



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 02:28 pm BST

PDB ID : 1PWP
Title : Crystal Structure of the Anthrax Lethal Factor complexed with Small Molecule Inhibitor NSC 12155
Authors : Wong, T.Y.; Schwarzenbacher, R.; Liddington, R.C.
Deposited on : 2003-07-02
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

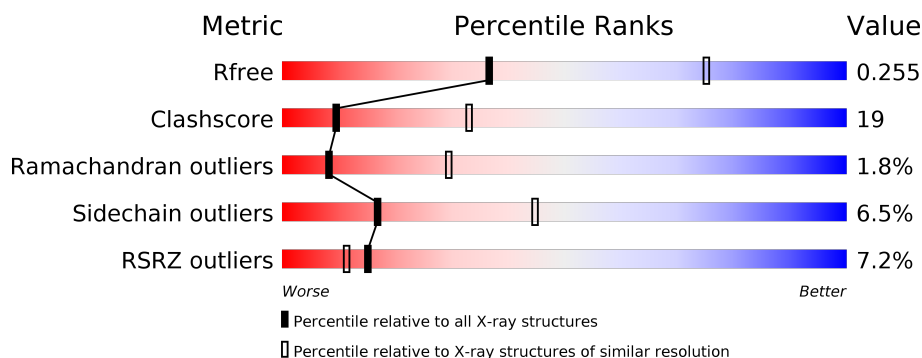
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	776	
1	B	776	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NSC	B	9003	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12177 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.

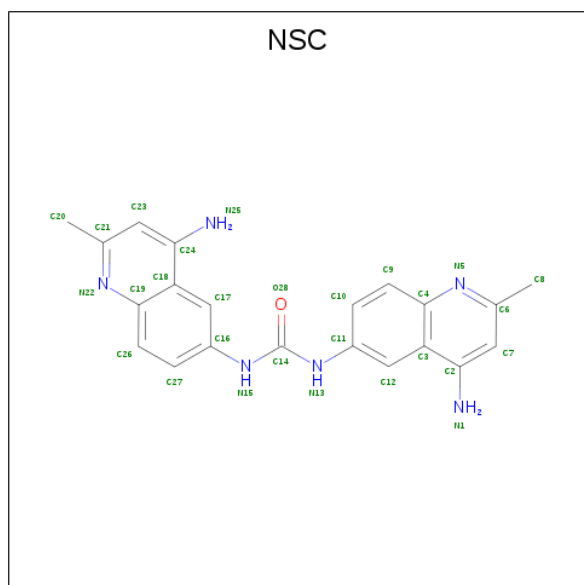
- Molecule 1 is a protein called Lethal factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	732	Total	C	N	O	S	0	0	0
			6014	3825	1011	1171	7			
1	B	743	Total	C	N	O	S	0	0	0
			6105	3877	1026	1195	7			

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

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

- Molecule 3 is N,N'-BIS(4-AMINO-2-METHYLQUINOLIN-6-YL)UREA (three-letter code: NSC) (formula: C₂₁H₂₀N₆O).

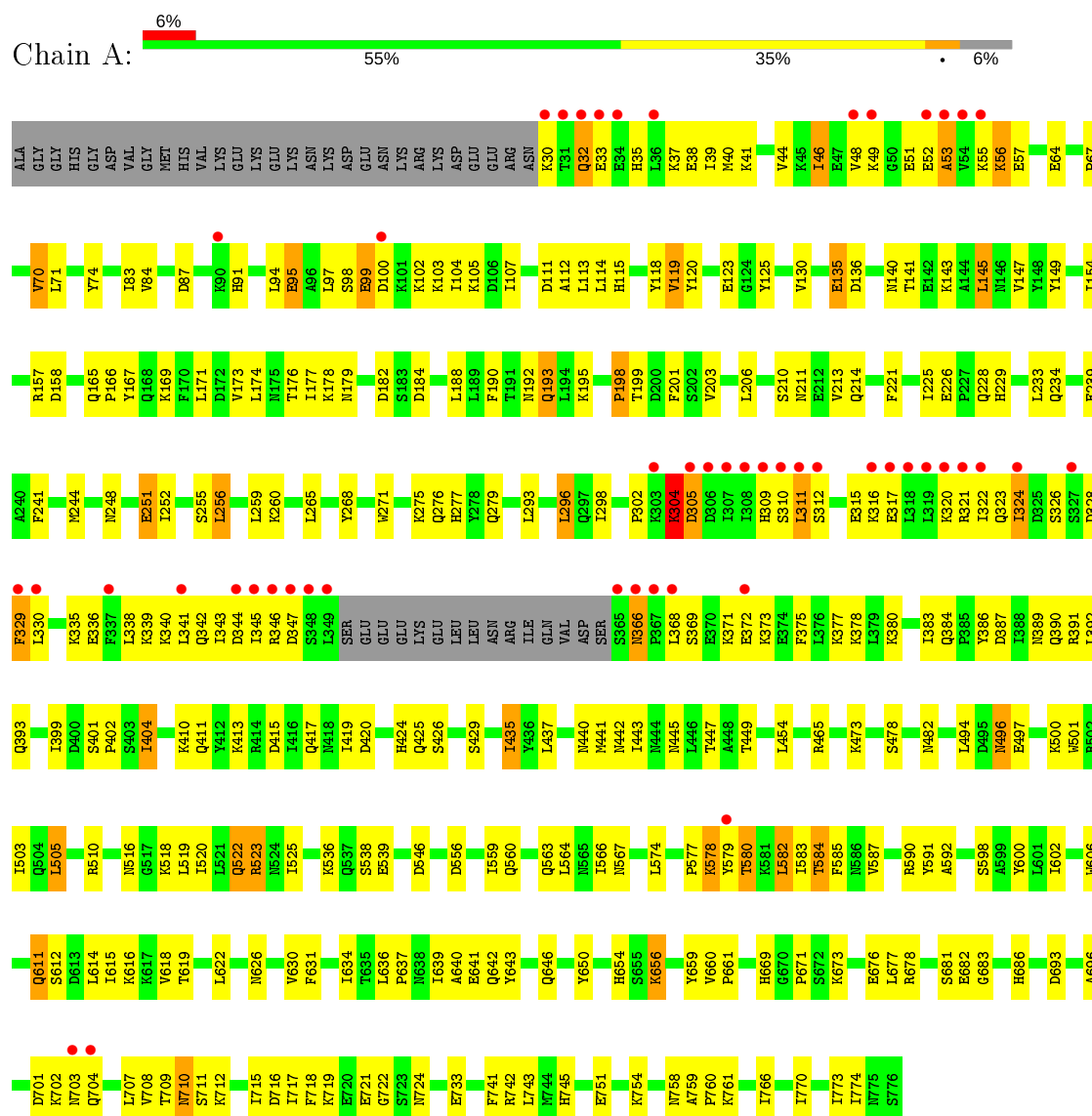


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	21	6	1		
3	B	1	Total	C	N	O	0	0
			28	21	6	1		

3 Residue-property plots

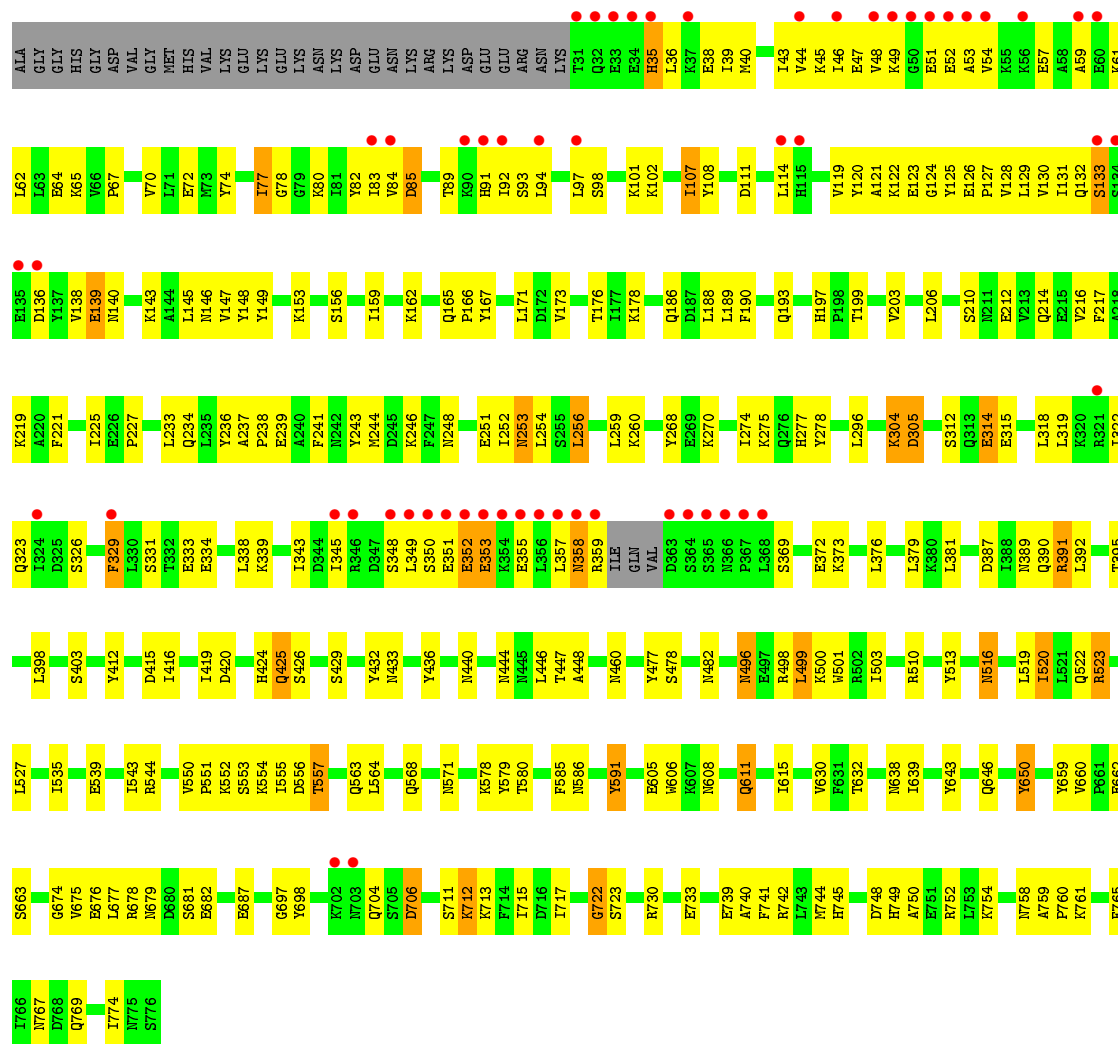
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Lethal factor



• Molecule 1: Lethal factor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.70 Å 137.40 Å 98.30 Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	23.83 – 2.90 46.05 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.1 (23.83-2.90) 94.1 (46.05-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.50	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.91 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.274 0.209 , 0.255	Depositor DCC
R_{free} test set	2595 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12177	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.38	0/6122	0.62	0/8246
1	B	0.39	0/6213	0.62	0/8368
All	All	0.39	0/12335	0.62	0/16614

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6014	0	6003	253	0
1	B	6105	0	6082	218	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	20	8	0
3	B	28	0	20	7	0
All	All	12177	0	12125	473	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 (473) 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:304:LYS:HD3	1:B:304:LYS:H	1.17	1.06
1:B:510:ARG:H	1:B:522:GLN:HE21	1.10	0.97
1:A:563:GLN:HE21	1:A:585:PHE:H	1.17	0.90
1:B:675:VAL:HG22	1:B:676:GLU:HG2	1.53	0.89
1:B:319:LEU:HD23	1:B:345:ILE:HG13	1.53	0.88
1:B:611:GLN:HE21	1:B:774:ILE:HD13	1.39	0.87
1:A:501:TRP:HB3	1:A:503:ILE:HD11	1.57	0.87
1:B:659:TYR:HB3	3:B:9003:NSC:H26	1.58	0.86
1:A:563:GLN:NE2	1:A:585:PHE:H	1.73	0.84
1:A:46:ILE:HD12	1:A:46:ILE:H	1.43	0.84
1:B:712:LYS:HD2	1:B:712:LYS:H	1.44	0.83
1:B:304:LYS:HD3	1:B:304:LYS:N	1.92	0.82
1:B:123:GLU:HG2	1:B:124:GLY:H	1.45	0.82
1:B:107:ILE:HG21	1:B:145:LEU:HD11	1.62	0.80
1:A:435:ILE:H	1:A:435:ILE:HD12	1.46	0.80
1:A:766:ILE:O	1:A:770:ILE:HG12	1.84	0.78
1:A:32:GLN:HG3	1:A:33:GLU:H	1.49	0.77
1:A:87:ASP:OD2	1:A:115:HIS:HA	1.85	0.77
1:B:176:THR:HG21	1:B:239:GLU:HG3	1.66	0.77
1:B:632:THR:HG21	1:B:639:ILE:HD11	1.68	0.76
1:B:563:GLN:NE2	1:B:585:PHE:H	1.85	0.75
1:A:107:ILE:HG21	1:A:145:LEU:HD13	1.67	0.75
1:A:435:ILE:HD12	1:A:435:ILE:N	2.00	0.75
1:A:659:TYR:HB3	3:A:9002:NSC:H26	1.69	0.74
1:B:97:LEU:HD23	1:B:101:LYS:HE3	1.69	0.74
1:A:277:HIS:CE1	1:A:425:GLN:HE21	2.05	0.74
1:A:30:LYS:HA	1:A:32:GLN:HG2	1.70	0.74
1:A:193:GLN:HE21	1:A:193:GLN:HA	1.52	0.74
1:B:126:GLU:N	1:B:127:PRO:HD3	2.03	0.74
1:B:349:LEU:HG	1:B:350:SER:H	1.52	0.73
1:B:712:LYS:HD2	1:B:712:LYS:N	2.03	0.73
1:A:304:LYS:HD3	1:A:304:LYS:H	1.53	0.72
1:A:567:ASN:HD21	1:A:583:ILE:H	1.36	0.72
1:B:679:ASN:HD21	1:B:681:SER:HB2	1.53	0.72
1:B:39:ILE:O	1:B:43:ILE:HG12	1.90	0.71
1:B:296:LEU:HD22	1:B:419:ILE:HD13	1.70	0.71
1:B:424:HIS:HA	1:B:510:ARG:HD2	1.70	0.71
1:A:99:GLU:OE1	1:A:102:LYS:HG3	1.91	0.71
1:B:712:LYS:CD	1:B:712:LYS:H	1.97	0.71
1:B:339:LYS:O	1:B:343:ILE:HG12	1.93	0.69
1:A:389:ASN:OD1	1:A:482:ASN:HB2	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ILE:HG12	1:A:56:LYS:HG2	1.75	0.69
1:A:770:ILE:O	1:A:774:ILE:HG12	1.92	0.69
1:B:611:GLN:NE2	1:B:774:ILE:HD13	2.08	0.68
1:A:277:HIS:CD2	1:A:429:SER:HB2	2.29	0.68
1:A:615:ILE:O	1:A:619:THR:HG23	1.92	0.68
1:A:634:ILE:HD11	1:A:639:ILE:HD12	1.75	0.68
1:B:233:LEU:HD22	1:B:237:ALA:HB3	1.75	0.67
1:B:535:ILE:HD13	1:B:544:ARG:HB2	1.75	0.67
1:B:136:ASP:O	1:B:140:ASN:HB3	1.95	0.67
1:B:759:ALA:N	1:B:760:PRO:HD3	2.10	0.66
1:A:733:GLU:H	1:A:733:GLU:CD	1.98	0.66
1:B:516:ASN:HD22	1:B:516:ASN:N	1.93	0.66
1:B:387:ASP:HB3	1:B:390:GLN:HB3	1.78	0.65
1:A:30:LYS:C	1:A:32:GLN:H	1.98	0.65
1:A:193:GLN:HE21	1:A:193:GLN:CA	2.10	0.65
1:A:577:PRO:O	1:A:580:THR:HG23	1.97	0.65
1:A:721:GLU:HA	1:A:724:ASN:HD21	1.61	0.64
1:B:206:LEU:O	1:B:206:LEU:HD23	1.97	0.64
1:B:440:ASN:HD21	1:B:500:LYS:NZ	1.94	0.64
1:A:721:GLU:HA	1:A:724:ASN:ND2	2.12	0.64
1:B:605:GLU:HG3	1:B:681:SER:OG	1.98	0.64
1:B:77:ILE:HD13	1:B:259:LEU:HD21	1.80	0.64
1:A:312:SER:O	1:A:316:LYS:HG3	1.98	0.63
1:A:707:LEU:HB3	1:A:709:THR:HG22	1.79	0.63
1:B:391:ARG:HG3	1:B:412:TYR:CD1	2.33	0.63
1:B:97:LEU:CD2	1:B:101:LYS:HE3	2.28	0.63
1:B:49:LYS:HG2	1:B:85:ASP:OD1	1.98	0.63
1:B:314:GLU:O	1:B:318:LEU:HD13	1.99	0.63
1:B:131:ILE:HG22	1:B:132:GLN:H	1.63	0.62
1:B:45:LYS:HD2	1:B:82:TYR:HE2	1.64	0.62
1:A:30:LYS:C	1:A:32:GLN:N	2.46	0.62
1:A:30:LYS:HE2	1:A:33:GLU:OE2	2.00	0.62
1:A:48:VAL:HG23	1:A:52:GLU:HG2	1.82	0.62
1:A:33:GLU:O	1:A:37:LYS:HG3	2.00	0.62
1:B:36:LEU:O	1:B:40:MET:HG3	2.00	0.62
1:B:478:SER:HB3	1:B:527:LEU:HB2	1.80	0.62
1:B:352:GLU:O	1:B:355:GLU:HB3	2.00	0.61
1:A:103:LYS:NZ	1:A:103:LYS:HB3	2.16	0.61
1:A:701:ASP:C	1:A:703:ASN:H	2.03	0.61
1:B:711:SER:O	1:B:715:ILE:HG13	2.00	0.61
1:A:107:ILE:HD12	1:A:149:TYR:HB2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:SER:O	1:A:214:GLN:HG3	2.00	0.61
1:A:741:PHE:O	1:A:745:HIS:HD2	1.84	0.61
1:A:188:LEU:HG	1:A:188:LEU:O	2.01	0.60
1:A:304:LYS:HD3	1:A:304:LYS:N	2.16	0.60
1:A:516:ASN:ND2	1:A:518:LYS:HD2	2.16	0.60
1:A:578:LYS:HB2	1:A:578:LYS:NZ	2.15	0.60
1:B:553:SER:O	1:B:557:THR:HG23	2.01	0.60
1:A:329:PHE:HA	3:A:9002:NSC:H83	1.83	0.60
1:B:277:HIS:CD2	1:B:429:SER:HB2	2.36	0.60
1:A:316:LYS:O	1:A:320:LYS:HG3	2.01	0.60
1:B:107:ILE:HG21	1:B:145:LEU:CD1	2.31	0.60
1:B:52:GLU:HG3	1:B:52:GLU:O	2.00	0.60
1:A:198:PRO:HG2	1:A:199:THR:H	1.67	0.60
1:B:171:LEU:HD21	1:B:206:LEU:HD12	1.84	0.60
1:B:46:ILE:HD13	1:B:83:ILE:HB	1.82	0.60
1:A:38:GLU:O	1:A:41:LYS:HG2	2.01	0.60
1:A:501:TRP:HB3	1:A:503:ILE:CD1	2.30	0.60
1:B:256:LEU:HD22	1:B:260:LYS:HE2	1.84	0.60
1:A:612:SER:O	1:A:616:LYS:HG3	2.02	0.59
1:A:70:VAL:HG12	1:A:252:ILE:HD11	1.84	0.59
1:A:256:LEU:HD22	1:A:260:LYS:HE3	1.84	0.59
1:A:522:GLN:HE21	1:A:525:ILE:HG13	1.67	0.59
1:A:759:ALA:N	1:A:760:PRO:HD3	2.17	0.59
1:A:304:LYS:HG2	1:A:305:ASP:H	1.66	0.59
1:A:393:GLN:HE22	1:A:445:ASN:HD21	1.50	0.59
1:A:496:ASN:C	1:A:496:ASN:HD22	2.04	0.59
1:B:253:ASN:N	1:B:253:ASN:HD22	1.99	0.59
1:A:614:LEU:HD22	1:A:770:ILE:HD12	1.83	0.59
1:B:403:SER:OG	1:B:638:ASN:ND2	2.34	0.59
1:A:56:LYS:HD3	1:A:56:LYS:O	2.01	0.59
1:A:125:TYR:HA	1:B:268:TYR:HE2	1.67	0.59
1:B:733:GLU:CD	1:B:733:GLU:H	2.06	0.58
1:B:91:HIS:CD2	1:B:93:SER:H	2.21	0.58
1:A:46:ILE:HD12	1:A:46:ILE:N	2.15	0.58
1:A:577:PRO:HD2	1:A:580:THR:HG21	1.84	0.58
1:A:369:SER:HB3	1:A:372:GLU:HB2	1.86	0.58
3:A:9002:NSC:H12	3:A:9002:NSC:O28	2.03	0.58
1:A:338:LEU:HD23	1:A:341:LEU:HD12	1.86	0.57
1:B:754:LYS:O	1:B:758:ASN:HB2	2.04	0.57
1:A:701:ASP:C	1:A:703:ASN:N	2.56	0.57
3:B:9003:NSC:H12	3:B:9003:NSC:O28	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:O	1:A:341:LEU:HB2	2.04	0.57
1:A:296:LEU:O	1:A:296:LEU:HD22	2.03	0.57
1:A:516:ASN:HD21	1:A:518:LYS:HD2	1.69	0.57
1:B:563:GLN:HE21	1:B:585:PHE:HB2	1.70	0.57
1:A:104:ILE:HG22	1:A:105:LYS:H	1.69	0.57
1:A:324:ILE:HG22	1:A:335:LYS:HG2	1.87	0.57
1:B:606:TRP:CE2	1:B:615:ILE:HD12	2.39	0.57
1:B:682:GLU:HG2	1:B:742:ARG:HD3	1.87	0.57
1:B:123:GLU:HG2	1:B:124:GLY:N	2.18	0.57
1:B:460:ASN:O	1:B:498:ARG:NH2	2.37	0.57
1:A:48:VAL:CG2	1:A:52:GLU:HG2	2.35	0.57
1:B:496:ASN:N	1:B:496:ASN:HD22	2.03	0.56
1:A:226:GLU:OE1	1:A:229:HIS:ND1	2.30	0.56
1:A:312:SER:HB3	1:A:315:GLU:HB2	1.87	0.56
1:B:513:TYR:HA	1:B:519:LEU:HD23	1.87	0.56
1:A:437:LEU:HD11	1:A:519:LEU:HD12	1.87	0.56
1:B:107:ILE:HG13	1:B:145:LEU:HD13	1.87	0.56
1:B:606:TRP:CH2	1:B:615:ILE:HG23	2.41	0.56
3:B:9003:NSC:O28	3:B:9003:NSC:H17	2.06	0.56
1:A:30:LYS:CA	1:A:32:GLN:HG2	2.35	0.55
1:B:212:GLU:O	1:B:216:VAL:HG23	2.05	0.55
1:A:711:SER:O	1:A:715:ILE:HG13	2.06	0.55
1:B:606:TRP:CZ2	1:B:615:ILE:HD12	2.41	0.55
1:B:45:LYS:HB2	1:B:82:TYR:CD2	2.41	0.55
1:A:696:ALA:HB3	1:A:708:VAL:HG11	1.88	0.55
1:A:70:VAL:HG12	1:A:252:ILE:CD1	2.36	0.55
1:B:237:ALA:N	1:B:238:PRO:HD3	2.22	0.55
1:A:48:VAL:HG21	1:A:55:LYS:HD2	1.89	0.55
1:A:611:GLN:OE1	1:A:770:ILE:HG21	2.07	0.55
1:A:701:ASP:O	1:A:703:ASN:N	2.39	0.55
1:A:754:LYS:O	1:A:758:ASN:HB2	2.06	0.55
1:B:477:TYR:HB2	1:B:555:ILE:HD13	1.88	0.55
1:B:643:TYR:HA	1:B:646:GLN:HG3	1.89	0.55
1:B:338:LEU:HD22	1:B:379:LEU:HD13	1.87	0.54
1:B:516:ASN:ND2	1:B:516:ASN:H	2.06	0.54
1:A:606:TRP:CH2	1:A:615:ILE:HG23	2.41	0.54
1:A:309:HIS:C	1:A:311:LEU:H	2.10	0.54
1:A:38:GLU:OE2	1:A:41:LYS:HE2	2.07	0.54
1:B:420:ASP:OD2	1:B:523:ARG:NH1	2.38	0.54
1:B:713:LYS:O	1:B:717:ILE:HG12	2.07	0.54
1:B:659:TYR:H	3:B:9003:NSC:C27	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HD13	1:A:115:HIS:HE1	1.73	0.54
1:A:53:ALA:O	1:A:57:GLU:HB2	2.08	0.54
3:A:9002:NSC:O28	3:A:9002:NSC:H17	2.06	0.54
1:B:444:ASN:ND2	1:B:448:ALA:HA	2.23	0.53
1:A:244:MET:HE3	1:A:244:MET:HA	1.90	0.53
1:A:302:PRO:HG2	1:A:383:ILE:O	2.08	0.53
1:A:426:SER:HA	1:A:510:ARG:HA	1.89	0.53
1:A:275:LYS:NZ	1:A:279:GLN:HE22	2.06	0.53
1:B:305:ASP:N	1:B:305:ASP:OD2	2.42	0.53
1:A:317:GLU:O	1:A:320:LYS:HB2	2.08	0.53
1:B:94:LEU:HD22	1:B:97:LEU:HD11	1.91	0.53
1:A:256:LEU:HD22	1:A:260:LYS:HG3	1.91	0.53
1:B:126:GLU:N	1:B:127:PRO:CD	2.72	0.53
1:B:552:LYS:HE2	1:B:556:ASP:OD1	2.09	0.53
1:B:769:GLN:HA	1:B:769:GLN:NE2	2.24	0.53
1:A:387:ASP:HB3	1:A:390:GLN:HB3	1.91	0.52
1:A:424:HIS:O	1:A:510:ARG:HD2	2.09	0.52
1:B:722:GLY:HA3	1:B:730:ARG:HH11	1.74	0.52
1:B:436:TYR:HA	1:B:503:ILE:O	2.10	0.52
1:A:339:LYS:O	1:A:343:ILE:HG12	2.10	0.52
1:A:686:HIS:HB2	1:A:742:ARG:HD3	1.92	0.52
1:A:701:ASP:OD2	1:A:704:GLN:HB3	2.10	0.52
1:B:107:ILE:HG12	1:B:149:TYR:CG	2.45	0.52
1:B:51:GLU:OE1	1:B:53:ALA:HB2	2.10	0.52
1:B:369:SER:O	1:B:373:LYS:HG3	2.10	0.51
1:A:234:GLN:NE2	1:A:241:PHE:CE1	2.79	0.51
1:A:618:VAL:O	1:A:622:LEU:HG	2.10	0.51
1:A:743:LEU:HD22	1:A:751:GLU:HG2	1.92	0.51
1:B:426:SER:HA	1:B:510:ARG:HA	1.93	0.51
1:A:100:ASP:C	1:A:102:LYS:H	2.14	0.51
1:B:501:TRP:HB3	1:B:503:ILE:HD11	1.93	0.51
1:A:659:TYR:HB3	3:A:9002:NSC:C26	2.39	0.51
1:B:516:ASN:ND2	1:B:516:ASN:N	2.56	0.51
1:A:123:GLU:HG3	1:A:157:ARG:CZ	2.41	0.51
1:B:107:ILE:HG22	1:B:108:TYR:CD1	2.46	0.51
1:B:586:ASN:HB3	1:B:632:THR:HB	1.93	0.51
1:A:373:LYS:O	1:A:377:LYS:HG3	2.10	0.51
1:B:392:LEU:HD21	1:B:416:ILE:HD13	1.93	0.51
1:B:510:ARG:H	1:B:522:GLN:NE2	1.94	0.51
1:A:315:GLU:HB3	1:A:375:PHE:CE1	2.46	0.51
1:A:640:ALA:O	1:A:642:GLN:N	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:TYR:C	1:B:238:PRO:HD3	2.32	0.50
1:A:342:GLN:O	1:A:345:ILE:HG22	2.11	0.50
1:A:40:MET:O	1:A:44:VAL:HB	2.11	0.50
1:B:312:SER:OG	1:B:315:GLU:HG3	2.11	0.50
1:A:443:ILE:CD1	1:A:454:LEU:HD22	2.41	0.50
1:B:167:TYR:OH	1:B:203:VAL:HG21	2.12	0.50
1:B:496:ASN:H	1:B:496:ASN:ND2	2.10	0.50
1:A:643:TYR:HA	1:A:646:GLN:HG3	1.93	0.50
1:B:65:LYS:HB2	1:B:148:TYR:OH	2.11	0.50
1:A:32:GLN:CG	1:A:33:GLU:H	2.20	0.50
1:B:304:LYS:CD	1:B:304:LYS:H	2.02	0.50
1:B:662:GLU:H	1:B:662:GLU:CD	2.13	0.50
1:A:583:ILE:HG23	1:A:631:PHE:HE1	1.77	0.49
1:B:107:ILE:HD13	1:B:219:LYS:HG2	1.94	0.49
1:A:602:ILE:HG23	1:A:681:SER:HA	1.93	0.49
1:B:578:LYS:O	1:B:579:TYR:HB2	2.12	0.49
1:A:614:LEU:HB2	1:A:774:ILE:HD11	1.94	0.49
1:A:566:ILE:HG13	1:A:600:TYR:CE2	2.47	0.49
1:B:94:LEU:HD21	1:B:120:TYR:HD2	1.77	0.49
1:B:121:ALA:HA	1:B:128:VAL:O	2.12	0.49
1:A:392:LEU:HD13	1:A:482:ASN:HA	1.93	0.49
1:B:496:ASN:H	1:B:496:ASN:HD22	1.59	0.49
1:B:47:GLU:O	1:B:84:VAL:HG23	2.12	0.49
1:A:410:LYS:HB3	1:A:410:LYS:NZ	2.27	0.49
1:B:564:LEU:O	1:B:568:GLN:HG3	2.12	0.49
1:A:317:GLU:HA	1:A:320:LYS:HD2	1.95	0.49
1:B:233:LEU:HD13	1:B:241:PHE:HB2	1.95	0.49
1:B:358:ASN:HD22	1:B:358:ASN:C	2.15	0.49
1:A:330:LEU:O	1:A:335:LYS:HE3	2.12	0.49
1:A:329:PHE:HA	3:A:9002:NSC:C8	2.42	0.49
1:A:293:LEU:HD22	1:A:520:ILE:HD12	1.95	0.48
1:B:630:VAL:HG11	1:B:639:ILE:HD13	1.95	0.48
1:B:440:ASN:HD21	1:B:500:LYS:HZ2	1.58	0.48
1:A:221:PHE:CE2	1:A:225:ILE:HG13	2.48	0.48
1:A:366:ASN:H	1:A:366:ASN:HD22	1.62	0.48
1:A:443:ILE:HD12	1:A:454:LEU:HD22	1.95	0.48
1:A:67:PRO:HG2	1:A:248:ASN:OD1	2.13	0.48
1:B:173:VAL:HG21	1:B:243:TYR:CD2	2.48	0.48
1:B:748:ASP:OD1	1:B:750:ALA:HB3	2.13	0.48
1:A:496:ASN:C	1:A:496:ASN:ND2	2.66	0.48
1:A:74:TYR:CZ	1:A:154:ILE:HD13	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:SER:HB2	1:B:372:GLU:HG3	1.94	0.48
1:B:741:PHE:O	1:B:745:HIS:HD2	1.96	0.48
1:A:496:ASN:HD22	1:A:497:GLU:N	2.11	0.48
1:B:234:GLN:HB2	1:B:241:PHE:CD2	2.49	0.48
1:B:89:THR:C	1:B:91:HIS:H	2.17	0.48
1:B:233:LEU:CD1	1:B:241:PHE:HA	2.44	0.48
1:B:774:ILE:O	1:B:774:ILE:HG22	2.13	0.48
1:A:437:LEU:CD1	1:A:519:LEU:HD12	2.43	0.48
1:B:149:TYR:CZ	1:B:153:LYS:HE3	2.49	0.48
1:B:165:GLN:HA	1:B:166:PRO:C	2.34	0.48
1:A:380:LYS:O	1:A:384:GLN:HG2	2.14	0.47
1:B:322:ILE:HD13	1:B:376:LEU:HD21	1.95	0.47
1:B:77:ILE:HG13	1:B:162:LYS:HE2	1.96	0.47
1:A:556:ASP:O	1:A:560:GLN:HG3	2.13	0.47
1:B:687:GLU:OE2	3:B:9003:NSC:H27	2.14	0.47
1:A:104:ILE:HG22	1:A:105:LYS:N	2.29	0.47
1:A:192:ASN:HA	1:A:195:LYS:HB2	1.97	0.47
1:A:203:VAL:HG21	1:A:465:ARG:NH2	2.30	0.47
1:B:178:LYS:HB2	1:B:190:PHE:HE1	1.79	0.47
1:B:722:GLY:HA3	1:B:730:ARG:NH1	2.28	0.47
1:B:97:LEU:HB2	1:B:102:LYS:HE3	1.95	0.47
1:A:94:LEU:HD11	1:A:130:VAL:HG21	1.97	0.47
1:B:62:LEU:HD21	1:B:147:VAL:HG11	1.96	0.47
1:B:674:GLY:HA3	1:B:677:LEU:HD12	1.97	0.47
1:B:84:VAL:O	1:B:132:GLN:HA	2.14	0.47
1:A:437:LEU:HD12	1:A:505:LEU:HD21	1.95	0.47
1:A:611:GLN:H	1:A:611:GLN:NE2	2.13	0.47
1:B:156:SER:HB2	1:B:217:PHE:CD2	2.50	0.47
1:B:446:LEU:HG	1:B:591:TYR:HB2	1.97	0.47
1:B:520:ILE:O	1:B:520:ILE:HG23	2.15	0.47
1:B:632:THR:CG2	1:B:639:ILE:HD11	2.42	0.47
1:B:74:TYR:HA	1:B:159:ILE:HD11	1.97	0.47
1:B:662:GLU:OE2	1:B:662:GLU:N	2.26	0.47
1:A:193:GLN:NE2	1:A:193:GLN:CA	2.78	0.47
1:A:268:TYR:CE2	1:B:125:TYR:HB3	2.50	0.47
1:A:48:VAL:HG11	1:A:55:LYS:HD3	1.97	0.47
1:A:710:ASN:O	1:A:710:ASN:ND2	2.48	0.47
1:B:107:ILE:HG13	1:B:145:LEU:CD1	2.45	0.47
1:B:252:ILE:HG23	1:B:253:ASN:N	2.30	0.47
1:B:759:ALA:N	1:B:760:PRO:CD	2.78	0.47
1:A:559:ILE:HD13	1:A:587:VAL:HB	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:VAL:HB	1:B:551:PRO:HD2	1.96	0.46
1:A:717:ILE:HG23	1:A:761:LYS:HB3	1.97	0.46
1:A:118:TYR:N	1:A:118:TYR:CD1	2.84	0.46
1:A:182:ASP:OD1	1:A:184:ASP:HB2	2.16	0.46
1:B:678:ARG:HG2	1:B:682:GLU:OE1	2.15	0.46
1:A:125:TYR:HA	1:B:268:TYR:CE2	2.50	0.46
1:A:141:THR:HG21	1:A:228:GLN:HG3	1.97	0.46
1:A:567:ASN:ND2	1:A:582:LEU:H	2.13	0.46
1:A:656:LYS:O	1:A:656:LYS:HD3	2.15	0.46
1:A:673:LYS:NZ	1:A:678:ARG:HA	2.30	0.46
1:B:331:SER:OG	1:B:334:GLU:HG3	2.15	0.46
1:B:659:TYR:H	3:B:9003:NSC:H27	1.79	0.46
1:A:119:VAL:HG11	1:A:147:VAL:HG13	1.98	0.46
1:A:598:SER:O	1:A:602:ILE:HG13	2.16	0.46
1:B:114:LEU:HD23	1:B:114:LEU:O	2.15	0.46
1:A:103:LYS:HG3	1:A:112:ALA:O	2.15	0.46
1:A:717:ILE:CD1	1:A:761:LYS:HD2	2.45	0.46
1:B:765:PHE:O	1:B:769:GLN:HG2	2.16	0.46
1:A:577:PRO:O	1:A:580:THR:CG2	2.63	0.46
1:B:91:HIS:CG	1:B:92:ILE:N	2.84	0.46
1:A:107:ILE:HG21	1:A:145:LEU:CD1	2.44	0.46
1:A:343:ILE:HG22	1:A:343:ILE:O	2.16	0.46
1:A:366:ASN:N	1:A:366:ASN:HD22	2.13	0.46
1:A:32:GLN:HG3	1:A:33:GLU:N	2.25	0.46
1:A:611:GLN:H	1:A:611:GLN:HE21	1.63	0.46
1:B:387:ASP:HB3	1:B:390:GLN:CB	2.46	0.46
1:B:40:MET:HA	1:B:44:VAL:HG23	1.98	0.46
1:A:378:LYS:HE2	1:A:650:TYR:CE2	2.51	0.45
1:B:122:LYS:HE2	1:B:128:VAL:HG22	1.97	0.45
1:A:135:GLU:N	1:A:135:GLU:CD	2.70	0.45
1:A:440:ASN:HD21	1:A:500:LYS:NZ	2.13	0.45
1:A:371:LYS:HD2	1:A:371:LYS:N	2.31	0.45
1:A:157:ARG:HG3	1:A:214:GLN:HE22	1.81	0.45
1:A:345:ILE:HG13	1:A:345:ILE:O	2.17	0.45
1:A:35:HIS:O	1:A:39:ILE:HG12	2.16	0.45
1:A:46:ILE:HG12	1:A:56:LYS:CG	2.45	0.45
1:A:176:THR:HG21	1:A:239:GLU:HG3	1.98	0.45
1:A:677:LEU:HD13	1:A:683:GLY:HA2	1.99	0.45
1:A:309:HIS:O	1:A:311:LEU:N	2.49	0.45
1:A:640:ALA:HA	1:A:643:TYR:CE2	2.52	0.45
1:A:226:GLU:OE1	1:A:228:GLN:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:HIS:CE1	1:A:425:GLN:NE2	2.80	0.45
1:A:584:THR:HG23	1:A:630:VAL:HG22	1.99	0.45
1:A:83:ILE:HD12	1:A:83:ILE:N	2.32	0.45
1:A:114:LEU:HD21	1:A:120:TYR:CD1	2.52	0.45
1:B:395:THR:HB	1:B:398:LEU:O	2.17	0.45
1:A:640:ALA:C	1:A:642:GLN:N	2.71	0.44
1:A:567:ASN:ND2	1:A:583:ILE:H	2.10	0.44
1:B:679:ASN:ND2	1:B:681:SER:HB2	2.26	0.44
1:B:119:VAL:HA	1:B:130:VAL:O	2.17	0.44
1:B:244:MET:HA	1:B:244:MET:HE3	1.98	0.44
1:B:444:ASN:HD22	1:B:448:ALA:HA	1.80	0.44
1:B:551:PRO:HG2	1:B:554:LYS:HG3	1.98	0.44
1:B:210:SER:O	1:B:214:GLN:HG3	2.17	0.44
1:B:571:ASN:ND2	1:B:580:THR:HB	2.32	0.44
1:B:739:GLU:OE1	1:B:739:GLU:HA	2.17	0.44
1:B:353:GLU:OE1	1:B:357:LEU:HG	2.18	0.44
1:A:171:LEU:HG	1:A:206:LEU:HD13	2.00	0.44
1:A:336:GLU:HG3	1:A:340:LYS:HE3	1.98	0.44
1:A:538:SER:O	1:A:539:GLU:HB2	2.17	0.44
1:B:717:ILE:HG23	1:B:761:LYS:HB2	1.98	0.44
1:A:311:LEU:HD23	1:A:316:LYS:HG2	2.00	0.44
1:A:391:ARG:NH1	1:A:404:ILE:HD12	2.33	0.44
1:B:304:LYS:HG2	1:B:305:ASP:H	1.81	0.44
1:B:516:ASN:HD22	1:B:516:ASN:H	1.60	0.44
1:B:188:LEU:HG	1:B:189:LEU:HG	1.98	0.44
1:B:197:HIS:HD2	1:B:199:THR:O	2.00	0.44
1:A:321:ARG:HA	1:A:321:ARG:HD2	1.75	0.44
1:B:496:ASN:ND2	1:B:496:ASN:N	2.65	0.44
1:A:401:SER:HA	1:A:402:PRO:HD3	1.73	0.43
1:A:614:LEU:O	1:A:618:VAL:HG23	2.18	0.43
1:B:54:VAL:HA	1:B:57:GLU:HB3	2.00	0.43
1:B:749:HIS:CE1	1:B:752:ARG:NH1	2.86	0.43
1:A:178:LYS:HD2	1:A:201:PHE:CE1	2.53	0.43
1:B:139:GLU:HG2	1:B:140:ASN:H	1.81	0.43
1:B:440:ASN:HD21	1:B:500:LYS:HZ3	1.63	0.43
1:A:174:LEU:HD11	1:A:213:VAL:HG13	2.00	0.43
1:B:740:ALA:O	1:B:744:MET:HG3	2.17	0.43
1:B:143:LYS:O	1:B:147:VAL:HG23	2.19	0.43
1:B:167:TYR:CZ	1:B:203:VAL:HG21	2.54	0.43
1:B:186:GLN:HG3	1:B:190:PHE:CD1	2.53	0.43
1:A:322:ILE:O	1:A:324:ILE:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ASP:OD1	1:A:523:ARG:HD3	2.19	0.43
1:A:424:HIS:HA	1:A:510:ARG:HD2	2.00	0.43
1:B:322:ILE:HD11	1:B:376:LEU:HD11	2.00	0.43
1:A:326:SER:O	1:A:368:LEU:HD21	2.19	0.43
1:B:318:LEU:O	1:B:322:ILE:HB	2.19	0.43
1:B:45:LYS:HE3	1:B:80:LYS:HD2	2.00	0.43
1:A:118:TYR:CZ	1:A:143:LYS:HG2	2.53	0.43
1:A:708:VAL:O	1:A:708:VAL:HG22	2.18	0.43
1:B:176:THR:CG2	1:B:239:GLU:HG3	2.43	0.42
1:B:244:MET:CE	1:B:248:ASN:HD21	2.32	0.42
1:B:35:HIS:CE1	1:B:38:GLU:HG2	2.54	0.42
1:B:45:LYS:HB2	1:B:82:TYR:HD2	1.81	0.42
1:B:83:ILE:CD1	1:B:131:ILE:HD12	2.49	0.42
1:B:65:LYS:HE2	1:B:227:PRO:HD3	2.02	0.42
1:A:386:TYR:OH	1:A:411:GLN:HG3	2.19	0.42
1:A:578:LYS:HD3	1:A:579:TYR:CZ	2.54	0.42
1:B:97:LEU:HB2	1:B:102:LYS:CE	2.49	0.42
1:B:389:ASN:OD1	1:B:482:ASN:HB2	2.18	0.42
1:B:723:SER:HB3	1:B:730:ARG:HD3	2.01	0.42
1:B:769:GLN:HA	1:B:769:GLN:HE21	1.84	0.42
1:A:98:SER:C	1:A:100:ASP:H	2.22	0.42
1:A:154:ILE:O	1:A:158:ASP:HB2	2.19	0.42
1:A:167:TYR:CZ	1:A:536:LYS:HB2	2.55	0.42
1:A:252:ILE:O	1:A:255:SER:HB2	2.19	0.42
1:A:393:GLN:NE2	1:A:445:ASN:HD21	2.15	0.42
1:A:51:GLU:N	1:A:51:GLU:CD	2.73	0.42
1:A:606:TRP:CZ2	1:A:615:ILE:HG23	2.55	0.42
1:A:516:ASN:HB2	1:B:539:GLU:CD	2.40	0.42
1:A:46:ILE:CD1	1:A:46:ILE:H	2.23	0.42
1:A:669:HIS:CE1	1:A:671:PRO:HB2	2.55	0.42
1:B:225:ILE:HD13	1:B:225:ILE:HA	1.89	0.42
1:B:270:LYS:O	1:B:274:ILE:HG12	2.20	0.42
1:A:640:ALA:HA	1:A:643:TYR:CD2	2.55	0.42
1:A:338:LEU:HA	1:A:341:LEU:HD12	2.02	0.42
1:A:437:LEU:HD12	1:A:505:LEU:HG	2.02	0.42
1:B:381:LEU:HD11	1:B:650:TYR:HA	2.02	0.42
1:A:165:GLN:HB3	1:A:166:PRO:HA	2.02	0.41
1:A:178:LYS:HG3	1:A:179:ASN:N	2.35	0.41
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.85	0.41
1:A:578:LYS:HB2	1:A:578:LYS:HZ3	1.84	0.41
1:A:64:GLU:HG2	1:A:64:GLU:O	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:GLU:OE2	1:A:742:ARG:NH1	2.52	0.41
1:B:139:GLU:HG2	1:B:140:ASN:N	2.35	0.41
1:A:103:LYS:HZ3	1:A:103:LYS:HB3	1.84	0.41
1:A:244:MET:CE	1:A:248:ASN:HD21	2.33	0.41
1:A:84:VAL:HG11	1:A:91:HIS:HD2	1.86	0.41
1:B:221:PHE:HD1	1:B:244:MET:HE1	1.84	0.41
1:B:278:TYR:CE2	1:B:425:GLN:HB3	2.55	0.41
1:A:271:TRP:O	1:A:271:TRP:HD1	2.03	0.41
1:A:339:LYS:O	1:A:342:GLN:HG2	2.21	0.41
1:A:440:ASN:HD21	1:A:500:LYS:HZ2	1.67	0.41
1:A:759:ALA:N	1:A:760:PRO:CD	2.82	0.41
3:A:9002:NSC:C12	3:A:9002:NSC:O28	2.68	0.41
1:B:237:ALA:N	1:B:238:PRO:CD	2.83	0.41
1:B:275:LYS:HG3	1:B:513:TYR:CZ	2.55	0.41
1:B:519:LEU:HD23	1:B:519:LEU:HA	1.94	0.41
1:B:717:ILE:HG23	1:B:761:LYS:CB	2.50	0.41
1:A:95:GLU:C	1:A:97:LEU:H	2.24	0.41
1:B:132:GLN:O	1:B:133:SER:C	2.58	0.41
1:B:675:VAL:O	1:B:676:GLU:HB2	2.21	0.41
1:A:173:VAL:O	1:A:177:ILE:HG12	2.20	0.41
1:A:309:HIS:C	1:A:311:LEU:N	2.73	0.41
1:A:399:ILE:HD12	1:A:413:LYS:HG3	2.01	0.41
1:A:298:ILE:HG13	1:A:298:ILE:O	2.20	0.41
1:A:660:VAL:HA	1:A:661:PRO:HD2	1.92	0.41
1:A:715:ILE:O	1:A:719:LYS:HG2	2.21	0.41
1:A:328:ASP:O	3:A:9002:NSC:H82	2.20	0.41
1:B:149:TYR:OH	1:B:153:LYS:HE3	2.20	0.41
1:A:157:ARG:HB2	1:A:214:GLN:NE2	2.36	0.41
1:A:693:ASP:CG	1:A:709:THR:HB	2.41	0.41
1:A:30:LYS:O	1:A:30:LYS:HG2	2.20	0.41
1:A:640:ALA:C	1:A:642:GLN:H	2.24	0.41
1:B:697:GLY:HA3	1:B:706:ASP:O	2.21	0.41
1:A:437:LEU:HD12	1:A:505:LEU:CD2	2.51	0.41
1:A:696:ALA:HB2	1:A:773:ILE:HD11	2.03	0.41
1:B:398:LEU:HD22	1:B:398:LEU:H	1.86	0.41
1:B:45:LYS:HB2	1:B:82:TYR:CE2	2.55	0.41
1:B:499:LEU:HD12	1:B:543:ILE:HB	2.02	0.41
1:A:169:LYS:NZ	1:A:251:GLU:OE2	2.54	0.41
1:A:275:LYS:HZ2	1:A:279:GLN:HE22	1.68	0.41
1:B:304:LYS:HG2	1:B:305:ASP:N	2.36	0.41
3:B:9003:NSC:C12	3:B:9003:NSC:O28	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ILE:CD1	1:A:413:LYS:HG3	2.51	0.40
1:A:718:PHE:O	1:A:722:GLY:HA3	2.21	0.40
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.91	0.40
1:B:415:ASP:O	1:B:419:ILE:HG13	2.21	0.40
1:B:67:PRO:HB2	1:B:70:VAL:HG23	2.03	0.40
1:A:119:VAL:HA	1:A:130:VAL:O	2.21	0.40
1:A:136:ASP:O	1:A:140:ASN:N	2.49	0.40
1:A:190:PHE:CD2	1:A:190:PHE:N	2.89	0.40
1:A:366:ASN:N	1:A:366:ASN:ND2	2.69	0.40
1:A:415:ASP:O	1:A:419:ILE:HG13	2.21	0.40
1:A:478:SER:OG	1:A:590:ARG:HA	2.22	0.40
1:B:48:VAL:HB	1:B:85:ASP:OD2	2.21	0.40
1:A:105:LYS:HE2	1:A:111:ASP:OD2	2.20	0.40
1:B:440:ASN:ND2	1:B:500:LYS:HZ3	2.19	0.40
1:B:660:VAL:HB	1:B:663:SER:OG	2.21	0.40
1:A:441:MET:HG2	1:A:442:ASN:N	2.36	0.40
1:A:637:PRO:HD3	1:A:654:HIS:HB2	2.03	0.40
1:A:716:ASP:O	1:A:719:LYS:HB2	2.21	0.40
1:B:40:MET:O	1:B:44:VAL:HB	2.22	0.40
1:B:553:SER:O	1:B:557:THR:CG2	2.68	0.40
1:B:59:ALA:C	1:B:61:LYS:H	2.25	0.40
1:A:323:GLN:O	1:A:324:ILE:C	2.59	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	728/776 (94%)	643 (88%)	69 (10%)	16 (2%)	6	24
1	B	739/776 (95%)	652 (88%)	76 (10%)	11 (2%)	10	34
All	All	1467/1552 (94%)	1295 (88%)	145 (10%)	27 (2%)	8	29

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	GLU
1	B	138	VAL
1	A	53	ALA
1	A	198	PRO
1	A	310	SER
1	A	311	LEU
1	A	329	PHE
1	A	473	LYS
1	A	592	ALA
1	B	98	SER
1	B	133	SER
1	B	326	SER
1	A	641	GLU
1	A	702	LYS
1	B	64	GLU
1	B	251	GLU
1	B	329	PHE
1	A	324	ILE
1	A	347	ASP
1	B	650	TYR
1	B	722	GLY
1	A	32	GLN
1	A	49	LYS
1	A	304	LYS
1	B	433	ASN
1	A	305	ASP
1	B	78	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	671/710 (94%)	626 (93%)	45 (7%)	16	43
1	B	682/710 (96%)	639 (94%)	43 (6%)	18	46
All	All	1353/1420 (95%)	1265 (94%)	88 (6%)	17	45

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	56	LYS
1	A	70	VAL
1	A	71	LEU
1	A	95	GLU
1	A	99	GLU
1	A	119	VAL
1	A	135	GLU
1	A	145	LEU
1	A	193	GLN
1	A	211	ASN
1	A	233	LEU
1	A	256	LEU
1	A	259	LEU
1	A	276	GLN
1	A	296	LEU
1	A	304	LYS
1	A	344	ASP
1	A	346	ARG
1	A	366	ASN
1	A	404	ILE
1	A	417	GLN
1	A	435	ILE
1	A	447	THR
1	A	449	THR
1	A	494	LEU
1	A	496	ASN
1	A	505	LEU
1	A	522	GLN
1	A	523	ARG
1	A	546	ASP
1	A	564	LEU
1	A	574	LEU
1	A	578	LYS
1	A	580	THR
1	A	582	LEU
1	A	584	THR
1	A	591	TYR
1	A	611	GLN
1	A	626	ASN
1	A	636	LEU
1	A	656	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	676	GLU
1	A	710	ASN
1	A	712	LYS
1	B	35	HIS
1	B	72	GLU
1	B	77	ILE
1	B	85	ASP
1	B	107	ILE
1	B	111	ASP
1	B	129	LEU
1	B	139	GLU
1	B	146	ASN
1	B	193	GLN
1	B	246	LYS
1	B	253	ASN
1	B	256	LEU
1	B	304	LYS
1	B	305	ASP
1	B	314	GLU
1	B	323	GLN
1	B	329	PHE
1	B	333	GLU
1	B	348	SER
1	B	351	GLU
1	B	352	GLU
1	B	353	GLU
1	B	358	ASN
1	B	359	ARG
1	B	391	ARG
1	B	425	GLN
1	B	432	TYR
1	B	447	THR
1	B	496	ASN
1	B	499	LEU
1	B	516	ASN
1	B	520	ILE
1	B	523	ARG
1	B	557	THR
1	B	591	TYR
1	B	608	ASN
1	B	611	GLN
1	B	698	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	704	GLN
1	B	706	ASP
1	B	712	LYS
1	B	767	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	A	140	ASN
1	A	164	ASN
1	A	193	GLN
1	A	197	HIS
1	A	209	ASN
1	A	214	GLN
1	A	234	GLN
1	A	242	ASN
1	A	262	GLN
1	A	277	HIS
1	A	279	GLN
1	A	366	ASN
1	A	393	GLN
1	A	440	ASN
1	A	496	ASN
1	A	504	GLN
1	A	522	GLN
1	A	524	ASN
1	A	563	GLN
1	A	567	ASN
1	A	571	ASN
1	A	608	ASN
1	A	611	GLN
1	A	652	GLN
1	A	710	ASN
1	A	724	ASN
1	A	745	HIS
1	A	767	ASN
1	A	769	GLN
1	B	42	HIS
1	B	91	HIS
1	B	164	ASN
1	B	197	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	209	ASN
1	B	214	GLN
1	B	228	GLN
1	B	234	GLN
1	B	242	ASN
1	B	248	ASN
1	B	250	GLN
1	B	253	ASN
1	B	262	GLN
1	B	297	GLN
1	B	313	GLN
1	B	323	GLN
1	B	358	ASN
1	B	440	ASN
1	B	444	ASN
1	B	445	ASN
1	B	496	ASN
1	B	504	GLN
1	B	516	ASN
1	B	522	GLN
1	B	524	ASN
1	B	533	GLN
1	B	563	GLN
1	B	571	ASN
1	B	608	ASN
1	B	609	ASN
1	B	611	GLN
1	B	638	ASN
1	B	645	HIS
1	B	679	ASN
1	B	704	GLN
1	B	745	HIS
1	B	756	GLN
1	B	769	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NSC	B	9003	-	31,31,31	1.48	6 (19%)	43,45,45	1.31	7 (16%)
3	NSC	A	9002	-	31,31,31	1.48	6 (19%)	43,45,45	1.31	9 (20%)

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	NSC	B	9003	-	-	0/8/8/8	0/4/4/4
3	NSC	A	9002	-	-	0/8/8/8	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	9003	NSC	C16-N15	-2.89	1.35	1.41
3	A	9002	NSC	C11-N13	-2.87	1.35	1.41
3	A	9002	NSC	C16-N15	-2.86	1.35	1.41
3	B	9003	NSC	C11-N13	-2.74	1.36	1.41
3	A	9002	NSC	C17-C16	2.42	1.42	1.37
3	B	9003	NSC	C17-C16	2.39	1.42	1.37
3	B	9003	NSC	C9-C10	2.35	1.41	1.36
3	B	9003	NSC	C12-C11	2.30	1.42	1.37
3	B	9003	NSC	C26-C27	2.30	1.41	1.36
3	A	9002	NSC	C9-C10	2.29	1.41	1.36
3	A	9002	NSC	C12-C11	2.28	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	9002	NSC	C26-C27	2.14	1.41	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	9002	NSC	C12-C3-C2	-2.59	120.98	123.08
3	B	9003	NSC	C12-C3-C2	-2.59	120.98	123.08
3	B	9003	NSC	C3-C4-N5	-2.58	120.07	122.81
3	A	9002	NSC	C3-C4-N5	-2.55	120.10	122.81
3	B	9003	NSC	C18-C19-N22	-2.50	120.16	122.81
3	A	9002	NSC	C23-C24-C18	2.43	119.64	117.96
3	A	9002	NSC	C18-C19-N22	-2.40	120.27	122.81
3	B	9003	NSC	C23-C24-C18	2.31	119.56	117.96
3	A	9002	NSC	C7-C2-C3	2.26	119.52	117.96
3	B	9003	NSC	C7-C2-C3	2.25	119.52	117.96
3	A	9002	NSC	C17-C18-C24	-2.20	121.30	123.08
3	B	9003	NSC	C17-C18-C24	-2.14	121.35	123.08
3	B	9003	NSC	C2-C3-C4	2.12	119.02	117.11
3	A	9002	NSC	C23-C21-N22	-2.11	120.07	122.57
3	A	9002	NSC	C7-C6-N5	-2.07	120.11	122.57
3	A	9002	NSC	C2-C3-C4	2.03	118.93	117.11

There are no chirality outliers.

There are no torsion outliers.

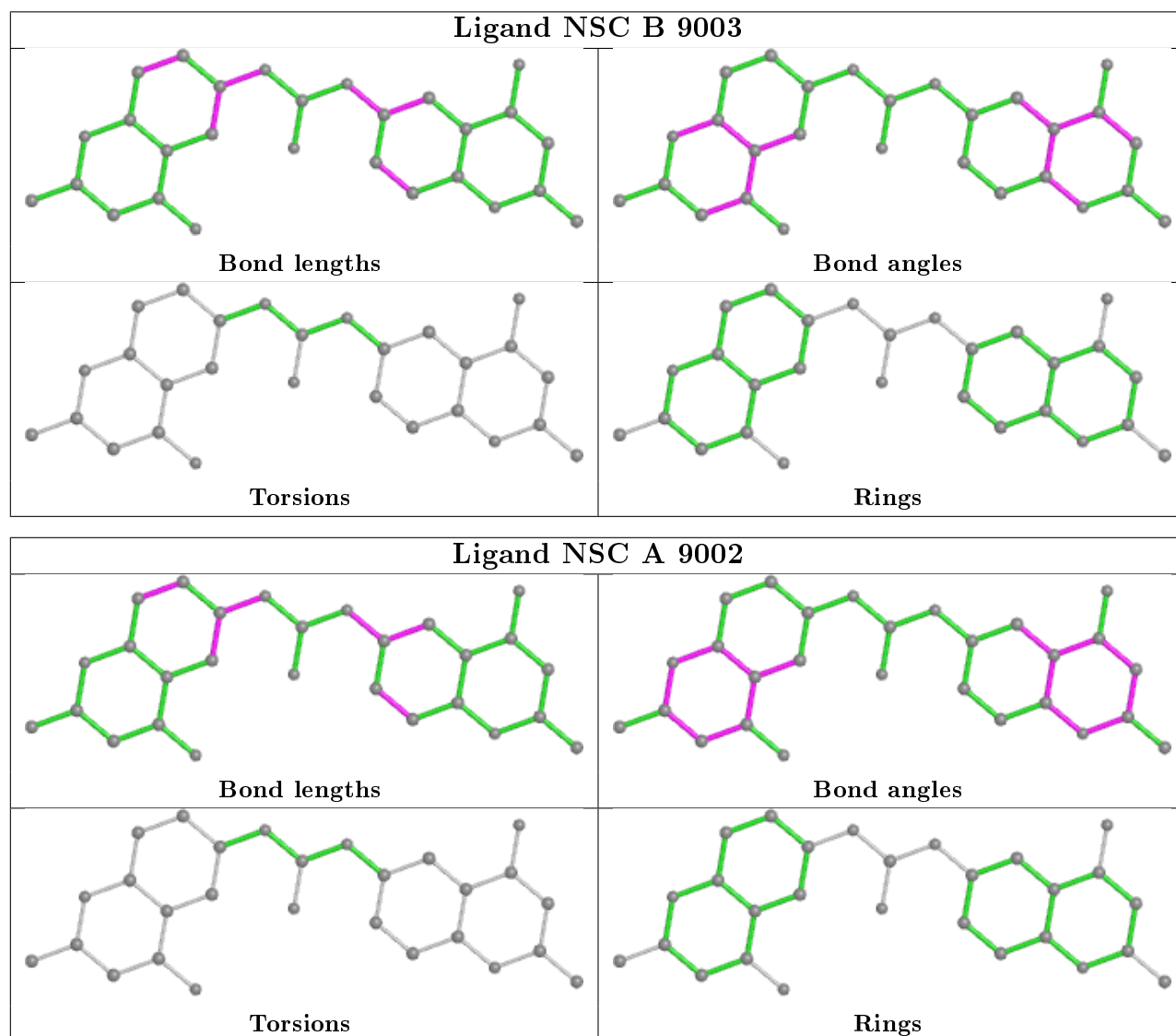
There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	9003	NSC	7	0
3	A	9002	NSC	8	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	732/776 (94%)	0.16	50 (6%) 17 13	8, 39, 94, 125	0
1	B	743/776 (95%)	0.17	56 (7%) 14 11	9, 37, 91, 101	0
All	All	1475/1552 (95%)	0.17	106 (7%) 15 11	8, 39, 92, 125	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	LEU	6.2
1	B	352	GLU	6.1
1	B	358	ASN	5.7
1	B	349	LEU	5.7
1	B	37	LYS	5.5
1	A	365	SER	5.3
1	B	356	LEU	5.0
1	B	364	SER	4.9
1	B	114	LEU	4.9
1	B	353	GLU	4.8
1	B	48	VAL	4.7
1	B	363	ASP	4.6
1	B	359	ARG	4.5
1	A	308	ILE	4.4
1	A	33	GLU	4.4
1	A	320	LYS	4.4
1	A	367	PRO	4.3
1	B	115	HIS	4.3
1	A	54	VAL	4.3
1	B	97	LEU	4.3
1	A	324	ILE	4.2
1	B	54	VAL	4.2
1	B	34	GLU	4.1
1	A	321	ARG	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	366	ASN	4.1
1	A	703	ASN	4.0
1	B	348	SER	3.9
1	A	318	LEU	3.8
1	A	309	HIS	3.8
1	A	322	ILE	3.7
1	B	355	GLU	3.6
1	B	49	LYS	3.6
1	A	310	SER	3.5
1	A	341	LEU	3.5
1	A	346	ARG	3.5
1	B	367	PRO	3.5
1	A	330	LEU	3.3
1	B	354	LYS	3.3
1	B	51	GLU	3.3
1	B	52	GLU	3.2
1	A	347	ASP	3.2
1	A	368	LEU	3.2
1	B	35	HIS	3.2
1	A	34	GLU	3.2
1	A	317	GLU	3.2
1	A	32	GLN	3.2
1	B	44	VAL	3.1
1	A	316	LYS	3.1
1	B	324	ILE	3.1
1	B	365	SER	3.1
1	B	59	ALA	3.1
1	A	48	VAL	3.1
1	B	33	GLU	3.1
1	A	53	ALA	3.0
1	B	84	VAL	3.0
1	B	135	GLU	2.9
1	A	344	ASP	2.9
1	B	345	ILE	2.9
1	A	348	SER	2.8
1	A	311	LEU	2.8
1	B	357	LEU	2.8
1	B	56	LYS	2.8
1	A	31	THR	2.8
1	A	36	LEU	2.7
1	B	321	ARG	2.7
1	B	703	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	31	THR	2.7
1	A	49	LYS	2.7
1	B	83	ILE	2.6
1	A	579	TYR	2.6
1	A	704	GLN	2.6
1	B	94	LEU	2.6
1	B	329	PHE	2.6
1	B	91	HIS	2.6
1	A	306	ASP	2.6
1	B	32	GLN	2.5
1	A	345	ILE	2.5
1	A	305	ASP	2.5
1	A	312	SER	2.5
1	A	303	LYS	2.5
1	A	307	ILE	2.4
1	B	133	SER	2.4
1	B	50	GLY	2.4
1	B	351	GLU	2.4
1	A	372	GLU	2.4
1	A	329	PHE	2.4
1	B	368	LEU	2.3
1	B	53	ALA	2.3
1	B	350	SER	2.3
1	A	90	LYS	2.3
1	B	346	ARG	2.3
1	B	60	GLU	2.3
1	A	100	ASP	2.2
1	A	30	LYS	2.2
1	B	702	LYS	2.2
1	A	349	LEU	2.2
1	A	327	SER	2.2
1	B	92	ILE	2.1
1	B	46	ILE	2.1
1	A	52	GLU	2.1
1	B	136	ASP	2.1
1	B	90	LYS	2.1
1	B	134	SER	2.1
1	A	55	LYS	2.1
1	A	366	ASN	2.1
1	A	337	PHE	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 carbohydrates in this entry.

6.4 Ligands [i](#)

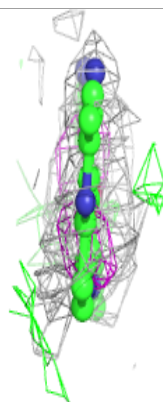
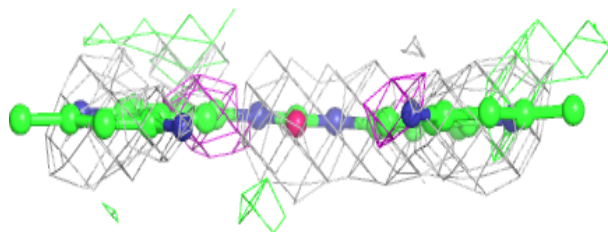
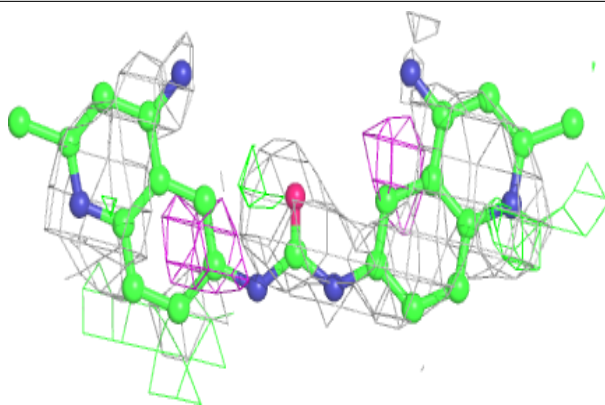
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NSC	B	9003	28/28	0.70	0.50	76,80,88,88	0
3	NSC	A	9002	28/28	0.78	0.40	75,80,87,87	0
2	ZN	B	9002	1/1	1.00	0.14	27,27,27,27	0
2	ZN	A	9001	1/1	1.00	0.20	37,37,37,37	0

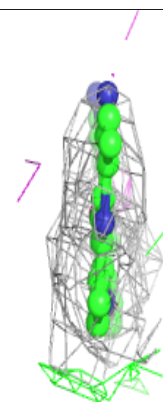
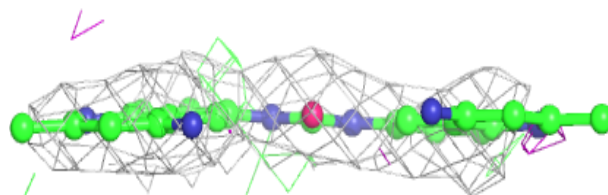
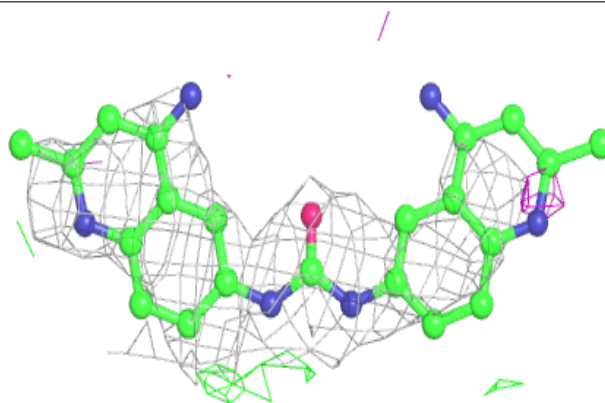
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NSC B 9003:

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

**Electron density around NSC A 9002:**

$2mF_o-DF_c$ (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.