mimics human aminopeptidase N (APN) as a target for anticancer drug development
Authors	:	Su, J.; Wang, Q.; Feng, J.; Zhang, C.; Zhu, D.; We, T.; Xu, W.; Gu, L.
Deposited on	:	2011-01-05
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 (i) 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 (i)) were used in the production of this report:

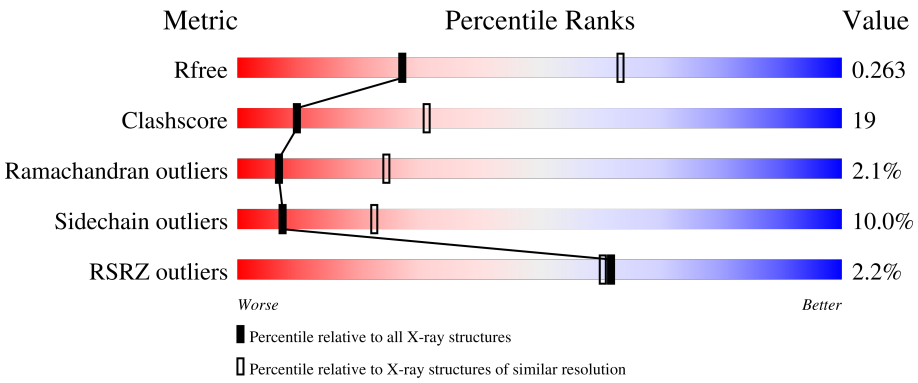
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (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 <=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	780	2% 62% 33% 5%
1	B	780	3% 60% 34% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12639 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 Tricorn protease-interacting factor F3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	780	6294	4008	1066	1189	31	2	0	0
1	B	780	6294	4008	1066	1189	31	8	0	0

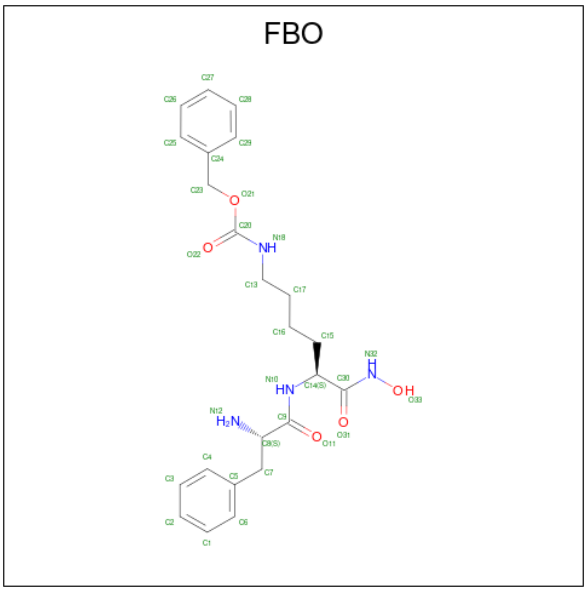
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	GLN	GLU	ENGINEERED MUTATION	UNP O93655
A	261	THR	ASN	ENGINEERED MUTATION	UNP O93655
B	101	GLN	GLU	ENGINEERED MUTATION	UNP O93655
B	261	THR	ASN	ENGINEERED MUTATION	UNP O93655

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is L-phenylalanyl-N6-[(benzyloxy)carbonyl]-N1-hydroxy-L-lysinamide (three-letter code: FBO) (formula: $C_{23}H_{30}N_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	32	23	4	5	0	0

- Molecule 4 is water.

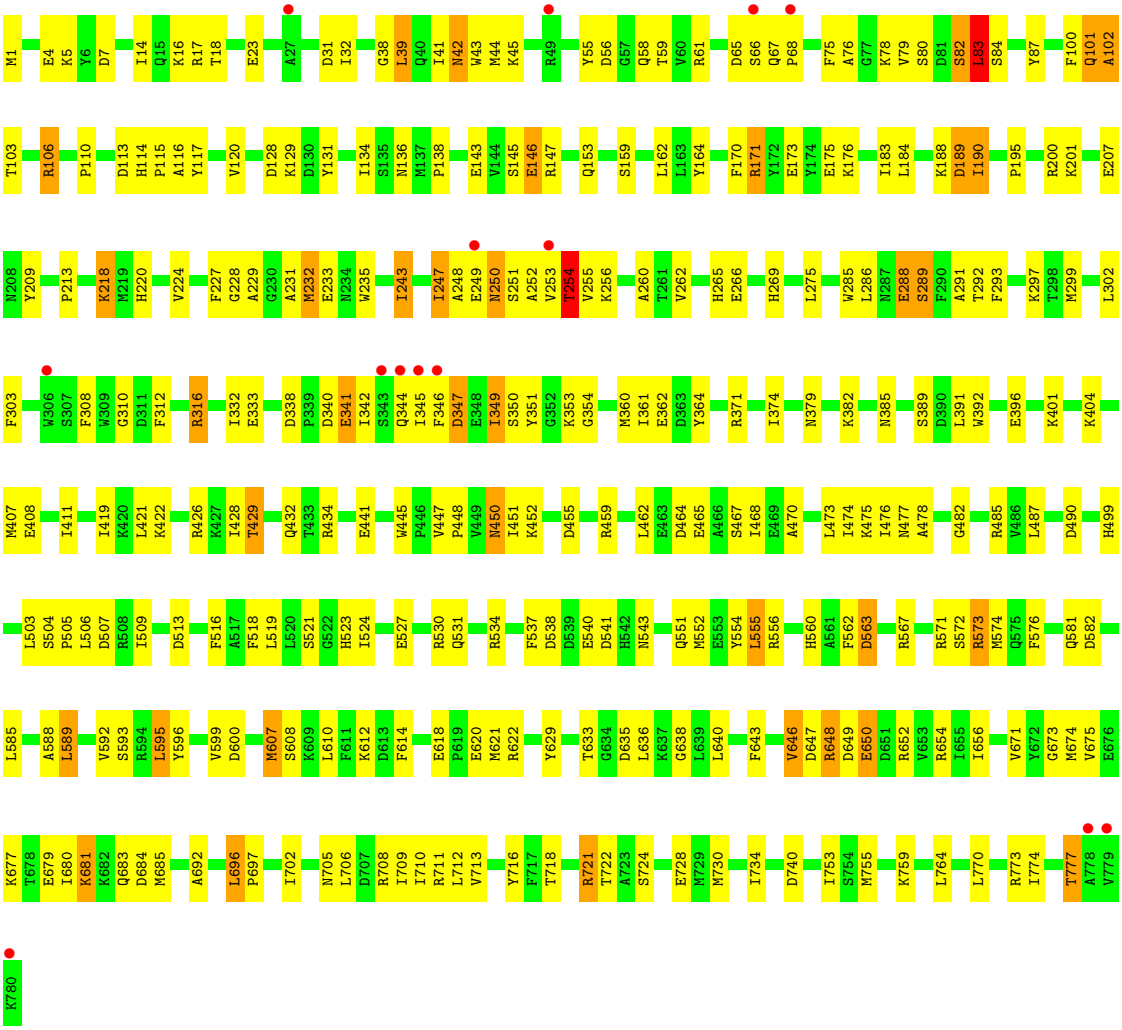
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	7	7	7	0	0
			Total	O		
4	B	10	10	10	0	0

3 Residue-property plots (i)

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

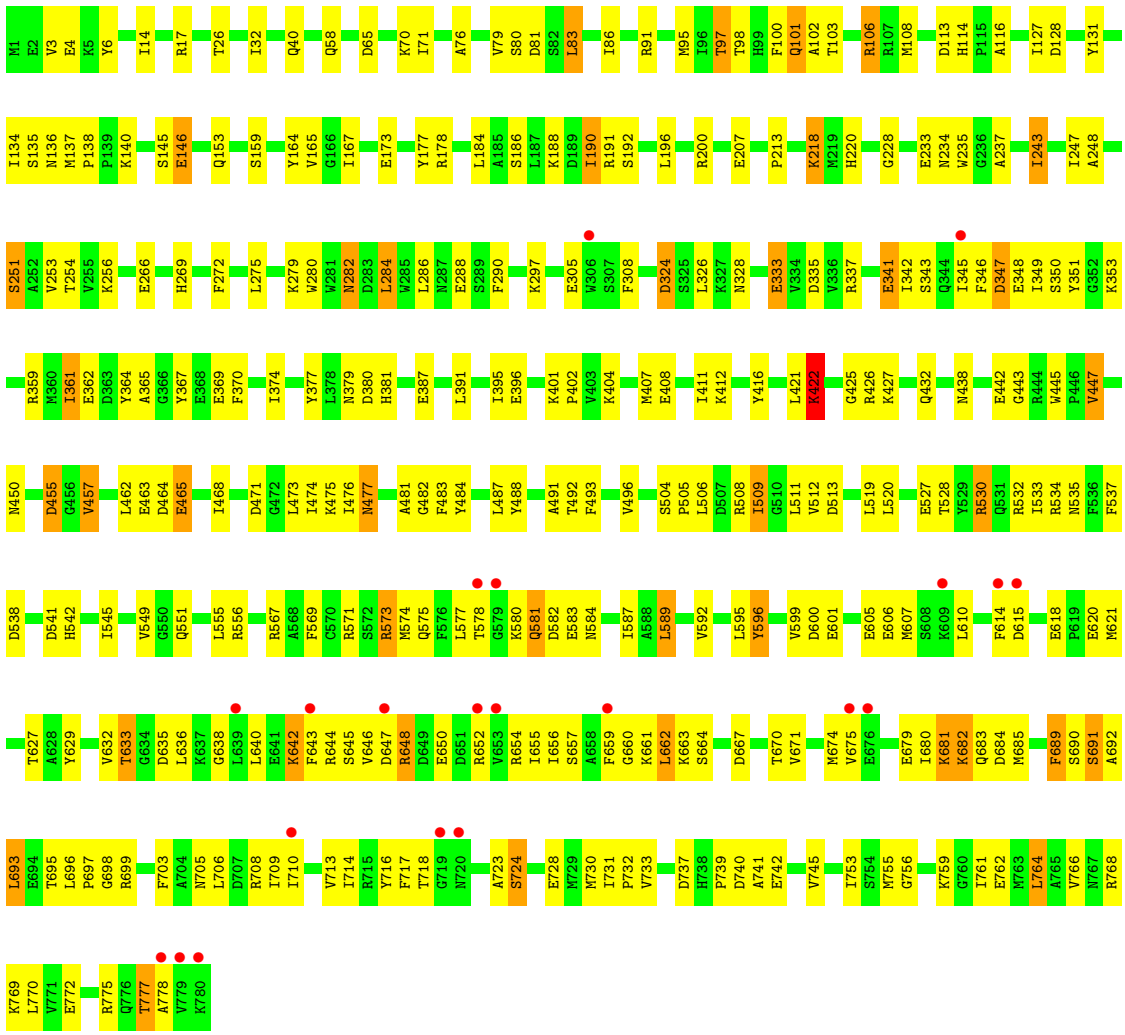
• Molecule 1: Tricorn protease-interacting factor F3

Chain A: 2% 62% 33% 5%



• Molecule 1: Tricorn protease-interacting factor F3

Chain B: 3% 60% 34% 5%


M1 E2 V3 E4 K5 Y6 I14 R17 T26 I32 Q40 Q68 D65 K70 I71 A76 V79 S80 D81 S82 L83 I86 R91 M95 I96 T97 T98 H99 F100 Q101 A102 T103 R106 R107 M108 D113 H114 P115 A116 I127 D128 Y131
I134 S135 N136 M137 P138 P139 K140 S145 E146 Q153 S159 Y164 V165 G166 I167 E173 Y177 R178 L184 A185 S186 L187 K188 D189 I190 R191 S192 L196 R200 E207 P213 K218 M219 H220 G228 E233 N234 W235 G236 A237 I243 I247 A248
S251 A252 V253 T254 V255 K256 E266 H269 F272 L275 K279 W280 W281 N282 D283 L284 W285 L286 N287 E288 S289 F290 K297 E305 W306 S307 F308 D324 S325 L326 K327 N328 E333 V334 D335 V336 R337 E341 I342 S343 Q344 I345 F346 D347 E348 I349 S350 Y351 G352 K353
R359 M360 I361 E362 D363 Y364 A365 G366 Y367 E368 E369 F370 I374 Y377 L378 N379 D380 H381 E387 L391 I395 E396 K401 P402 V403 K404 M407 E408 I411 K412 Y416 L421 K422 G425 R426 K427 Q432 N438 E442 G443 R444 W445 P446 V447
N450 D455 G456 V457 L462 E463 D464 E465 I468 D471 G472 L473 I474 K475 I476 N477 A481 G482 F483 Y484 L487 Y488 A491 T492 F493 V496 S504 P505 L506 D507 R508 I509 G510 L511 V512 D513 L519 L520 E527 T528 Y529 R530 Q531 R532 I533 R534 N535 F536 F537
D538 D541 H542 I545 V549 G550 Q551 L555 R556 R567 A568 F569 C570 R571 S572 R573 M574 Q575 F576 L577 T578 G579 K580 Q581 D582 E583 N584 I587 A588 L589 V592 L595 Y596 V599 D600 E601 E605 E606 M607 S608 K609 L610 F614 D615 E618 F619 E620 M621
T627 A628 Y629 V632 T633 G634 D635 L636 K637 G638 L639 L640 E641 K642 F643 R644 S645 V646 D647 R648 D649 E650 D651 R652 V653 R654 I655 I656 S657 A658 F659 G660 K661 L662 K663 S664 D667 T670 V671 M674 V675 E676 E679 I680 K681 K682 Q683 D684 M685 F689 S690 S691 A692
L693 E694 T695 L696 P697 G698 R699 F703 A704 N705 L706 D707 R708 I709 I710 V713 I714 R715 Y716 F717 T718 G719 N720 A723 S724 E728 M729 M730 I731 P732 V733 D737 H738 P739 D740 A741 E742 V745 I753 S754 M755 G756 K759 G760 I761 E762 M763 L764 A765 V766 N767 R768
K769 L770 V771 E772 R775 Q776 T777 A778 V779 K780

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	114.72Å 183.10Å 105.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.95 – 2.91 48.61 – 2.91	Depositor EDS
% Data completeness (in resolution range)	96.1 (47.95-2.91) 99.5 (48.61-2.91)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.202 , 0.271 0.197 , 0.263	Depositor DCC
R_{free} test set	2488 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	53.0	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12639	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, FBO

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	0.46	0/6428	0.62	0/8676
1	B	0.44	0/6428	0.59	0/8676
All	All	0.45	0/12856	0.61	0/17352

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	101	GLN	Peptide

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	6294	0	6209	226	0
1	B	6294	0	6209	254	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	32	0	30	12	0
4	A	7	0	0	0	0
4	B	10	0	0	2	0
All	All	12639	0	12448	481	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 19.

All (481) 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:B:573:ARG:HE	1:B:573:ARG:HA	1.25	1.01
1:A:527:GLU:HG2	1:A:530:ARG:HH21	1.31	0.96
1:B:136:ASN:HD21	1:B:164:TYR:H	1.12	0.93
1:A:101:GLN:HG2	3:A:900:FBO:H6	1.52	0.92
1:A:247:ILE:HD13	1:A:247:ILE:H	1.35	0.90
1:A:705:ASN:O	1:A:709:ILE:HG12	1.72	0.89
1:A:421:LEU:HD23	1:A:428:ILE:HG21	1.53	0.89
1:A:351:TYR:HB2	3:A:900:FBO:H23A	1.56	0.87
1:A:195:PRO:HG3	1:A:247:ILE:HD11	1.57	0.87
1:A:521:SER:OG	1:A:523:HIS:HD2	1.60	0.84
1:B:365:ALA:O	1:B:369:GLU:HG3	1.78	0.83
1:A:432:GLN:HE22	1:A:445:TRP:H	1.26	0.82
1:B:581:GLN:H	1:B:581:GLN:HE21	1.27	0.81
1:A:114:HIS:HD2	1:A:116:ALA:H	1.25	0.81
1:A:136:ASN:HD21	1:A:164:TYR:H	1.29	0.81
1:B:191:ARG:HH21	1:B:248:ALA:HB2	1.44	0.80
1:B:573:ARG:HA	1:B:573:ARG:NE	1.96	0.80
1:B:618:GLU:HB3	1:B:620:GLU:OE2	1.83	0.79
1:A:721:ARG:HB3	1:A:721:ARG:CZ	2.10	0.78
1:A:374:ILE:HD13	1:A:391:LEU:HD11	1.65	0.78
1:B:114:HIS:HD2	1:B:116:ALA:H	1.28	0.77
1:B:103:THR:O	1:B:106:ARG:HD3	1.85	0.76
1:A:450:ASN:HD21	1:A:478:ALA:H	1.33	0.76
1:A:721:ARG:HB3	1:A:721:ARG:NH1	2.01	0.75
1:B:573:ARG:HE	1:B:573:ARG:CA	1.98	0.74
1:B:567:ARG:HD3	1:B:599:VAL:O	1.86	0.74
1:A:207:GLU:HG2	1:A:213:PRO:HA	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:709:ILE:O	1:B:713:VAL:HG23	1.86	0.74
1:A:516:PHE:HZ	1:A:554:TYR:CD2	2.05	0.74
1:B:682:LYS:NZ	1:B:716:TYR:HB3	2.03	0.73
1:A:101:GLN:CG	3:A:900:FBO:H6	2.19	0.72
1:A:288:GLU:OE1	1:A:288:GLU:HA	1.89	0.72
1:B:695:THR:O	1:B:699:ARG:HG3	1.90	0.72
1:B:341:GLU:HB2	1:B:345:ILE:HG22	1.70	0.71
1:B:728:GLU:OE1	1:B:759:LYS:HD3	1.90	0.71
1:A:103:THR:O	1:A:106:ARG:HD3	1.90	0.71
1:B:581:GLN:HE21	1:B:581:GLN:N	1.88	0.70
1:A:23:GLU:OE1	1:A:110:PRO:HG2	1.92	0.70
1:B:520:LEU:HD23	1:B:770:LEU:HD22	1.74	0.70
1:A:721:ARG:HH11	1:A:722:THR:H	1.37	0.70
1:A:530:ARG:HD2	1:A:534:ARG:NH1	2.06	0.69
1:A:629:TYR:CE1	1:A:633:THR:HG21	2.27	0.69
1:B:606:GLU:HG2	1:B:607:MET:HE3	1.75	0.69
1:A:171:ARG:HG3	1:A:171:ARG:HH11	1.57	0.69
1:B:404:LYS:O	1:B:408:GLU:HG3	1.93	0.69
1:B:253:VAL:HB	1:B:583:GLU:HG2	1.75	0.69
1:B:359:ARG:NH2	1:B:481:ALA:HA	2.07	0.69
1:B:737:ASP:O	1:B:739:PRO:HD3	1.93	0.69
1:B:297:LYS:HE3	1:B:362:GLU:OE1	1.93	0.69
1:A:516:PHE:HZ	1:A:554:TYR:HD2	1.40	0.68
1:B:614:PHE:CZ	1:B:655:ILE:HD11	2.28	0.68
1:A:101:GLN:HG2	3:A:900:FBO:C6	2.23	0.68
1:B:346:PHE:HD1	1:B:351:TYR:CE2	2.11	0.68
1:B:192:SER:HB3	1:B:247:ILE:O	1.94	0.67
1:A:114:HIS:CD2	1:A:116:ALA:H	2.08	0.67
1:A:260:ALA:HB1	1:A:299:MET:SD	2.35	0.67
1:B:114:HIS:CD2	1:B:116:ALA:H	2.10	0.67
1:B:680:ILE:O	1:B:681:LYS:O	2.13	0.67
1:A:82:SER:O	1:A:84:SER:N	2.28	0.66
1:B:636:LEU:HD21	1:B:670:THR:HG21	1.78	0.66
1:B:83:LEU:HD23	1:B:83:LEU:O	1.95	0.66
1:A:347:ASP:HB3	1:A:349:ILE:H	1.61	0.66
1:A:477:ASN:HD21	1:A:482:GLY:H	1.43	0.66
1:B:364:TYR:OH	1:B:402:PRO:HD2	1.96	0.65
1:B:577:LEU:O	1:B:589:LEU:HD13	1.97	0.65
1:A:184:LEU:HD22	1:A:190:ILE:HD12	1.77	0.65
1:B:184:LEU:HB2	1:B:196:LEU:HD21	1.78	0.65
1:B:173:GLU:HG2	1:B:190:ILE:HG13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ARG:HB3	1:A:79:VAL:HB	1.77	0.64
1:B:636:LEU:HD13	1:B:667:ASP:HB3	1.79	0.64
1:A:728:GLU:HG3	1:A:759:LYS:HB3	1.80	0.64
1:B:32:ILE:HD11	1:B:71:ILE:HD12	1.80	0.64
1:B:3:VAL:HG11	1:B:6:TYR:CE2	2.33	0.64
1:A:656:ILE:HD12	1:A:684:ASP:HB3	1.80	0.64
1:B:581:GLN:H	1:B:581:GLN:NE2	1.96	0.64
1:B:589:LEU:HD21	1:B:621:MET:SD	2.38	0.63
1:A:218:LYS:NZ	1:A:220:HIS:HD2	1.95	0.63
1:A:39:LEU:HB3	1:A:76:ALA:O	1.98	0.63
1:A:635:ASP:OD1	1:A:638:GLY:HA3	1.99	0.63
1:A:247:ILE:HD13	1:A:247:ILE:N	2.12	0.63
1:A:341:GLU:HG2	1:A:344:GLN:HE21	1.65	0.62
1:B:4:GLU:HB3	1:B:26:THR:HG22	1.81	0.62
1:A:614:PHE:CZ	1:A:622:ARG:HG2	2.34	0.62
1:B:508:ARG:O	1:B:512:VAL:HG23	1.99	0.62
1:B:140:LYS:HB2	1:B:153:GLN:HG3	1.81	0.62
1:A:581:GLN:HA	1:A:581:GLN:NE2	2.14	0.61
1:B:136:ASN:ND2	1:B:164:TYR:H	1.91	0.61
1:B:663:LYS:HD3	1:B:697:PRO:HG3	1.83	0.61
1:A:16:LYS:HB3	1:A:18:THR:HG23	1.83	0.61
1:B:675:VAL:HG11	1:B:685:MET:HG3	1.81	0.61
1:A:530:ARG:HD2	1:A:534:ARG:HH11	1.65	0.61
1:B:359:ARG:HH22	1:B:481:ALA:HA	1.64	0.61
1:B:218:LYS:NZ	1:B:220:HIS:CD2	2.69	0.61
1:B:136:ASN:HD21	1:B:164:TYR:N	1.92	0.60
1:B:682:LYS:NZ	1:B:716:TYR:CD1	2.69	0.60
1:B:682:LYS:HZ1	1:B:716:TYR:HB3	1.66	0.60
1:B:696:LEU:N	1:B:697:PRO:HD2	2.16	0.60
1:A:138:PRO:HD2	1:A:153:GLN:HE21	1.66	0.60
1:A:106:ARG:NH1	1:A:113:ASP:HB3	2.16	0.60
1:A:421:LEU:HD23	1:A:428:ILE:CG2	2.28	0.60
1:A:473:LEU:HD13	1:A:474:ILE:N	2.18	0.59
1:B:627:THR:HG22	1:B:661:LYS:HG2	1.84	0.59
1:B:755:MET:CE	1:B:759:LYS:HE3	2.33	0.59
1:B:661:LYS:NZ	1:B:691:SER:HB2	2.17	0.59
1:B:689:PHE:CZ	1:B:709:ILE:HG13	2.38	0.59
1:B:627:THR:CG2	1:B:661:LYS:HG2	2.33	0.59
1:B:218:LYS:NZ	1:B:220:HIS:HD2	1.99	0.59
1:A:341:GLU:HB2	1:A:344:GLN:HB3	1.85	0.59
1:B:374:ILE:HD13	1:B:391:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:THR:O	1:B:496:VAL:HG23	2.03	0.59
1:A:83:LEU:CD1	1:A:228:GLY:H	2.16	0.58
1:B:106:ARG:HD2	1:B:113:ASP:OD2	2.04	0.58
1:A:55:TYR:HD1	1:A:59:THR:O	1.85	0.58
1:A:537:PHE:O	1:A:573:ARG:HD3	2.02	0.58
1:A:101:GLN:HG3	1:A:102:ALA:N	2.17	0.58
1:B:346:PHE:HD1	1:B:351:TYR:HE2	1.52	0.58
1:B:537:PHE:CE1	1:B:569:PHE:HB2	2.39	0.58
1:A:171:ARG:HG3	1:A:171:ARG:NH1	2.19	0.58
1:A:450:ASN:ND2	1:A:478:ALA:H	2.00	0.57
1:B:541:ASP:O	1:B:545:ILE:HG12	2.04	0.57
1:B:601:GLU:O	1:B:605:GLU:HG3	2.04	0.57
1:A:450:ASN:HD21	1:A:478:ALA:CB	2.17	0.57
1:A:42:ASN:H	1:A:42:ASN:ND2	2.02	0.57
1:B:730:MET:C	1:B:732:PRO:HD2	2.25	0.57
1:B:632:VAL:HG12	1:B:633:THR:HG22	1.87	0.57
1:A:114:HIS:HB3	1:A:117:TYR:HD1	1.70	0.57
1:B:218:LYS:HZ3	1:B:220:HIS:CD2	2.23	0.57
1:B:667:ASP:O	1:B:671:VAL:HG23	2.05	0.57
1:A:42:ASN:H	1:A:42:ASN:HD22	1.53	0.57
1:A:42:ASN:HD22	1:A:42:ASN:N	2.00	0.57
1:A:249:GLU:HA	1:A:256:LYS:HE2	1.87	0.57
1:B:184:LEU:HD13	1:B:190:ILE:HG21	1.87	0.57
1:A:773:ARG:O	1:A:777:THR:HG22	2.05	0.56
1:B:380:ASP:HB2	1:B:381:HIS:CD2	2.40	0.56
1:A:218:LYS:HZ3	1:A:220:HIS:CD2	2.23	0.56
1:A:721:ARG:NH1	1:A:722:THR:H	2.03	0.56
1:A:333:GLU:HB2	1:A:411:ILE:HG22	1.86	0.56
1:A:588:ALA:O	1:A:592:VAL:HG23	2.06	0.56
1:A:173:GLU:HG2	1:A:190:ILE:HG13	1.88	0.56
1:A:360:MET:HB2	1:A:482:GLY:HA2	1.87	0.56
1:B:473:LEU:HD23	1:B:474:ILE:N	2.21	0.56
1:B:764:LEU:HD11	1:B:768:ARG:NH2	2.21	0.56
1:A:231:ALA:O	3:A:900:FBO:H8	2.05	0.56
1:B:186:SER:OG	1:B:190:ILE:HD13	2.06	0.56
1:B:71:ILE:HD13	1:B:71:ILE:N	2.20	0.56
1:B:243:ILE:CG2	4:B:781:HOH:O	2.54	0.55
1:B:346:PHE:CD1	1:B:351:TYR:HE2	2.24	0.55
1:A:541:ASP:OD2	1:A:543:ASN:HB2	2.06	0.55
1:A:560:HIS:HA	1:A:563:ASP:OD2	2.06	0.55
1:B:741:ALA:O	1:B:745:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ALA:O	1:A:255:VAL:HG22	2.06	0.55
1:A:551:GLN:O	1:A:555:LEU:HD22	2.05	0.55
1:B:280:TRP:HD1	1:B:282:ASN:HD22	1.55	0.55
1:B:675:VAL:CG1	1:B:685:MET:HG3	2.36	0.55
1:A:538:ASP:HA	1:A:573:ARG:NH2	2.22	0.54
1:A:432:GLN:NE2	1:A:445:TRP:H	1.99	0.54
1:B:682:LYS:NZ	1:B:716:TYR:HD1	2.06	0.54
1:A:44:MET:HG2	1:A:45:LYS:H	1.71	0.54
1:B:650:GLU:HG2	1:B:654:ARG:NH1	2.22	0.54
1:A:218:LYS:NZ	1:A:220:HIS:CD2	2.75	0.54
1:B:408:GLU:O	1:B:412:LYS:HG3	2.08	0.54
1:B:682:LYS:HZ2	1:B:716:TYR:HB3	1.72	0.54
1:A:44:MET:HG2	1:A:45:LYS:N	2.22	0.54
1:A:101:GLN:OE1	3:A:900:FBO:H6	2.08	0.54
1:A:302:LEU:O	1:A:303:PHE:HD2	1.90	0.54
1:B:681:LYS:HD2	1:B:683:GLN:NE2	2.23	0.54
1:B:475:LYS:HE2	1:B:476:ILE:O	2.08	0.53
1:A:618:GLU:HB3	1:A:620:GLU:OE1	2.07	0.53
1:B:607:MET:HE2	1:B:607:MET:HA	1.89	0.53
1:A:477:ASN:HD21	1:A:482:GLY:N	2.07	0.53
1:A:652:ARG:O	1:A:656:ILE:HG13	2.09	0.53
1:B:279:LYS:HE3	1:B:387:GLU:HG2	1.91	0.53
1:B:146:GLU:H	1:B:146:GLU:CD	2.12	0.53
1:A:421:LEU:HD21	1:A:476:ILE:HD11	1.91	0.53
1:A:518:PHE:HB3	1:A:524:ILE:HG12	1.90	0.53
1:A:521:SER:OG	1:A:523:HIS:CD2	2.49	0.53
1:A:83:LEU:HD13	1:A:228:GLY:H	1.74	0.53
1:B:512:VAL:HG12	1:B:551:GLN:NE2	2.24	0.53
1:A:724:SER:HA	1:A:753:ILE:HG22	1.89	0.53
1:A:106:ARG:HD2	1:A:113:ASP:OD2	2.08	0.52
1:A:396:GLU:HG3	1:A:401:LYS:O	2.09	0.52
1:B:457:VAL:HG12	1:B:457:VAL:O	2.09	0.52
1:B:642:LYS:HA	1:B:645:SER:HB3	1.91	0.52
1:A:429:THR:HG22	1:A:467:SER:OG	2.09	0.52
1:B:97:THR:HG22	1:B:164:TYR:HE1	1.74	0.52
1:B:706:LEU:CD2	1:B:741:ALA:HB1	2.39	0.52
1:A:38:GLY:C	1:A:39:LEU:HD23	2.30	0.52
1:A:43:TRP:CZ3	1:A:45:LYS:HG3	2.45	0.52
1:A:23:GLU:HG2	1:A:75:PHE:HE2	1.73	0.52
1:B:682:LYS:HZ1	1:B:716:TYR:CB	2.23	0.52
1:A:67:GLN:HB3	1:A:68:PRO:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLU:HG3	1:A:176:LYS:H	1.74	0.52
1:B:477:ASN:HD21	1:B:482:GLY:H	1.58	0.52
1:A:428:ILE:HG13	1:A:470:ALA:HB2	1.92	0.52
1:A:516:PHE:CD1	1:A:551:GLN:HG2	2.45	0.51
1:B:177:TYR:HE2	1:B:207:GLU:OE1	1.93	0.51
1:B:650:GLU:HG2	1:B:654:ARG:HH11	1.75	0.51
1:A:347:ASP:C	1:A:349:ILE:H	2.14	0.51
1:B:100:PHE:HZ	1:B:108:MET:CE	2.24	0.51
1:B:648:ARG:HG2	1:B:650:GLU:HB2	1.92	0.51
1:B:670:THR:O	1:B:674:MET:HG3	2.11	0.51
1:B:297:LYS:CE	1:B:362:GLU:OE1	2.59	0.51
1:B:353:LYS:HG3	1:B:483:PHE:CE2	2.46	0.51
1:B:681:LYS:HB2	1:B:684:ASP:OD1	2.10	0.51
1:A:292:THR:OG1	3:A:900:FBO:H13	2.10	0.51
1:A:292:THR:OG1	3:A:900:FBO:N18	2.44	0.50
1:A:518:PHE:CB	1:A:524:ILE:HG12	2.41	0.50
1:A:572:SER:OG	1:A:573:ARG:NH2	2.44	0.50
1:B:145:SER:HB3	1:B:146:GLU:OE2	2.11	0.50
1:B:207:GLU:HG2	1:B:213:PRO:HA	1.94	0.50
1:B:272:PHE:CE1	1:B:377:TYR:CE1	2.99	0.50
1:B:97:THR:HG22	1:B:164:TYR:CE1	2.47	0.50
1:B:534:ARG:HA	1:B:537:PHE:CD2	2.47	0.50
1:B:705:ASN:HD22	1:B:708:ARG:HD2	1.77	0.50
1:A:675:VAL:HA	1:A:680:ILE:HB	1.93	0.50
1:B:693:LEU:HD22	1:B:733:VAL:HG11	1.93	0.50
1:A:341:GLU:HG2	1:A:344:GLN:NE2	2.25	0.50
1:B:32:ILE:CD1	1:B:71:ILE:HD12	2.42	0.50
1:B:341:GLU:C	1:B:343:SER:H	2.15	0.50
1:B:527:GLU:OE2	1:B:527:GLU:HA	2.11	0.50
1:B:724:SER:N	1:B:753:ILE:HG22	2.27	0.50
1:A:530:ARG:HG3	1:A:562:PHE:CE2	2.46	0.50
1:B:98:THR:HG21	1:B:108:MET:HE1	1.94	0.50
1:B:618:GLU:HB3	1:B:620:GLU:CD	2.32	0.50
1:B:647:ASP:O	1:B:648:ARG:C	2.50	0.50
1:B:462:LEU:HD23	1:B:463:GLU:N	2.27	0.49
1:B:83:LEU:CD1	1:B:228:GLY:H	2.24	0.49
1:B:284:LEU:O	1:B:284:LEU:HD22	2.12	0.49
1:B:361:ILE:HG13	1:B:407:MET:SD	2.52	0.49
1:B:659:PHE:O	1:B:662:LEU:HB2	2.12	0.49
1:A:374:ILE:CD1	1:A:391:LEU:HD11	2.38	0.49
1:B:178:ARG:NH2	1:B:207:GLU:OE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:GLN:HE22	1:B:445:TRP:H	1.59	0.49
1:B:482:GLY:HA3	1:B:484:TYR:CE2	2.47	0.49
1:B:692:ALA:O	1:B:698:GLY:HA3	2.12	0.49
1:B:574:MET:HE1	1:B:589:LEU:HG	1.94	0.49
1:B:728:GLU:HB2	1:B:756:GLY:HA2	1.94	0.49
1:A:229:ALA:HB1	3:A:900:FBO:C3	2.43	0.49
3:A:900:FBO:O22	3:A:900:FBO:H25	2.13	0.49
1:B:674:MET:CB	1:B:680:ILE:HG12	2.43	0.49
1:A:136:ASN:H	1:A:136:ASN:HD22	1.60	0.49
1:A:351:TYR:CB	3:A:900:FBO:H23A	2.37	0.49
1:B:636:LEU:HB2	1:B:667:ASP:OD1	2.13	0.49
1:A:175:GLU:HG3	1:A:176:LYS:N	2.28	0.49
1:B:98:THR:HG23	1:B:165:VAL:O	2.12	0.49
1:B:629:TYR:CE2	1:B:635:ASP:HB3	2.48	0.49
1:B:755:MET:HE1	1:B:759:LYS:HE3	1.95	0.49
1:A:42:ASN:ND2	1:A:42:ASN:N	2.61	0.48
1:B:537:PHE:CD1	1:B:569:PHE:HB2	2.48	0.48
1:B:723:ALA:HB1	1:B:753:ILE:HG21	1.94	0.48
1:A:302:LEU:C	1:A:303:PHE:HD2	2.17	0.48
1:A:608:SER:OG	1:A:629:TYR:HA	2.13	0.48
1:B:40:GLN:HG2	1:B:76:ALA:HB3	1.96	0.48
1:B:324:ASP:HB3	1:B:416:TYR:CD1	2.48	0.48
1:B:530:ARG:O	1:B:534:ARG:HG3	2.13	0.48
1:B:652:ARG:O	1:B:656:ILE:HG13	2.12	0.48
1:A:83:LEU:CD1	1:A:228:GLY:N	2.75	0.48
1:A:692:ALA:HB3	1:A:702:ILE:HD11	1.95	0.48
1:B:346:PHE:CD1	1:B:351:TYR:CE2	2.96	0.48
1:B:251:SER:H	1:B:256:LYS:HE3	1.79	0.48
1:B:643:PHE:CE2	1:B:680:ILE:HD13	2.48	0.48
1:A:103:THR:HB	1:A:106:ARG:NH1	2.29	0.48
1:B:620:GLU:HG2	1:B:621:MET:N	2.28	0.48
1:A:233:GLU:HG3	1:A:269:HIS:HB3	1.96	0.48
1:A:432:GLN:HE22	1:A:445:TRP:N	2.04	0.48
1:B:14:ILE:HD12	1:B:128:ASP:CG	2.35	0.48
1:B:341:GLU:O	1:B:343:SER:N	2.47	0.48
1:B:346:PHE:O	1:B:347:ASP:CB	2.62	0.47
1:B:567:ARG:HD2	1:B:600:ASP:HB2	1.96	0.47
1:B:660:GLY:HA3	1:B:691:SER:OG	2.14	0.47
1:B:690:SER:O	1:B:693:LEU:HB2	2.14	0.47
1:B:742:GLU:HG3	1:B:761:ILE:HD11	1.96	0.47
1:B:17:ARG:HB3	1:B:79:VAL:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:MET:HB3	1:B:680:ILE:HG12	1.96	0.47
1:A:101:GLN:HG3	1:A:102:ALA:H	1.79	0.47
1:B:528:THR:O	1:B:532:ARG:HG2	2.13	0.47
1:A:128:ASP:HB2	1:A:131:TYR:HD1	1.80	0.47
1:A:452:LYS:HG3	1:A:478:ALA:HB2	1.95	0.47
1:A:349:ILE:O	1:A:353:LYS:HB3	2.14	0.47
1:B:282:ASN:HD22	1:B:282:ASN:H	1.60	0.47
1:A:188:LYS:O	1:A:189:ASP:O	2.33	0.47
1:A:248:ALA:HB1	1:A:250:ASN:OD1	2.14	0.47
1:B:253:VAL:CB	1:B:583:GLU:HG2	2.43	0.47
1:B:504:SER:O	1:B:508:ARG:HD3	2.14	0.47
1:B:538:ASP:HA	1:B:573:ARG:NH1	2.30	0.47
1:A:136:ASN:H	1:A:136:ASN:ND2	2.13	0.47
1:A:82:SER:O	1:A:83:LEU:C	2.54	0.47
1:A:302:LEU:C	1:A:303:PHE:CD2	2.88	0.47
1:B:775:ARG:HG2	1:B:775:ARG:O	2.14	0.47
1:A:224:VAL:HB	1:A:227:PHE:HB2	1.97	0.46
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.70	0.46
1:B:506:LEU:HD23	1:B:506:LEU:HA	1.74	0.46
1:A:450:ASN:HD21	1:A:478:ALA:N	2.08	0.46
1:B:290:PHE:CE1	1:B:374:ILE:HD12	2.51	0.46
1:B:580:LYS:HD2	1:B:581:GLN:NE2	2.31	0.46
1:B:724:SER:O	1:B:756:GLY:HA3	2.16	0.46
1:A:200:ARG:NH2	1:A:201:LYS:HE3	2.31	0.46
1:A:379:ASN:O	1:A:382:LYS:HG2	2.16	0.46
1:A:5:LYS:HA	1:A:120:VAL:O	2.16	0.46
1:B:234:ASN:HB2	1:B:237:ALA:O	2.15	0.46
1:A:285:TRP:O	1:A:289:SER:HB2	2.16	0.46
1:A:540:GLU:HG2	1:A:576:PHE:CE1	2.51	0.46
1:A:404:LYS:HE2	1:A:408:GLU:OE1	2.16	0.45
1:B:243:ILE:HG22	4:B:781:HOH:O	2.16	0.45
1:B:288:GLU:OE2	1:B:288:GLU:HA	2.13	0.45
1:B:367:TYR:N	1:B:367:TYR:CD2	2.83	0.45
1:B:571:ARG:HG2	1:B:596:TYR:OH	2.16	0.45
1:A:392:TRP:HB3	1:A:404:LYS:HA	1.99	0.45
1:A:451:ILE:HD13	1:A:468:ILE:HD13	1.98	0.45
1:B:438:ASN:ND2	1:B:769:LYS:HE3	2.32	0.45
1:A:475:LYS:HD2	1:A:503:LEU:HD22	1.99	0.45
1:B:95:MET:CE	1:B:97:THR:HG23	2.45	0.45
1:B:269:HIS:HA	1:B:272:PHE:O	2.16	0.45
1:A:708:ARG:HB3	1:A:711:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLU:C	1:A:251:SER:H	2.20	0.45
1:A:421:LEU:HD21	1:A:476:ILE:CD1	2.47	0.45
1:B:100:PHE:HZ	1:B:108:MET:HE1	1.81	0.45
1:B:432:GLN:HE21	1:B:443:GLY:HA3	1.82	0.45
1:B:542:HIS:CG	1:B:584:ASN:HB3	2.51	0.45
1:A:341:GLU:O	1:A:341:GLU:OE2	2.35	0.45
1:B:266:GLU:O	1:B:269:HIS:HB2	2.17	0.45
1:A:332:ILE:HD11	1:A:353:LYS:HG2	1.99	0.44
1:A:675:VAL:HG11	1:A:685:MET:HG3	1.99	0.44
1:B:14:ILE:HD12	1:B:128:ASP:OD1	2.17	0.44
1:B:421:LEU:O	1:B:422:LYS:HB3	2.17	0.44
1:B:605:GLU:HA	1:B:632:VAL:HG21	1.98	0.44
1:B:642:LYS:O	1:B:646:VAL:HG13	2.17	0.44
1:A:774:ILE:O	1:A:777:THR:HG23	2.17	0.44
1:B:772:GLU:OE2	1:B:772:GLU:HA	2.17	0.44
1:A:289:SER:OG	1:A:354:GLY:HA3	2.17	0.44
1:B:367:TYR:N	1:B:367:TYR:HD2	2.15	0.44
1:B:407:MET:O	1:B:411:ILE:HG13	2.17	0.44
1:B:556:ARG:O	1:B:556:ARG:HG2	2.16	0.44
1:B:755:MET:HE3	1:B:759:LYS:HE3	1.98	0.44
1:A:450:ASN:HD21	1:A:478:ALA:HB3	1.81	0.44
1:B:341:GLU:C	1:B:343:SER:N	2.70	0.44
1:B:545:ILE:HD12	1:B:573:ARG:HD3	2.00	0.44
1:B:477:ASN:HB2	1:B:484:TYR:OH	2.17	0.44
1:B:650:GLU:O	1:B:654:ARG:HG3	2.18	0.44
1:A:607:MET:HE2	1:A:621:MET:CE	2.48	0.44
1:A:607:MET:HE2	1:A:621:MET:HE1	2.00	0.44
1:B:447:VAL:HG13	1:B:462:LEU:HB3	2.00	0.44
1:B:656:ILE:HD13	1:B:680:ILE:HG23	2.00	0.44
1:B:731:ILE:N	1:B:732:PRO:CD	2.80	0.44
1:A:83:LEU:HD13	1:A:228:GLY:N	2.32	0.44
1:A:128:ASP:OD1	1:A:147:ARG:NH2	2.50	0.44
1:B:468:ILE:HD12	1:B:468:ILE:O	2.17	0.44
1:B:488:TYR:O	1:B:532:ARG:NH1	2.45	0.44
1:A:134:ILE:HD12	1:A:170:PHE:CE2	2.52	0.44
1:A:392:TRP:CE3	1:A:407:MET:HG3	2.53	0.44
1:B:114:HIS:CE1	1:B:280:TRP:CE3	3.06	0.44
1:A:573:ARG:N	1:A:573:ARG:HD2	2.32	0.44
1:A:589:LEU:HD21	1:A:621:MET:SD	2.58	0.44
1:A:650:GLU:HG2	1:A:654:ARG:HH11	1.82	0.44
1:A:730:MET:O	1:A:734:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:THR:HG22	1:B:98:THR:H	1.83	0.44
1:B:349:ILE:HG22	1:B:350:SER:N	2.33	0.44
1:B:421:LEU:O	1:B:422:LYS:CB	2.65	0.44
1:B:512:VAL:HG13	1:B:533:ILE:HD11	2.00	0.44
1:B:731:ILE:N	1:B:732:PRO:HD2	2.33	0.44
1:A:474:ILE:HG12	1:A:499:HIS:CD2	2.53	0.43
1:A:504:SER:HB3	1:A:507:ASP:OD1	2.17	0.43
1:A:17:ARG:NH2	1:A:17:ARG:HG3	2.32	0.43
1:A:136:ASN:ND2	1:A:164:TYR:H	2.06	0.43
1:B:442:GLU:H	1:B:442:GLU:HG2	1.55	0.43
1:B:538:ASP:C	1:B:573:ARG:HH12	2.21	0.43
1:A:41:ILE:O	1:A:42:ASN:C	2.57	0.43
1:B:696:LEU:H	1:B:697:PRO:HD2	1.82	0.43
1:A:262:VAL:O	1:A:265:HIS:HB3	2.18	0.43
1:A:265:HIS:CE1	1:A:291:ALA:HB3	2.53	0.43
1:A:567:ARG:HD2	1:A:599:VAL:O	2.19	0.43
1:A:696:LEU:HB3	1:A:697:PRO:CD	2.49	0.43
1:A:116:ALA:HA	1:A:385:ASN:ND2	2.34	0.43
1:A:505:PRO:HB3	1:A:541:ASP:OD1	2.19	0.43
1:A:552:MET:HB2	1:A:595:LEU:HD11	2.00	0.43
1:B:282:ASN:H	1:B:282:ASN:ND2	2.17	0.43
1:B:681:LYS:HB3	1:B:682:LYS:H	1.60	0.43
1:A:17:ARG:HG3	1:A:17:ARG:HH21	1.83	0.43
1:A:607:MET:CE	1:A:621:MET:CE	2.96	0.43
1:B:661:LYS:HZ3	1:B:691:SER:HB2	1.84	0.43
1:A:14:ILE:O	1:A:17:ARG:HD3	2.18	0.43
1:A:66:SER:O	1:A:67:GLN:NE2	2.51	0.43
1:A:101:GLN:HB2	1:A:232:MET:CE	2.49	0.43
1:A:643:PHE:O	1:A:646:VAL:HG22	2.19	0.43
1:B:359:ARG:NH1	1:B:506:LEU:HD13	2.34	0.43
1:A:310:GLY:HA2	1:A:506:LEU:HD21	2.01	0.43
1:A:582:ASP:HB3	1:A:585:LEU:HD12	2.00	0.43
1:A:183:ILE:HD12	1:A:183:ILE:N	2.34	0.43
1:A:452:LYS:NZ	1:A:507:ASP:OD1	2.48	0.43
1:B:83:LEU:O	1:B:83:LEU:CD2	2.64	0.43
1:B:95:MET:HE3	1:B:97:THR:HG23	2.01	0.43
1:A:709:ILE:O	1:A:713:VAL:HG23	2.18	0.42
1:B:577:LEU:HB3	1:B:589:LEU:HB2	2.00	0.42
1:B:640:LEU:O	1:B:644:ARG:HD2	2.18	0.42
1:B:724:SER:CA	1:B:753:ILE:HG22	2.49	0.42
1:B:134:ILE:HG22	1:B:135:SER:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:MET:HB3	1:B:138:PRO:CD	2.49	0.42
1:B:703:PHE:C	1:B:705:ASN:H	2.23	0.42
1:B:127:ILE:HG21	1:B:167:ILE:HG12	2.01	0.42
1:B:396:GLU:HG3	1:B:401:LYS:O	2.19	0.42
1:B:530:ARG:HA	1:B:533:ILE:HG22	2.01	0.42
1:A:252:ALA:O	1:A:254:THR:N	2.49	0.42
1:A:345:ILE:O	1:A:350:SER:HB2	2.19	0.42
1:A:614:PHE:CE1	1:A:622:ARG:HG2	2.54	0.42
1:B:682:LYS:O	1:B:717:PHE:HZ	2.01	0.42
1:A:146:GLU:CD	1:A:146:GLU:H	2.22	0.42
1:B:574:MET:HG2	1:B:592:VAL:HG11	2.01	0.42
1:A:297:LYS:HE3	1:A:362:GLU:OE1	2.19	0.42
1:A:649:ASP:O	1:A:650:GLU:C	2.57	0.42
1:B:545:ILE:O	1:B:549:VAL:HG23	2.19	0.42
1:B:705:ASN:O	1:B:709:ILE:HD13	2.20	0.42
1:A:83:LEU:HA	1:A:87:TYR:CE2	2.55	0.42
1:A:706:LEU:O	1:A:710:ILE:HG12	2.19	0.42
1:B:664:SER:HB3	1:B:667:ASP:HB2	2.02	0.42
1:B:682:LYS:HD3	1:B:717:PHE:CE1	2.55	0.42
1:A:673:GLY:O	1:A:677:LYS:HG3	2.19	0.42
1:A:679:GLU:O	1:A:681:LYS:HE2	2.20	0.42
1:A:712:LEU:HD23	1:A:712:LEU:C	2.40	0.42
1:B:365:ALA:O	1:B:369:GLU:CG	2.60	0.42
1:B:391:LEU:O	1:B:395:ILE:HG13	2.19	0.42
1:B:464:ASP:O	1:B:465:GLU:C	2.58	0.42
1:A:67:GLN:O	1:A:68:PRO:C	2.58	0.42
1:A:249:GLU:HA	1:A:256:LYS:CE	2.49	0.42
1:A:361:ILE:HD12	1:A:361:ILE:HA	1.92	0.42
1:A:421:LEU:N	1:A:421:LEU:HD12	2.35	0.42
1:B:432:GLN:O	1:B:432:GLN:HG3	2.20	0.42
1:A:100:PHE:O	1:A:101:GLN:C	2.58	0.42
1:A:574:MET:CE	1:A:593:SER:HA	2.49	0.42
1:A:607:MET:CE	1:A:621:MET:HE1	2.49	0.42
1:B:346:PHE:O	1:B:347:ASP:CG	2.58	0.42
1:B:361:ILE:HD13	1:B:361:ILE:HA	1.90	0.42
1:B:505:PRO:O	1:B:509:ILE:HB	2.20	0.42
1:A:32:ILE:O	1:A:61:ARG:HA	2.20	0.41
1:A:129:LYS:HB2	1:A:129:LYS:HE3	1.78	0.41
1:A:647:ASP:O	1:A:648:ARG:CB	2.68	0.41
1:A:209:TYR:CZ	1:A:371:ARG:HG3	2.55	0.41
1:B:512:VAL:HG12	1:B:551:GLN:HE22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:PHE:O	1:B:374:ILE:HG12	2.20	0.41
1:B:587:ILE:HA	1:B:587:ILE:HD13	1.79	0.41
1:A:434:ARG:HB3	1:A:441:GLU:HB2	2.02	0.41
1:A:567:ARG:HG2	1:A:600:ASP:HB2	2.02	0.41
1:A:595:LEU:O	1:A:599:VAL:HG22	2.21	0.41
1:A:675:VAL:HG22	1:A:680:ILE:HG21	2.02	0.41
1:B:422:LYS:NZ	1:B:422:LYS:HB2	2.36	0.41
1:B:438:ASN:HD21	1:B:769:LYS:HE3	1.85	0.41
1:B:473:LEU:HD23	1:B:474:ILE:C	2.40	0.41
1:A:712:LEU:HD21	1:A:716:TYR:CE2	2.54	0.41
1:B:100:PHE:O	1:B:101:GLN:C	2.56	0.41
1:B:326:LEU:HB3	1:B:762:GLU:OE2	2.20	0.41
1:A:41:ILE:O	1:A:41:ILE:HG22	2.20	0.41
1:B:135:SER:OG	1:B:136:ASN:N	2.54	0.41
1:B:764:LEU:HD11	1:B:768:ARG:CZ	2.50	0.41
1:A:115:PRO:HA	1:A:159:SER:HB3	2.03	0.41
1:A:347:ASP:C	1:A:349:ILE:N	2.74	0.41
1:A:374:ILE:HD13	1:A:374:ILE:HA	1.90	0.41
1:A:516:PHE:CG	1:A:551:GLN:HG2	2.56	0.41
1:B:184:LEU:HD13	1:B:190:ILE:CG2	2.51	0.41
1:B:333:GLU:HB2	1:B:411:ILE:HG22	2.02	0.41
1:B:477:ASN:HD21	1:B:482:GLY:N	2.19	0.41
1:B:538:ASP:C	1:B:573:ARG:NH1	2.74	0.41
1:B:710:ILE:O	1:B:714:ILE:HG13	2.21	0.41
1:A:342:ILE:O	1:A:342:ILE:HG12	2.20	0.41
1:B:177:TYR:HB2	1:B:200:ARG:HG3	2.03	0.41
1:B:607:MET:HE2	1:B:610:LEU:HD12	2.03	0.41
1:B:635:ASP:OD1	1:B:638:GLY:HA3	2.21	0.41
1:A:312:PHE:O	1:A:316:ARG:HB2	2.21	0.40
1:B:475:LYS:HE3	1:B:511:LEU:HD21	2.03	0.40
1:A:671:VAL:O	1:A:674:MET:HB2	2.21	0.40
1:B:493:PHE:CE2	1:B:532:ARG:HD2	2.56	0.40
1:A:243:ILE:O	1:A:243:ILE:HG13	2.14	0.40
1:A:292:THR:OG1	3:A:900:FBO:C13	2.68	0.40
1:A:338:ASP:C	1:A:340:ASP:H	2.25	0.40
1:A:636:LEU:O	1:A:640:LEU:N	2.37	0.40
1:B:128:ASP:HB2	1:B:131:TYR:CD1	2.55	0.40
1:B:476:ILE:HG22	1:B:477:ASN:N	2.36	0.40
1:A:266:GLU:O	1:A:269:HIS:HB2	2.22	0.40
1:A:293:PHE:HZ	1:A:362:GLU:OE2	2.05	0.40
1:A:145:SER:HB3	1:A:146:GLU:OE1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:TYR:CD1	1:A:448:PRO:HB3	2.55	0.40
1:B:233:GLU:O	1:B:234:ASN:C	2.60	0.40
1:B:573:ARG:C	1:B:575:GLN:N	2.74	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	778/780 (100%)	696 (90%)	68 (9%)	14 (2%)	8 28
1	B	778/780 (100%)	675 (87%)	84 (11%)	19 (2%)	6 21
All	All	1556/1560 (100%)	1371 (88%)	152 (10%)	33 (2%)	7 24

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	83	LEU
1	A	189	ASP
1	B	83	LEU
1	B	347	ASP
1	B	422	LYS
1	B	681	LYS
1	A	42	ASN
1	A	102	ALA
1	A	253	VAL
1	A	465	GLU
1	A	718	THR
1	B	102	ALA
1	B	477	ASN
1	B	689	PHE

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Mol	Chain	Res	Type
1	B	777	THR
1	A	254	THR
1	A	556	ARG
1	A	610	LEU
1	B	80	SER
1	B	427	LYS
1	B	455	ASP
1	B	740	ASP
1	A	31	ASP
1	A	250	ASN
1	B	425	GLY
1	B	465	GLU
1	B	491	ALA
1	A	650	GLU
1	B	342	ILE
1	B	535	ASN
1	B	582	ASP
1	B	778	ALA

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	677/677 (100%)	607 (90%)	70 (10%)	7 21
1	B	677/677 (100%)	611 (90%)	66 (10%)	8 24
All	All	1354/1354 (100%)	1218 (90%)	136 (10%)	7 22

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	GLU
1	A	7	ASP
1	A	39	LEU
1	A	56	ASP

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Mol	Chain	Res	Type
1	A	58	GLN
1	A	65	ASP
1	A	78	LYS
1	A	82	SER
1	A	83	LEU
1	A	101	GLN
1	A	106	ARG
1	A	143	GLU
1	A	146	GLU
1	A	171	ARG
1	A	190	ILE
1	A	218	LYS
1	A	232	MET
1	A	235	TRP
1	A	243	ILE
1	A	247	ILE
1	A	254	THR
1	A	275	LEU
1	A	286	LEU
1	A	288	GLU
1	A	289	SER
1	A	308	PHE
1	A	316	ARG
1	A	341	GLU
1	A	346	PHE
1	A	347	ASP
1	A	349	ILE
1	A	389	SER
1	A	419	ILE
1	A	422	LYS
1	A	426	ARG
1	A	429	THR
1	A	447	VAL
1	A	450	ASN
1	A	455	ASP
1	A	459	ARG
1	A	462	LEU
1	A	464	ASP
1	A	485	ARG
1	A	487	LEU
1	A	490	ASP
1	A	509	ILE

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Mol	Chain	Res	Type
1	A	513	ASP
1	A	519	LEU
1	A	531	GLN
1	A	555	LEU
1	A	563	ASP
1	A	571	ARG
1	A	573	ARG
1	A	589	LEU
1	A	595	LEU
1	A	596	TYR
1	A	607	MET
1	A	612	LYS
1	A	646	VAL
1	A	648	ARG
1	A	681	LYS
1	A	683	GLN
1	A	696	LEU
1	A	721	ARG
1	A	740	ASP
1	A	755	MET
1	A	764	LEU
1	A	770	LEU
1	A	777	THR
1	B	58	GLN
1	B	65	ASP
1	B	70	LYS
1	B	81	ASP
1	B	86	ILE
1	B	91	ARG
1	B	97	THR
1	B	106	ARG
1	B	146	GLU
1	B	159	SER
1	B	188	LYS
1	B	190	ILE
1	B	218	LYS
1	B	235	TRP
1	B	243	ILE
1	B	251	SER
1	B	254	THR
1	B	275	LEU
1	B	282	ASN

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Mol	Chain	Res	Type
1	B	284	LEU
1	B	286	LEU
1	B	305	GLU
1	B	308	PHE
1	B	324	ASP
1	B	328	ASN
1	B	333	GLU
1	B	335	ASP
1	B	337	ARG
1	B	341	GLU
1	B	348	GLU
1	B	361	ILE
1	B	379	ASN
1	B	422	LYS
1	B	426	ARG
1	B	447	VAL
1	B	450	ASN
1	B	455	ASP
1	B	457	VAL
1	B	471	ASP
1	B	487	LEU
1	B	509	ILE
1	B	513	ASP
1	B	519	LEU
1	B	530	ARG
1	B	555	LEU
1	B	573	ARG
1	B	578	THR
1	B	581	GLN
1	B	589	LEU
1	B	595	LEU
1	B	596	TYR
1	B	615	ASP
1	B	633	THR
1	B	642	LYS
1	B	648	ARG
1	B	657	SER
1	B	662	LEU
1	B	679	GLU
1	B	682	LYS
1	B	691	SER
1	B	693	LEU

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Mol	Chain	Res	Type
1	B	718	THR
1	B	724	SER
1	B	764	LEU
1	B	766	VAL
1	B	777	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	40	GLN
1	A	42	ASN
1	A	47	ASN
1	A	58	GLN
1	A	69	GLN
1	A	114	HIS
1	A	136	ASN
1	A	153	GLN
1	A	220	HIS
1	A	234	ASN
1	A	258	ASN
1	A	265	HIS
1	A	287	ASN
1	A	344	GLN
1	A	381	HIS
1	A	432	GLN
1	A	438	ASN
1	A	450	ASN
1	A	477	ASN
1	A	523	HIS
1	A	535	ASN
1	A	575	GLN
1	A	581	GLN
1	A	683	GLN
1	A	738	HIS
1	B	42	ASN
1	B	58	GLN
1	B	114	HIS
1	B	136	ASN
1	B	220	HIS
1	B	258	ASN
1	B	282	ASN

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Mol	Chain	Res	Type
1	B	287	ASN
1	B	381	HIS
1	B	432	GLN
1	B	438	ASN
1	B	477	ASN
1	B	581	GLN
1	B	705	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FBO	A	900	2	33,33,33	1.92	3 (9%)	40,41,41	1.84	10 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FBO	A	900	2	-	16/31/31/31	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FBO	C30-N32	8.31	1.44	1.33
3	A	900	FBO	O21-C20	4.00	1.42	1.35
3	A	900	FBO	O33-N32	-3.15	1.32	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	900	FBO	O21-C20-N18	5.26	118.80	110.61
3	A	900	FBO	O21-C23-C24	4.07	119.17	109.39
3	A	900	FBO	C5-C7-C8	3.75	121.93	114.13
3	A	900	FBO	O22-C20-N18	-3.52	119.57	124.96
3	A	900	FBO	C13-N18-C20	-3.28	116.62	121.89
3	A	900	FBO	C17-C13-N18	2.87	120.41	112.21
3	A	900	FBO	C14-N10-C9	-2.27	116.80	121.67
3	A	900	FBO	C7-C8-C9	2.24	114.22	108.97
3	A	900	FBO	C14-C30-N32	-2.05	112.19	116.69
3	A	900	FBO	C23-O21-C20	2.01	120.41	115.93

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	900	FBO	C7-C8-C9-N10
3	A	900	FBO	C7-C8-C9-O11
3	A	900	FBO	C17-C13-N18-C20
3	A	900	FBO	O21-C20-N18-C13
3	A	900	FBO	N18-C20-O21-C23
3	A	900	FBO	O22-C20-N18-C13
3	A	900	FBO	O22-C20-O21-C23
3	A	900	FBO	N18-C13-C17-C16
3	A	900	FBO	C4-C5-C7-C8
3	A	900	FBO	C14-C15-C16-C17
3	A	900	FBO	C6-C5-C7-C8
3	A	900	FBO	N12-C8-C9-N10
3	A	900	FBO	N12-C8-C9-O11
3	A	900	FBO	N10-C14-C30-O31
3	A	900	FBO	C15-C16-C17-C13

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Mol	Chain	Res	Type	Atoms
3	A	900	FBO	N10-C14-C30-N32

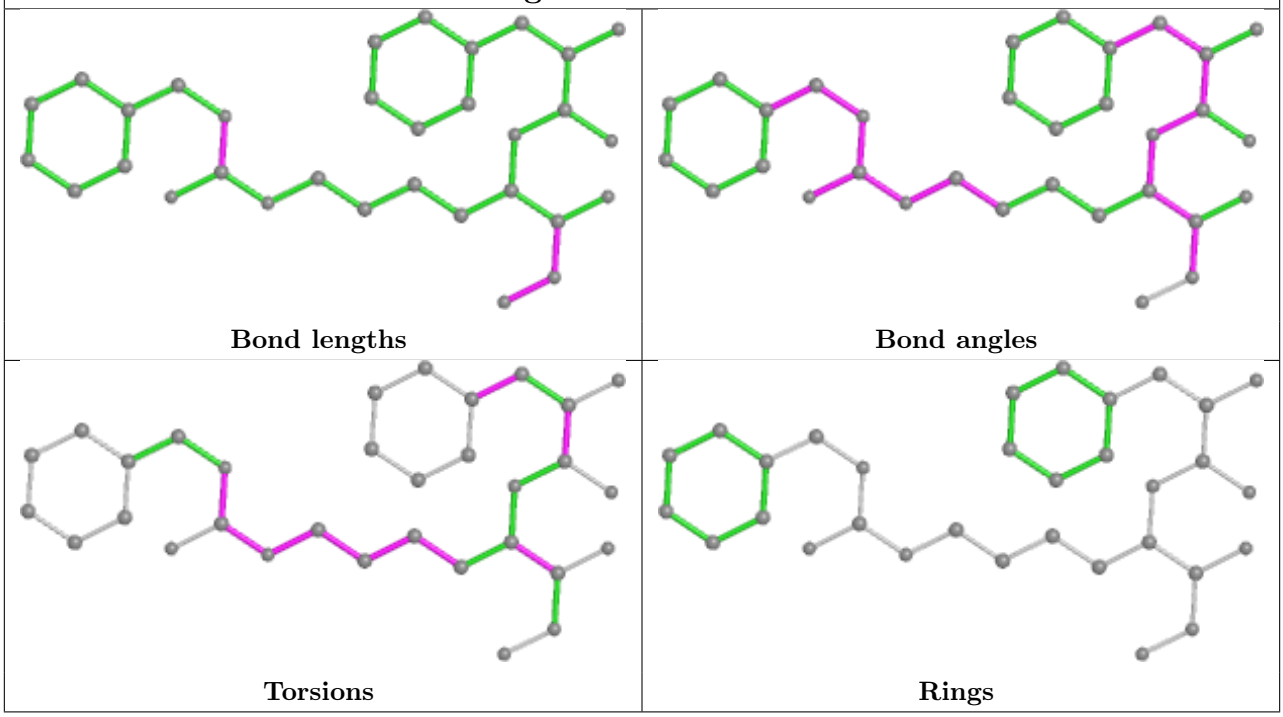
There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	FBO	12	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 then 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.

Ligand FBO A 900



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	780/780 (100%)	-0.24	14 (1%)	68	67	24, 44, 80, 120	1 (0%)
1	B	780/780 (100%)	-0.09	21 (2%)	54	51	26, 46, 91, 124	4 (0%)
All	All	1560/1560 (100%)	-0.16	35 (2%)	62	60	24, 45, 88, 124	5 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	779	VAL	8.0
1	A	344	GLN	6.9
1	B	780	LYS	6.3
1	A	779	VAL	5.9
1	B	778	ALA	4.8
1	A	345	ILE	4.6
1	B	659	PHE	4.2
1	B	345	ILE	4.1
1	B	676	GLU	4.0
1	A	346	PHE	3.9
1	B	643	PHE	3.6
1	B	639	LEU	3.5
1	A	306	TRP	3.2
1	B	710	ILE	2.9
1	B	306	TRP	2.8
1	A	66	SER	2.8
1	B	719	GLY	2.8
1	A	778	ALA	2.7
1	A	49	ARG	2.7
1	A	249	GLU	2.7
1	B	675	VAL	2.6
1	A	780	LYS	2.6
1	A	68	PRO	2.6
1	B	647	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	720	ASN	2.6
1	A	343	SER	2.5
1	B	653	VAL	2.4
1	B	579	GLY	2.4
1	B	578	THR	2.4
1	B	652	ARG	2.3
1	B	614	PHE	2.3
1	B	609	LYS	2.2
1	A	253	VAL	2.1
1	B	615	ASP	2.1
1	A	27	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

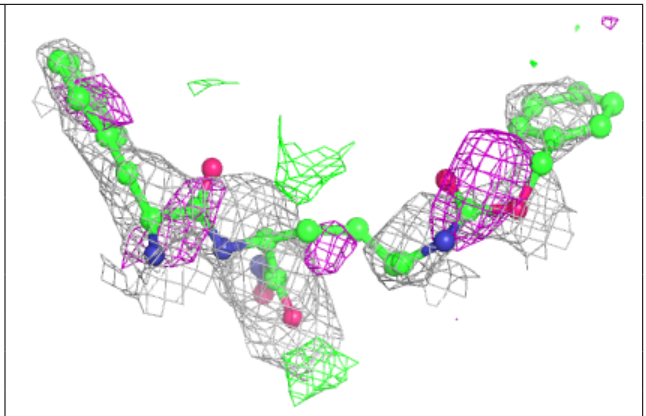
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

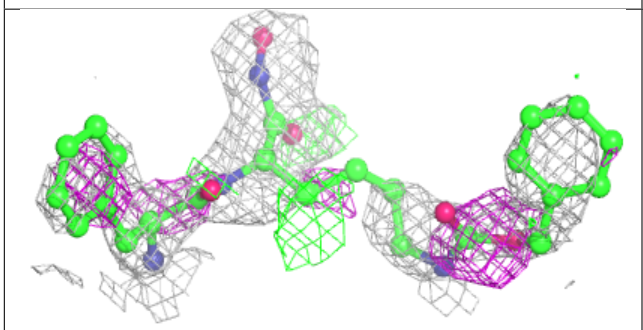
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FBO	A	900	32/32	0.82	0.36	47,63,72,74	0
2	ZN	B	800	1/1	0.96	0.13	47,47,47,47	0
2	ZN	A	800	1/1	0.99	0.13	46,46,46,46	0

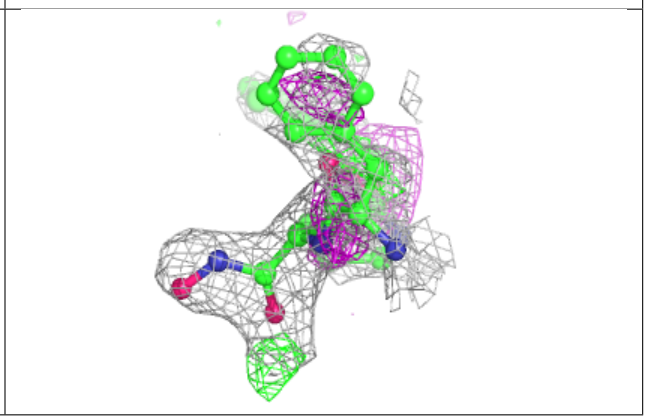
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FBO A 900:

$2mF_o$-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.