



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 04:16 AM EDT

PDB ID : 2P9E
Title : Crystal Structure of G336V mutant of E.coli phosphoglycerate dehydrogenase
Authors : Dey, S.; Sacchettini, J.C.
Deposited on : 2007-03-25
Resolution : 2.60 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 : 2.23.2
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) : 2.23.2

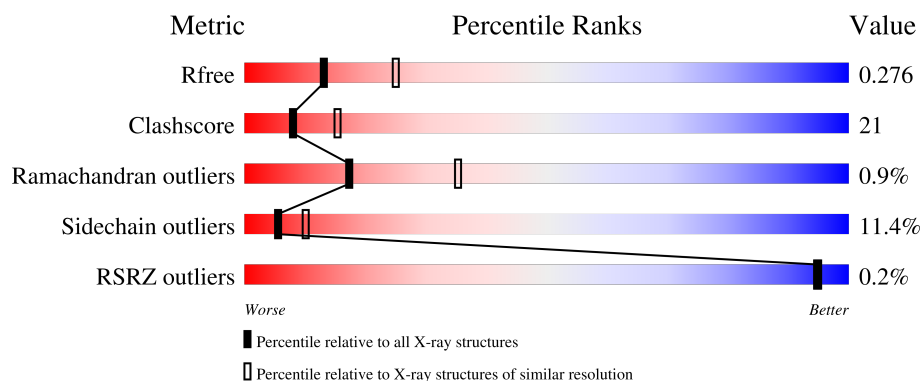
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	410	
1	B	410	
1	C	410	
1	D	410	

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
2	PO4	B	499	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12648 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 D-3-phosphoglycerate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3076	1950	534	584	8			
1	B	404	Total	C	N	O	S	0	0	0
			3062	1941	532	581	8			
1	C	406	Total	C	N	O	S	0	0	0
			3076	1950	534	584	8			
1	D	403	Total	C	N	O	S	0	0	0
			3053	1936	531	578	8			

There are 20 discrepancies between the modelled and reference sequences:

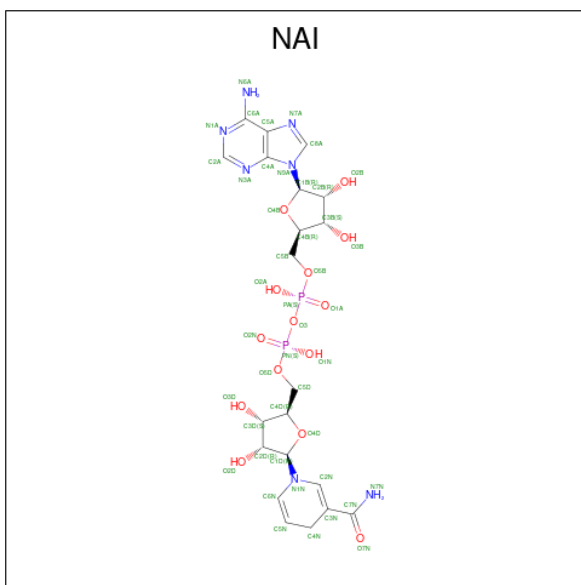
Chain	Residue	Modelled	Actual	Comment	Reference
A	81	ALA	CYS	engineered mutation	UNP P0A9T0
A	83	ALA	CYS	engineered mutation	UNP P0A9T0
A	250	ALA	CYS	engineered mutation	UNP P0A9T0
A	282	ALA	CYS	engineered mutation	UNP P0A9T0
A	336	VAL	GLY	engineered mutation	UNP P0A9T0
B	81	ALA	CYS	engineered mutation	UNP P0A9T0
B	83	ALA	CYS	engineered mutation	UNP P0A9T0
B	250	ALA	CYS	engineered mutation	UNP P0A9T0
B	282	ALA	CYS	engineered mutation	UNP P0A9T0
B	336	VAL	GLY	engineered mutation	UNP P0A9T0
C	81	ALA	CYS	engineered mutation	UNP P0A9T0
C	83	ALA	CYS	engineered mutation	UNP P0A9T0
C	250	ALA	CYS	engineered mutation	UNP P0A9T0
C	282	ALA	CYS	engineered mutation	UNP P0A9T0
C	336	VAL	GLY	engineered mutation	UNP P0A9T0
D	81	ALA	CYS	engineered mutation	UNP P0A9T0
D	83	ALA	CYS	engineered mutation	UNP P0A9T0
D	250	ALA	CYS	engineered mutation	UNP P0A9T0
D	282	ALA	CYS	engineered mutation	UNP P0A9T0
D	336	VAL	GLY	engineered mutation	UNP P0A9T0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



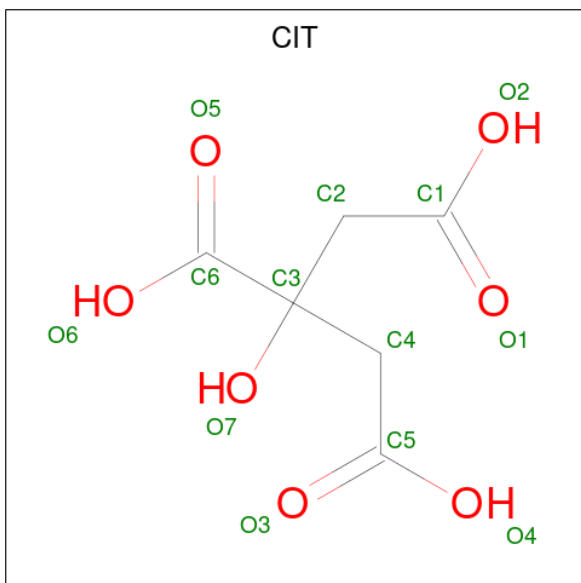
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



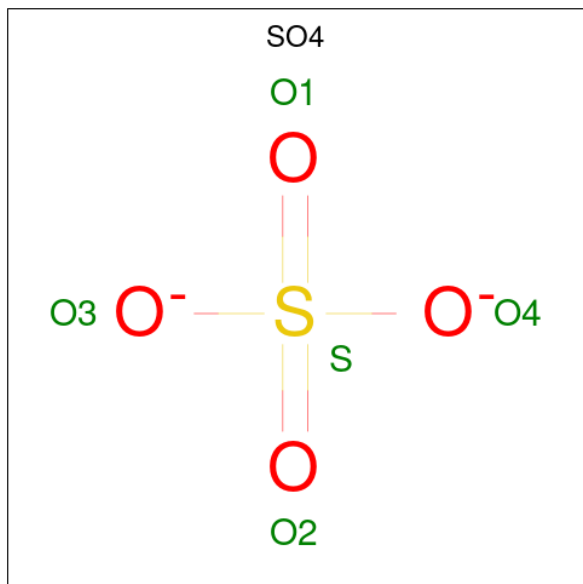
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	D	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0
4	A	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0
4	C	1	Total C O 13 6 7	0	0
4	C	1	Total C O 13 6 7	0	0
4	D	1	Total C O 13 6 7	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	24	Total O 24 24	0	0
6	B	16	Total O 16 16	0	0
6	C	15	Total O 15 15	0	0

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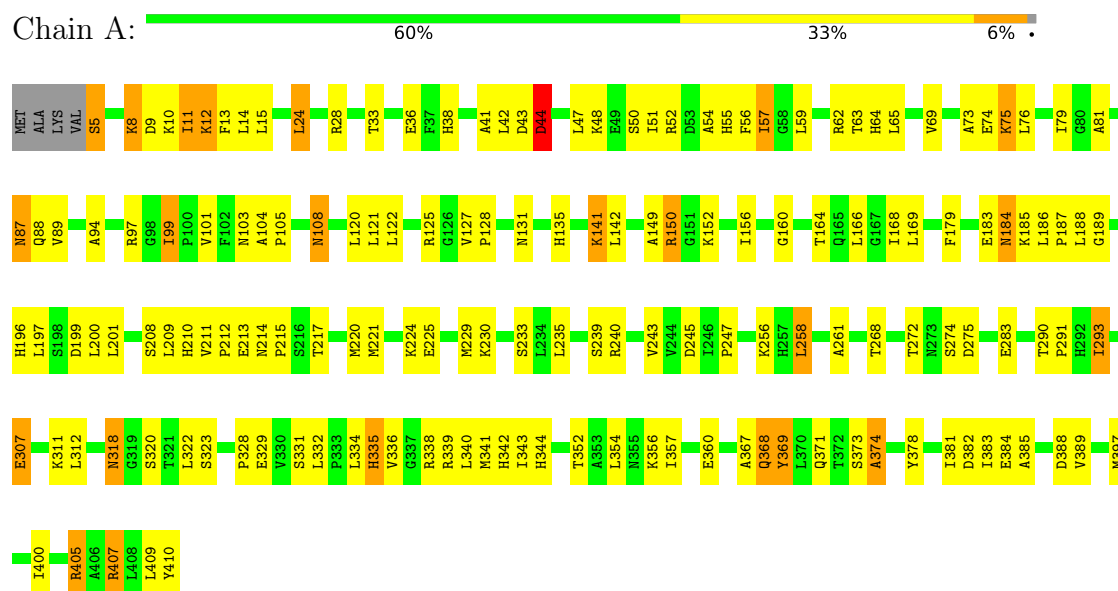
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	27	Total	O	0	0
			27	27		

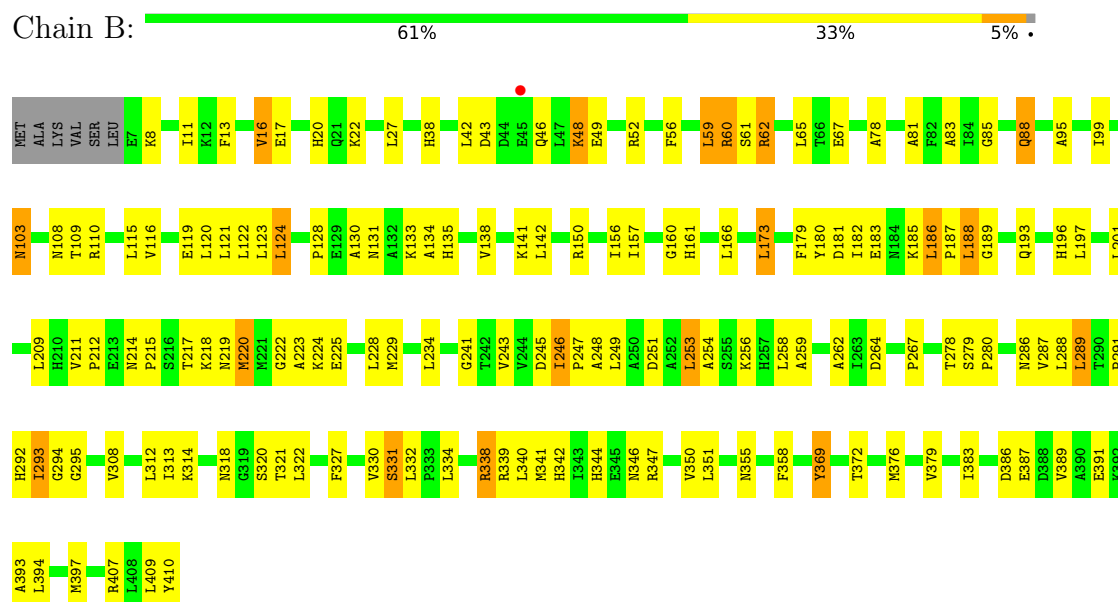
3 Residue-property plots

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: D-3-phosphoglycerate dehydrogenase

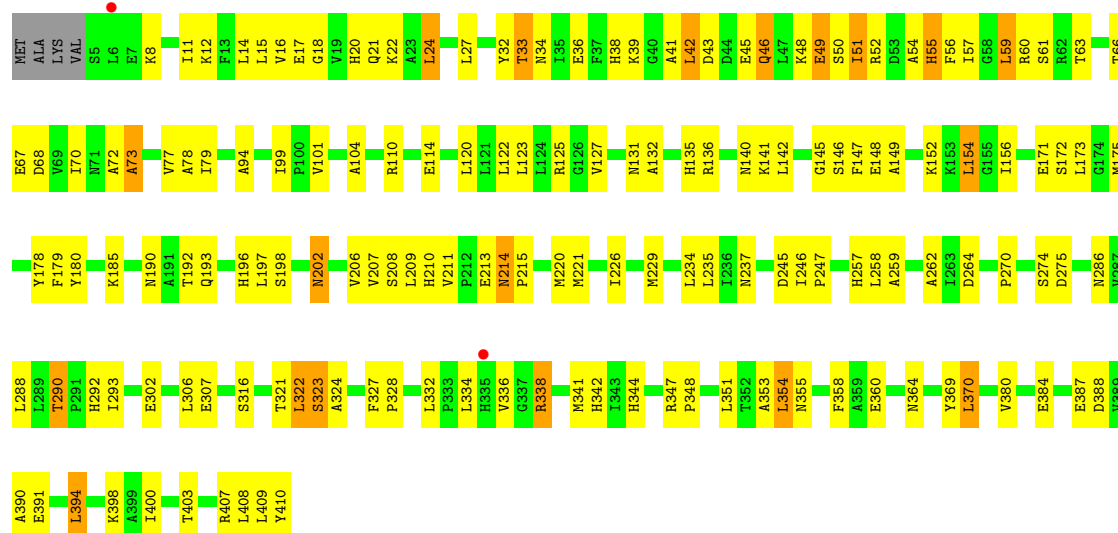


• Molecule 1: D-3-phosphoglycerate dehydrogenase



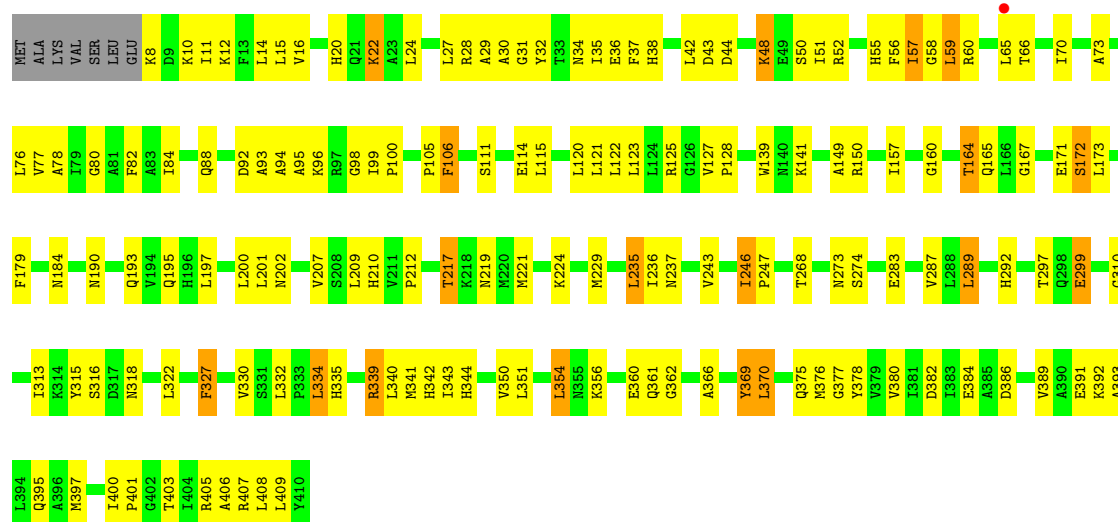
• Molecule 1: D-3-phosphoglycerate dehydrogenase

Chain C:  60% 35% 5% .



• Molecule 1: D-3-phosphoglycerate dehydrogenase

Chain D:  60% 34% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	76.24Å 76.24Å 353.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.60 42.11 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.00-2.60) 99.5 (42.11-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.279 0.203 , 0.276	Depositor DCC
R_{free} test set	3107 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 12.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.215 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12648	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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: CIT, PO4, NAI, SO4

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	0.74	0/3129	0.88	0/4241
1	B	0.79	1/3115 (0.0%)	0.88	0/4222
1	C	0.78	0/3129	0.94	2/4241 (0.0%)
1	D	0.79	0/3106	0.89	1/4210 (0.0%)
All	All	0.78	1/12479 (0.0%)	0.90	3/16914 (0.0%)

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	185	LYS	CE-NZ	6.13	1.64	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	207	VAL	CB-CA-C	-5.25	101.42	111.40
1	C	370	LEU	CA-CB-CG	5.20	127.26	115.30
1	D	200	LEU	CB-CG-CD1	-5.02	102.47	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	334	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3076	0	3122	144	0
1	B	3062	0	3106	140	0
1	C	3076	0	3122	139	0
1	D	3053	0	3100	127	0
2	A	10	0	0	0	0
2	B	10	0	0	3	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	44	0	27	2	0
3	B	44	0	27	4	0
3	C	44	0	27	0	0
3	D	44	0	27	1	0
4	A	26	0	10	7	0
4	B	13	0	5	3	0
4	C	26	0	10	6	0
4	D	13	0	5	3	0
5	C	5	0	0	1	0
6	A	24	0	0	4	0
6	B	16	0	0	0	0
6	C	15	0	0	1	0
6	D	27	0	0	2	0
All	All	12648	0	12588	539	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 21.

All (539) 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:268:THR:HB	6:D:590:HOH:O	1.39	1.17
1:C:342:HIS:CD2	1:C:344:HIS:HD2	1.63	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:HIS:HB3	2:B:499:PO4:O4	1.52	1.09
1:B:214:ASN:HB2	1:B:215:PRO:HD3	1.42	1.01
1:A:62:ARG:HH21	1:A:272:THR:HB	1.25	1.00
1:B:62:ARG:HH11	1:B:62:ARG:CG	1.76	0.99
1:B:62:ARG:HH11	1:B:62:ARG:HG3	0.84	0.98
1:B:62:ARG:HG3	1:B:62:ARG:NH1	1.64	0.98
1:B:342:HIS:ND1	1:B:344:HIS:HD2	1.62	0.97
1:C:20:HIS:HD2	1:C:22:LYS:H	1.10	0.96
1:B:88:GLN:N	1:B:88:GLN:HE21	1.64	0.95
1:C:342:HIS:CD2	1:C:344:HIS:CD2	2.55	0.94
1:C:342:HIS:HD2	1:C:344:HIS:HD2	1.09	0.93
1:A:59:LEU:HD23	1:A:59:LEU:H	1.31	0.92
1:B:161:HIS:HD2	3:B:509:NAI:O2A	1.52	0.92
1:B:214:ASN:HB2	1:B:215:PRO:CD	1.99	0.92
1:A:342:HIS:HD2	1:A:344:HIS:HD2	1.06	0.91
1:A:94:ALA:HB1	1:A:99:ILE:HB	1.53	0.90
1:B:88:GLN:HE21	1:B:88:GLN:H	0.98	0.90
1:C:322:LEU:O	1:C:323:SER:HB3	1.72	0.89
1:C:229:MET:CE	1:C:235:LEU:HD13	2.03	0.88
1:B:88:GLN:H	1:B:88:GLN:NE2	1.71	0.88
1:A:335:HIS:HB3	6:A:571:HOH:O	1.74	0.87
1:B:180:TYR:CD1	1:B:197:LEU:HD13	2.09	0.87
1:B:409:LEU:O	1:B:410:TYR:HB3	1.74	0.86
1:A:11:ILE:HG23	1:A:55:HIS:CG	2.10	0.86
1:B:42:LEU:HB3	1:B:46:GLN:HG3	1.57	0.86
1:D:12:LYS:H	1:D:55:HIS:HD2	1.20	0.85
1:A:141:LYS:O	1:A:141:LYS:HG3	1.79	0.82
1:A:342:HIS:HD2	1:A:344:HIS:CD2	1.94	0.82
1:A:125:ARG:HB2	1:A:127:VAL:HG23	1.62	0.82
1:A:150:ARG:CG	1:A:150:ARG:HH11	1.93	0.82
1:C:342:HIS:HD2	1:C:344:HIS:CD2	1.94	0.82
1:B:342:HIS:ND1	1:B:344:HIS:CD2	2.46	0.82
1:A:62:ARG:NH2	1:A:272:THR:HB	1.93	0.81
1:C:20:HIS:CD2	1:C:22:LYS:H	1.97	0.81
1:B:332:LEU:HB3	1:B:339:ARG:NH2	1.95	0.80
1:C:229:MET:HE1	1:C:235:LEU:HD13	1.62	0.80
1:C:78:ALA:HA	1:C:99:ILE:HG23	1.64	0.80
1:B:83:ALA:HB1	4:B:516:CIT:H41	1.64	0.79
4:C:517:CIT:C6	4:C:517:CIT:O3	2.25	0.79
1:D:212:PRO:O	1:D:217:THR:HG21	1.82	0.79
1:D:339:ARG:HD2	1:D:380:VAL:CG1	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:CD1	1:A:369:TYR:HB2	2.12	0.78
1:C:51:ILE:HD13	1:C:73:ALA:HB2	1.64	0.78
1:A:150:ARG:HG3	1:A:150:ARG:NH1	1.99	0.78
1:A:11:ILE:HG22	1:A:55:HIS:HB2	1.67	0.77
1:B:291:PRO:HD2	1:B:293:ILE:HD13	1.66	0.77
1:D:339:ARG:HD3	1:D:382:ASP:OD1	1.83	0.77
1:A:150:ARG:HH11	1:A:150:ARG:HG3	1.48	0.77
1:A:342:HIS:CD2	1:A:344:HIS:HD2	1.97	0.77
1:D:160:GLY:O	1:D:164:THR:HB	1.84	0.76
1:B:201:LEU:HD23	1:B:225:GLU:O	1.86	0.76
1:A:291:PRO:HD2	1:A:293:ILE:HG12	1.66	0.76
1:C:45:GLU:O	1:C:49:GLU:HB2	1.86	0.76
1:C:11:ILE:HG23	1:C:55:HIS:CD2	2.20	0.75
1:A:332:LEU:HD13	1:A:369:TYR:HB2	1.67	0.75
1:B:196:HIS:CB	2:B:499:PO4:O4	2.31	0.75
1:A:38:HIS:CD2	1:A:42:LEU:HD21	2.21	0.74
1:B:212:PRO:O	1:B:217:THR:HG21	1.87	0.74
1:C:38:HIS:HD2	1:C:42:LEU:HD21	1.52	0.74
1:B:340:LEU:HD13	1:B:397:MET:HE2	1.68	0.74
1:C:322:LEU:O	1:C:323:SER:CB	2.33	0.74
1:B:248:ALA:O	1:B:251:ASP:HB2	1.88	0.74
1:B:85:GLY:N	4:B:516:CIT:O4	2.21	0.74
1:C:123:LEU:HB3	1:C:234:LEU:HD13	1.70	0.74
1:A:213:GLU:HB2	1:A:240:ARG:HD2	1.70	0.73
1:C:8:LYS:HA	1:C:11:ILE:HD12	1.69	0.73
1:B:156:ILE:HG12	1:B:166:LEU:HD23	1.71	0.73
1:C:226:ILE:O	1:C:229:MET:HB2	1.88	0.73
1:D:57:ILE:HG21	1:D:65:LEU:HD11	1.71	0.73
1:B:201:LEU:CD2	1:B:225:GLU:O	2.37	0.72
1:A:36:GLU:OE2	1:A:50:SER:HB2	1.90	0.72
4:A:514:CIT:C6	4:A:514:CIT:O3	2.37	0.72
1:D:179:PHE:CZ	1:D:193:GLN:HB2	2.25	0.71
1:C:21:GLN:O	1:C:24:LEU:N	2.23	0.71
1:B:340:LEU:HD13	1:B:397:MET:CE	2.21	0.71
1:D:125:ARG:HB2	1:D:127:VAL:HG23	1.71	0.71
1:A:388:ASP:OD1	1:A:389:VAL:N	2.25	0.70
1:B:355:ASN:ND2	1:C:351:LEU:HB3	2.06	0.70
1:D:12:LYS:HD2	1:D:34:ASN:HD21	1.56	0.70
1:A:11:ILE:CG2	1:A:55:HIS:CB	2.68	0.70
1:C:20:HIS:HD2	1:C:22:LYS:N	1.87	0.70
4:D:513:CIT:C6	4:D:513:CIT:O1	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:TYR:HD1	1:B:197:LEU:HD13	1.56	0.69
1:C:229:MET:HE3	1:C:235:LEU:HD13	1.73	0.68
1:D:59:LEU:HD23	1:D:59:LEU:H	1.57	0.68
1:A:209:LEU:C	1:A:210:HIS:CD2	2.68	0.68
1:B:161:HIS:CD2	3:B:509:NAI:O2A	2.42	0.68
1:A:131:ASN:O	1:A:135:HIS:HD2	1.76	0.67
1:B:201:LEU:HD23	1:B:228:LEU:HB2	1.75	0.67
1:D:38:HIS:CD2	1:D:42:LEU:HD11	2.29	0.67
1:D:342:HIS:CE1	1:D:403:THR:HG23	2.29	0.67
1:A:272:THR:N	1:A:275:ASP:OD1	2.27	0.67
1:A:290:THR:HB	1:A:293:ILE:HD11	1.76	0.67
1:A:197:LEU:O	1:A:201:LEU:HG	1.94	0.67
1:D:24:LEU:HD23	1:D:28:ARG:NH2	2.09	0.67
1:A:409:LEU:O	1:A:410:TYR:HB3	1.95	0.66
1:A:150:ARG:CG	1:A:150:ARG:NH1	2.57	0.66
1:A:33:THR:O	1:A:33:THR:HG22	1.94	0.66
1:C:104:ALA:HA	1:C:307:GLU:OE1	1.96	0.66
1:A:214:ASN:HB2	1:A:215:PRO:HD2	1.78	0.66
1:A:59:LEU:HD23	1:A:59:LEU:N	2.05	0.66
1:C:59:LEU:HD12	1:C:60:ARG:O	1.96	0.65
1:C:213:GLU:O	1:C:214:ASN:HB3	1.95	0.65
1:A:245:ASP:OD1	1:A:247:PRO:HD2	1.97	0.65
1:A:14:LEU:HD23	1:A:57:ILE:HG13	1.78	0.65
1:B:249:LEU:CD1	1:B:253:LEU:HD22	2.26	0.65
1:A:11:ILE:HG23	1:A:55:HIS:CB	2.25	0.65
1:B:157:ILE:HB	1:B:209:LEU:HD23	1.78	0.65
1:B:339:ARG:HG2	1:B:409:LEU:HD12	1.79	0.65
1:B:108:ASN:ND2	1:B:295:GLY:HA3	2.11	0.64
4:C:515:CIT:O1	4:C:515:CIT:C6	2.41	0.64
1:B:27:LEU:HD23	1:B:313:ILE:HD11	1.79	0.64
1:A:11:ILE:CG2	1:A:55:HIS:HB2	2.27	0.64
1:B:123:LEU:HD23	1:B:128:PRO:HG2	1.80	0.64
1:C:125:ARG:HH12	1:D:115:LEU:HB2	1.62	0.64
1:D:287:VAL:HG12	1:D:289:LEU:HD13	1.78	0.64
1:A:328:PRO:HB3	1:A:371:GLN:HG3	1.80	0.64
1:B:108:ASN:HD22	1:B:295:GLY:HA3	1.62	0.64
1:C:209:LEU:HD12	1:C:237:ASN:HB2	1.79	0.64
1:A:342:HIS:CD2	1:A:344:HIS:CD2	2.80	0.63
4:C:517:CIT:C6	4:C:517:CIT:O1	2.47	0.63
1:B:42:LEU:HB3	1:B:46:GLN:CG	2.27	0.63
1:C:61:SER:HB3	4:C:517:CIT:O3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ALA:O	1:B:103:ASN:HA	1.98	0.63
1:A:367:ALA:HB3	1:A:382:ASP:HB2	1.79	0.63
1:B:279:SER:OG	1:B:280:PRO:HD2	1.99	0.62
1:A:5:SER:HA	1:A:8:LYS:HG3	1.81	0.62
1:C:147:PHE:HB3	1:C:152:LYS:HE2	1.81	0.62
1:A:185:LYS:O	1:A:187:PRO:HD3	1.98	0.62
1:C:154:LEU:HD23	1:C:206:VAL:HB	1.81	0.62
1:B:116:VAL:CG1	1:B:166:LEU:HD11	2.29	0.62
1:D:376:MET:HG2	1:D:377:GLY:N	2.13	0.62
1:B:386:ASP:OD1	1:B:389:VAL:HG23	1.99	0.62
1:C:229:MET:O	1:C:257:HIS:CE1	2.53	0.62
1:D:318:ASN:HB2	1:D:339:ARG:HH11	1.65	0.62
1:A:164:THR:CG2	1:A:188:LEU:HD11	2.30	0.61
1:D:15:LEU:CD1	1:D:35:ILE:HG23	2.30	0.61
1:C:211:VAL:HG11	1:C:220:MET:HE1	1.80	0.61
1:C:391:GLU:HG2	1:C:408:LEU:HD22	1.82	0.61
1:A:120:LEU:C	1:A:120:LEU:HD12	2.21	0.61
1:B:181:ASP:OD1	3:B:509:NAI:H1B	2.01	0.60
1:D:70:ILE:O	1:D:73:ALA:HB3	2.00	0.60
1:A:196:HIS:ND1	4:A:514:CIT:O5	2.34	0.60
1:A:38:HIS:HD2	1:A:42:LEU:HD21	1.66	0.60
1:B:120:LEU:O	1:B:121:LEU:C	2.40	0.60
1:D:66:THR:O	1:D:70:ILE:HG13	2.01	0.60
1:D:48:LYS:O	1:D:52:ARG:HB3	2.01	0.60
1:A:186:LEU:HD12	1:A:187:PRO:HD2	1.84	0.59
1:C:179:PHE:CZ	1:C:193:GLN:HB2	2.37	0.59
1:A:332:LEU:HB3	1:A:339:ARG:NH1	2.17	0.59
1:C:123:LEU:HB3	1:C:234:LEU:CD1	2.31	0.59
1:C:125:ARG:NH2	1:D:111:SER:O	2.35	0.59
1:D:105:PRO:HB2	1:D:106:PHE:CD2	2.37	0.59
1:B:217:THR:OG1	1:B:243:VAL:HG22	2.02	0.59
1:B:308:VAL:O	1:B:312:LEU:HG	2.02	0.59
1:D:59:LEU:H	1:D:59:LEU:CD2	2.16	0.59
1:D:12:LYS:HD2	1:D:34:ASN:ND2	2.18	0.59
1:B:214:ASN:CB	1:B:215:PRO:CD	2.76	0.58
1:A:208:SER:OG	1:A:210:HIS:NE2	2.30	0.58
1:D:20:HIS:HD2	1:D:22:LYS:HB2	1.67	0.58
1:A:73:ALA:O	1:A:97:ARG:NH1	2.31	0.58
1:C:171:GLU:OE1	1:C:190:ASN:HB2	2.04	0.58
1:C:11:ILE:HG23	1:C:55:HIS:HD2	1.67	0.58
1:C:245:ASP:OD1	1:C:247:PRO:HD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:LEU:HD11	1:B:253:LEU:HD22	1.86	0.58
1:C:38:HIS:CD2	1:C:42:LEU:HD21	2.37	0.58
1:C:43:ASP:H	1:C:46:GLN:HE21	1.51	0.58
1:C:122:LEU:HD22	1:C:127:VAL:HG11	1.85	0.58
1:B:342:HIS:CE1	1:B:344:HIS:HB3	2.38	0.57
1:B:253:LEU:HD13	1:B:258:LEU:HB2	1.87	0.57
1:C:264:ASP:OD1	1:C:290:THR:HB	2.03	0.57
1:D:92:ASP:O	1:D:93:ALA:C	2.41	0.57
1:A:334:LEU:O	1:A:335:HIS:CD2	2.57	0.57
1:C:148:GLU:HG3	1:D:299:GLU:HG2	1.85	0.57
1:C:347:ARG:O	1:C:348:PRO:C	2.39	0.57
1:A:12:LYS:HB3	1:A:54:ALA:HA	1.86	0.57
1:C:12:LYS:HD2	1:C:54:ALA:HA	1.87	0.57
1:C:132:ALA:O	1:C:136:ARG:HG2	2.05	0.57
1:D:229:MET:HE3	1:D:235:LEU:HG	1.87	0.57
1:A:407:ARG:HD2	6:A:588:HOH:O	2.04	0.56
1:D:197:LEU:HB3	4:D:513:CIT:O7	2.05	0.56
1:D:287:VAL:HG12	1:D:289:LEU:CD1	2.36	0.56
1:B:211:VAL:HB	1:B:212:PRO:HD2	1.87	0.56
1:D:171:GLU:OE2	1:D:190:ASN:HB2	2.04	0.56
1:B:181:ASP:C	1:B:183:GLU:H	2.08	0.56
1:B:332:LEU:HB3	1:B:339:ARG:HH22	1.71	0.56
1:D:229:MET:CE	1:D:235:LEU:HG	2.36	0.56
1:A:8:LYS:O	1:A:10:LYS:N	2.38	0.56
1:A:12:LYS:NZ	1:A:12:LYS:HB2	2.21	0.56
1:A:24:LEU:HD23	1:A:24:LEU:H	1.71	0.55
1:B:17:GLU:OE1	1:B:60:ARG:N	2.38	0.55
1:B:369:TYR:O	1:B:379:VAL:HA	2.07	0.55
1:C:154:LEU:HD13	1:C:156:ILE:HG13	1.89	0.55
1:B:59:LEU:HD22	1:B:65:LEU:HD11	1.88	0.55
1:A:373:SER:O	1:A:374:ALA:C	2.45	0.55
1:C:41:ALA:O	1:C:42:LEU:HD12	2.06	0.55
1:B:314:LYS:O	1:B:318:ASN:N	2.33	0.55
1:C:122:LEU:HD12	1:D:122:LEU:HD12	1.88	0.55
1:C:148:GLU:CG	1:D:299:GLU:HG2	2.37	0.55
1:A:384:GLU:O	1:A:385:ALA:HB2	2.07	0.55
1:B:103:ASN:N	1:B:103:ASN:HD22	2.05	0.55
1:C:125:ARG:HE	1:D:297:THR:HG21	1.72	0.55
1:A:76:LEU:O	1:A:99:ILE:HD13	2.07	0.54
1:A:332:LEU:HD13	1:A:369:TYR:CB	2.35	0.54
1:B:287:VAL:HG12	1:B:289:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:VAL:HG13	1:D:369:TYR:CG	2.42	0.54
1:D:24:LEU:HD23	1:D:28:ARG:HH21	1.72	0.54
1:B:179:PHE:CE1	1:B:193:GLN:HB2	2.42	0.54
1:C:16:VAL:HG23	1:C:17:GLU:HG3	1.88	0.54
1:C:229:MET:HE1	1:C:235:LEU:CD1	2.35	0.54
1:B:78:ALA:HA	1:B:99:ILE:HG23	1.88	0.54
1:C:123:LEU:CB	1:C:234:LEU:HD13	2.38	0.54
1:D:105:PRO:HB2	1:D:106:PHE:CE2	2.43	0.54
1:B:115:LEU:O	1:B:119:GLU:HG3	2.08	0.54
1:D:32:TYR:HH	1:D:316:SER:HG	1.53	0.54
1:C:36:GLU:OE2	1:C:50:SER:HB2	2.07	0.54
1:B:340:LEU:HD22	1:B:397:MET:HE1	1.90	0.53
1:A:33:THR:O	1:A:33:THR:CG2	2.56	0.53
1:C:246:ILE:N	1:C:247:PRO:CD	2.71	0.53
1:A:164:THR:HG21	1:A:188:LEU:HD11	1.90	0.53
1:B:201:LEU:HG	1:B:229:MET:HG3	1.89	0.53
1:B:342:HIS:CE1	1:B:344:HIS:CD2	2.95	0.53
1:C:56:PHE:CZ	1:C:316:SER:HB2	2.44	0.53
1:C:211:VAL:HG21	1:C:220:MET:CE	2.38	0.53
1:A:65:LEU:HD23	1:A:69:VAL:HG11	1.91	0.53
1:B:409:LEU:O	1:B:410:TYR:CB	2.49	0.53
1:C:178:TYR:CD2	1:C:192:THR:HB	2.44	0.53
4:C:517:CIT:O6	4:C:517:CIT:C5	2.54	0.53
1:D:342:HIS:HD2	1:D:344:HIS:CD2	2.25	0.53
1:D:43:ASP:C	1:D:43:ASP:OD1	2.47	0.52
1:C:131:ASN:OD1	1:C:135:HIS:HE1	1.91	0.52
1:A:212:PRO:HD2	1:A:217:THR:HG21	1.91	0.52
1:A:405:ARG:HD3	6:A:588:HOH:O	2.09	0.52
1:B:160:GLY:HA3	3:B:509:NAI:O5B	2.09	0.52
1:C:11:ILE:HG23	1:C:55:HIS:CB	2.38	0.52
1:B:124:LEU:HD13	1:B:234:LEU:HD12	1.90	0.52
1:C:33:THR:HG23	1:C:33:THR:O	2.08	0.52
1:D:120:LEU:HD12	1:D:121:LEU:N	2.24	0.52
1:A:28:ARG:HD2	6:A:544:HOH:O	2.09	0.52
1:D:77:VAL:O	1:D:100:PRO:HD2	2.10	0.52
1:A:225:GLU:OE1	1:A:225:GLU:N	2.39	0.52
1:B:201:LEU:HD21	1:B:225:GLU:O	2.10	0.52
1:D:350:VAL:HG12	1:D:354:LEU:CD2	2.40	0.52
1:B:17:GLU:HB2	1:B:60:ARG:HG2	1.92	0.52
1:C:110:ARG:HE	1:C:114:GLU:HG3	1.75	0.52
1:A:87:ASN:HD22	1:A:87:ASN:H	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:HIS:HD2	1:B:22:LYS:H	1.56	0.51
1:B:116:VAL:HG11	1:B:166:LEU:HD11	1.92	0.51
1:B:124:LEU:HD13	1:B:234:LEU:CD1	2.41	0.51
1:C:20:HIS:CE1	1:C:302:GLU:HB2	2.45	0.51
1:A:196:HIS:HB3	4:A:514:CIT:O3	2.11	0.51
1:A:210:HIS:CD2	1:A:210:HIS:N	2.78	0.51
1:C:259:ALA:O	1:C:286:ASN:ND2	2.39	0.51
1:C:338:ARG:HG3	1:C:410:TYR:O	2.10	0.51
1:A:12:LYS:HB2	1:A:12:LYS:HZ3	1.75	0.51
1:C:196:HIS:HB3	4:C:515:CIT:O5	2.11	0.51
1:A:131:ASN:O	1:A:135:HIS:CD2	2.62	0.51
1:C:22:LYS:HB3	1:C:306:LEU:HD21	1.92	0.51
1:C:146:SER:C	1:C:147:PHE:CD2	2.85	0.51
1:B:264:ASP:O	1:B:292:HIS:HA	2.10	0.51
1:A:51:ILE:O	1:A:52:ARG:C	2.49	0.50
1:B:214:ASN:CB	1:B:215:PRO:HD3	2.27	0.50
1:A:164:THR:CG2	1:A:188:LEU:CD1	2.89	0.50
1:C:270:PRO:HB3	1:C:275:ASP:HB2	1.94	0.50
1:B:8:LYS:HA	1:B:11:ILE:HD12	1.93	0.50
1:B:156:ILE:CG1	1:B:166:LEU:HD23	2.41	0.50
1:B:259:ALA:O	1:B:286:ASN:ND2	2.35	0.50
1:B:246:ILE:HB	1:B:247:PRO:HD3	1.93	0.50
1:C:148:GLU:HA	1:D:114:GLU:OE2	2.12	0.50
1:D:56:PHE:CE2	1:D:78:ALA:HB3	2.46	0.50
1:B:13:PHE:CZ	1:B:56:PHE:CD1	3.00	0.50
1:C:211:VAL:HG21	1:C:220:MET:HE2	1.94	0.50
1:A:239:SER:OG	1:A:240:ARG:N	2.45	0.50
1:B:59:LEU:HD22	1:B:65:LEU:CD1	2.42	0.50
1:B:62:ARG:CG	1:B:62:ARG:NH1	2.48	0.50
1:B:181:ASP:O	1:B:183:GLU:N	2.45	0.50
1:D:167:GLY:O	1:D:171:GLU:HG3	2.12	0.50
1:A:59:LEU:N	1:A:59:LEU:CD2	2.74	0.49
1:D:351:LEU:HA	1:D:354:LEU:HD23	1.94	0.49
1:B:218:LYS:O	1:B:219:ASN:HB2	2.11	0.49
1:B:254:ALA:C	1:B:256:LYS:H	2.14	0.49
1:C:43:ASP:H	1:C:46:GLN:NE2	2.10	0.49
1:B:133:LYS:HB3	1:B:138:VAL:HB	1.92	0.49
1:C:11:ILE:HG23	1:C:55:HIS:CG	2.46	0.49
1:C:125:ARG:HE	1:D:297:THR:CG2	2.24	0.49
1:C:131:ASN:OD1	1:C:135:HIS:CE1	2.64	0.49
1:D:44:ASP:OD1	1:D:44:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:LEU:HD23	1:D:149:ALA:HB2	1.93	0.49
1:D:393:ALA:O	1:D:397:MET:HG3	2.11	0.49
1:B:16:VAL:HG23	1:B:59:LEU:HA	1.93	0.49
1:D:342:HIS:CE1	1:D:403:THR:CG2	2.95	0.49
1:C:41:ALA:C	1:C:42:LEU:HD12	2.33	0.49
1:B:188:LEU:O	1:B:189:GLY:C	2.50	0.49
1:D:340:LEU:HD23	1:D:408:LEU:HB2	1.93	0.49
1:A:291:PRO:HD3	1:B:130:ALA:HB1	1.95	0.49
1:A:360:GLU:O	1:A:360:GLU:HG2	2.12	0.48
1:A:368:GLN:NE2	1:A:381:ILE:HG12	2.27	0.48
1:C:141:LYS:HE3	1:D:292:HIS:O	2.13	0.48
1:D:14:LEU:HD13	1:D:50:SER:HB3	1.95	0.48
1:D:95:ALA:O	1:D:98:GLY:N	2.33	0.48
1:B:214:ASN:N	1:B:217:THR:HG22	2.28	0.48
1:D:342:HIS:HD2	1:D:344:HIS:HD2	1.61	0.48
1:A:55:HIS:HA	1:A:75:LYS:O	2.14	0.48
1:C:110:ARG:HE	1:C:114:GLU:CG	2.26	0.48
1:D:243:VAL:O	1:D:243:VAL:HG12	2.13	0.48
1:A:51:ILE:O	1:A:54:ALA:N	2.47	0.48
1:A:318:ASN:HD21	1:A:320:SER:HB2	1.79	0.48
1:A:409:LEU:O	1:A:410:TYR:CB	2.58	0.48
1:B:338:ARG:HA	1:B:410:TYR:O	2.13	0.48
1:D:43:ASP:OD1	1:D:43:ASP:O	2.31	0.48
1:B:358:PHE:CE1	1:B:383:ILE:HG21	2.48	0.48
1:C:16:VAL:HG21	1:C:63:THR:OG1	2.14	0.48
1:D:376:MET:CG	1:D:377:GLY:N	2.75	0.48
1:D:407:ARG:NH1	1:D:409:LEU:HD22	2.29	0.48
1:A:318:ASN:O	1:A:339:ARG:NH2	2.40	0.48
1:B:83:ALA:HA	4:B:516:CIT:O6	2.14	0.48
1:D:28:ARG:NH1	1:D:35:ILE:HD12	2.29	0.48
1:C:246:ILE:HB	1:C:247:PRO:HD3	1.95	0.47
1:A:235:LEU:O	1:A:261:ALA:HA	2.14	0.47
1:C:264:ASP:OD1	1:C:290:THR:CB	2.61	0.47
1:A:340:LEU:HD22	1:A:397:MET:SD	2.54	0.47
1:B:201:LEU:HD23	1:B:228:LEU:CB	2.44	0.47
1:C:59:LEU:HD13	1:C:63:THR:HB	1.96	0.47
1:C:292:HIS:HB3	1:D:141:LYS:HE2	1.96	0.47
1:D:207:VAL:HB	1:D:229:MET:HE1	1.96	0.47
1:A:243:VAL:HG12	1:A:243:VAL:O	2.13	0.47
1:C:214:ASN:HB2	1:C:215:PRO:HD2	1.96	0.47
1:A:168:ILE:HD11	1:A:188:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LEU:HB3	2:B:499:PO4:O2	2.15	0.47
1:C:327:PHE:CG	1:C:328:PRO:HD2	2.49	0.47
1:D:327:PHE:HZ	1:D:343:ILE:HD13	1.79	0.47
1:A:230:LYS:O	1:A:233:SER:HB3	2.14	0.47
1:D:82:PHE:N	1:D:82:PHE:CD1	2.82	0.47
1:B:291:PRO:HD2	1:B:293:ILE:CD1	2.39	0.47
1:D:11:ILE:HA	1:D:55:HIS:CD2	2.50	0.47
1:D:157:ILE:HB	1:D:209:LEU:HD23	1.97	0.47
1:D:209:LEU:HB2	1:D:237:ASN:HD22	1.80	0.47
1:C:120:LEU:C	1:C:120:LEU:HD12	2.35	0.47
1:A:122:LEU:HD12	1:B:122:LEU:HD12	1.97	0.46
1:B:222:GLY:O	1:B:223:ALA:C	2.52	0.46
1:D:339:ARG:HD2	1:D:380:VAL:HG12	1.94	0.46
1:A:240:ARG:HB2	1:A:243:VAL:HG23	1.97	0.46
1:A:341:MET:HE1	1:A:378:TYR:CE1	2.50	0.46
1:C:12:LYS:NZ	1:C:50:SER:O	2.43	0.46
1:A:43:ASP:O	1:A:44:ASP:C	2.53	0.46
1:A:169:LEU:HD22	1:B:173:LEU:HD12	1.97	0.46
1:A:211:VAL:HB	1:A:212:PRO:CD	2.45	0.46
1:B:48:LYS:HG3	1:B:49:GLU:N	2.29	0.46
1:B:254:ALA:C	1:B:256:LYS:N	2.68	0.46
1:D:332:LEU:HB3	1:D:339:ARG:NH2	2.30	0.46
1:B:42:LEU:HD22	1:B:46:GLN:HE21	1.81	0.46
1:B:241:GLY:O	1:B:267:PRO:HD3	2.15	0.46
1:A:38:HIS:CG	4:A:518:CIT:O5	2.68	0.46
1:D:15:LEU:CD1	1:D:35:ILE:CG2	2.93	0.46
1:A:120:LEU:HD12	1:A:121:LEU:N	2.31	0.46
1:C:24:LEU:N	1:C:24:LEU:HD23	2.30	0.46
1:C:38:HIS:HB3	5:C:506:SO4:O4	2.15	0.46
1:B:264:ASP:OD1	1:B:293:ILE:N	2.46	0.46
1:C:94:ALA:HB1	1:C:99:ILE:HB	1.98	0.46
1:A:38:HIS:ND1	4:A:518:CIT:O5	2.49	0.46
1:B:115:LEU:HD22	1:B:294:GLY:HA2	1.98	0.46
1:C:292:HIS:O	1:C:292:HIS:CD2	2.69	0.46
1:A:24:LEU:H	1:A:24:LEU:CD2	2.28	0.46
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.81	0.46
1:B:220:MET:HG2	1:B:243:VAL:HG13	1.97	0.46
1:C:20:HIS:CD2	1:C:21:GLN:N	2.84	0.46
1:C:354:LEU:O	1:C:358:PHE:CD2	2.69	0.46
1:D:77:VAL:CG1	1:D:315:TYR:HE2	2.28	0.46
1:A:156:ILE:HG12	1:A:166:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PHE:C	1:A:179:PHE:CD1	2.88	0.46
1:A:196:HIS:O	1:A:199:ASP:HB2	2.15	0.46
1:C:208:SER:OG	1:C:210:HIS:NE2	2.42	0.46
1:A:13:PHE:CD2	1:A:56:PHE:HB2	2.51	0.45
1:C:14:LEU:C	1:C:15:LEU:HD23	2.37	0.45
1:C:214:ASN:C	1:C:214:ASN:OD1	2.54	0.45
1:C:407:ARG:NH2	6:C:539:HOH:O	2.45	0.45
1:A:24:LEU:CD2	1:A:24:LEU:N	2.79	0.45
1:D:37:PHE:CD1	1:D:37:PHE:C	2.89	0.45
1:D:287:VAL:CG1	1:D:289:LEU:CD1	2.94	0.45
1:C:154:LEU:HD13	1:C:156:ILE:CG1	2.45	0.45
1:C:258:LEU:N	1:C:258:LEU:HD12	2.31	0.45
1:D:370:LEU:HA	1:D:378:TYR:O	2.16	0.45
1:A:8:LYS:C	1:A:10:LYS:H	2.19	0.45
1:A:88:GLN:HG2	1:A:89:VAL:HG23	1.99	0.45
1:B:95:ALA:HB1	1:B:376:MET:CE	2.45	0.45
1:B:95:ALA:HB1	1:B:376:MET:HE1	1.98	0.45
1:A:214:ASN:HB2	1:A:215:PRO:CD	2.46	0.45
1:D:197:LEU:O	1:D:201:LEU:HG	2.17	0.45
1:C:214:ASN:HB2	1:C:215:PRO:CD	2.46	0.45
1:B:344:HIS:CD2	1:B:350:VAL:HG11	2.52	0.45
1:D:14:LEU:HD23	1:D:57:ILE:HG12	1.98	0.45
1:C:323:SER:O	1:C:324:ALA:C	2.56	0.44
1:D:14:LEU:HB3	1:D:57:ILE:HG12	1.98	0.44
1:D:405:ARG:HG2	1:D:406:ALA:N	2.32	0.44
1:A:104:ALA:HA	1:A:307:GLU:OE2	2.17	0.44
1:C:79:ILE:O	1:C:101:VAL:HA	2.17	0.44
1:D:209:LEU:HD11	1:D:221:MET:HG3	1.99	0.44
1:D:12:LYS:H	1:D:55:HIS:CD2	2.12	0.44
1:D:400:ILE:O	1:D:401:PRO:C	2.54	0.44
1:D:59:LEU:CD2	1:D:59:LEU:N	2.79	0.44
1:D:334:LEU:HD13	1:D:334:LEU:O	2.17	0.44
1:A:188:LEU:O	1:A:189:GLY:C	2.56	0.44
1:A:341:MET:HE1	1:A:378:TYR:HE1	1.83	0.44
1:A:383:ILE:O	1:A:383:ILE:HG13	2.16	0.44
1:C:321:THR:O	1:C:322:LEU:C	2.55	0.44
1:D:310:GLY:HA3	6:D:565:HOH:O	2.17	0.44
1:A:103:ASN:OD1	1:A:105:PRO:HD3	2.18	0.44
1:D:15:LEU:HD12	1:D:35:ILE:HG23	1.99	0.44
1:D:120:LEU:HD12	1:D:120:LEU:C	2.38	0.44
1:B:186:LEU:HD12	1:B:187:PRO:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:LEU:HG	1:C:398:LYS:HE2	1.99	0.44
3:D:511:NAI:H2D	3:D:511:NAI:H6N	1.69	0.44
1:A:57:ILE:HD12	1:A:65:LEU:HD11	1.98	0.44
1:B:16:VAL:HG12	1:B:38:HIS:HB2	1.98	0.44
1:C:141:LYS:H	1:D:273:ASN:ND2	2.16	0.44
1:D:29:ALA:C	1:D:31:GLY:H	2.21	0.44
1:A:322:LEU:HA	1:A:329:GLU:HG2	2.00	0.43
1:C:27:LEU:O	1:C:32:TYR:HB2	2.18	0.43
1:D:57:ILE:HG21	1:D:65:LEU:CD1	2.46	0.43
1:D:100:PRO:HG3	1:D:315:TYR:CE1	2.52	0.43
1:C:409:LEU:HD23	1:C:409:LEU:HA	1.82	0.43
1:D:123:LEU:HD23	1:D:128:PRO:HG2	2.00	0.43
1:C:270:PRO:HG2	1:D:139:TRP:CG	2.53	0.43
1:A:36:GLU:CD	1:A:50:SER:HB2	2.38	0.43
4:A:514:CIT:O1	4:A:514:CIT:O7	2.36	0.43
1:B:314:LYS:HG2	1:B:318:ASN:HD21	1.84	0.43
1:D:246:ILE:N	1:D:247:PRO:CD	2.82	0.43
1:B:355:ASN:HD21	1:C:351:LEU:HB3	1.83	0.43
1:D:58:GLY:HA2	1:D:80:GLY:O	2.18	0.43
1:D:350:VAL:HG12	1:D:354:LEU:HD22	2.00	0.43
1:C:125:ARG:NH1	1:D:115:LEU:HB2	2.30	0.43
1:D:16:VAL:HA	1:D:38:HIS:HB2	1.99	0.43
1:D:334:LEU:O	1:D:335:HIS:ND1	2.51	0.43
1:D:386:ASP:OD1	1:D:389:VAL:HG23	2.18	0.43
1:C:353:ALA:HB3	1:C:400:ILE:HD13	1.99	0.43
1:D:20:HIS:HD2	1:D:22:LYS:H	1.67	0.43
1:D:27:LEU:HD23	1:D:313:ILE:HD11	2.01	0.43
1:D:34:ASN:ND2	1:D:34:ASN:C	2.72	0.43
1:A:12:LYS:NZ	1:A:12:LYS:CB	2.82	0.43
1:A:43:ASP:OD2	1:A:44:ASP:N	2.52	0.43
4:A:514:CIT:O6	4:A:514:CIT:C5	2.62	0.43
1:D:209:LEU:O	1:D:210:HIS:CG	2.71	0.43
1:A:74:GLU:OE2	1:A:74:GLU:HA	2.18	0.43
1:A:108:ASN:N	1:A:108:ASN:HD22	2.17	0.43
1:B:133:LYS:O	1:B:134:ALA:C	2.54	0.43
1:C:293:ILE:HD12	1:C:293:ILE:C	2.40	0.43
1:D:340:LEU:CD2	1:D:408:LEU:HB2	2.49	0.43
1:A:209:LEU:HD11	1:A:221:MET:HG3	2.01	0.42
1:A:341:MET:HE1	1:A:343:ILE:HD11	2.01	0.42
1:B:228:LEU:HD23	1:B:228:LEU:HA	1.84	0.42
1:C:42:LEU:N	1:C:42:LEU:CD1	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:LEU:HD23	1:B:27:LEU:HA	1.78	0.42
1:B:201:LEU:HG	1:B:229:MET:CG	2.49	0.42
1:B:214:ASN:H	1:B:217:THR:CG2	2.32	0.42
1:B:321:THR:O	1:B:322:LEU:C	2.55	0.42
1:C:70:ILE:C	1:C:72:ALA:H	2.21	0.42
1:C:262:ALA:HA	1:C:288:LEU:O	2.19	0.42
1:B:214:ASN:H	1:B:217:THR:HG22	1.84	0.42
1:B:393:ALA:C	1:B:397:MET:HE3	2.39	0.42
1:D:76:LEU:O	1:D:99:ILE:HD11	2.18	0.42
1:D:235:LEU:HD22	1:D:236:ILE:N	2.35	0.42
1:B:330:VAL:HG12	1:B:331:SER:N	2.35	0.42
1:C:66:THR:O	1:C:70:ILE:HG13	2.18	0.42
1:C:229:MET:O	1:C:257:HIS:HE1	2.02	0.42
1:D:92:ASP:O	1:D:94:ALA:N	2.53	0.42
4:D:513:CIT:O1	4:D:513:CIT:O6	2.37	0.42
1:A:311:LYS:HE2	1:A:323:SER:OG	2.20	0.42
1:C:22:LYS:HE3	1:C:306:LEU:HD11	2.02	0.42
1:C:41:ALA:C	1:C:42:LEU:CD1	2.88	0.42
1:C:172:SER:HB3	1:D:172:SER:HB3	2.01	0.42
1:C:198:SER:O	1:C:202:ASN:HB2	2.20	0.42
1:A:160:GLY:HA3	3:A:508:NAI:O5B	2.19	0.42
1:B:131:ASN:O	1:B:135:HIS:HD2	2.03	0.42
1:B:214:ASN:N	1:B:217:THR:CG2	2.83	0.42
1:B:249:LEU:HD12	1:B:253:LEU:HD22	2.01	0.42
1:B:394:LEU:HD12	1:B:394:LEU:HA	1.86	0.42
1:A:65:LEU:CD2	1:A:69:VAL:HG11	2.50	0.42
1:A:258:LEU:HD12	1:A:258:LEU:HA	1.73	0.42
1:B:262:ALA:HA	1:B:288:LEU:O	2.20	0.42
1:D:55:HIS:HA	1:D:76:LEU:HA	2.02	0.42
1:A:41:ALA:O	1:A:42:LEU:HD12	2.20	0.42
1:A:169:LEU:HA	1:A:169:LEU:HD23	1.76	0.42
1:A:229:MET:HE2	1:A:258:LEU:HD11	2.02	0.42
1:B:393:ALA:O	1:B:394:LEU:C	2.56	0.42
1:C:173:LEU:HD11	1:D:173:LEU:HD11	2.00	0.42
1:A:81:ALA:O	1:A:103:ASN:HA	2.19	0.42
1:D:38:HIS:HD2	1:D:42:LEU:HD11	1.80	0.42
1:A:152:LYS:HD3	1:A:152:LYS:HA	1.77	0.41
1:A:357:ILE:HD12	1:A:400:ILE:HD11	2.02	0.41
1:C:149:ALA:O	1:C:175:MET:HG2	2.20	0.41
1:A:59:LEU:HB2	1:A:63:THR:HB	2.02	0.41
1:B:109:THR:O	1:B:110:ARG:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:LEU:HD12	1:C:380:VAL:HG12	2.01	0.41
1:C:145:GLY:O	1:C:147:PHE:CE2	2.72	0.41
1:C:398:LYS:HA	1:C:403:THR:HG21	2.02	0.41
1:A:127:VAL:HB	1:A:128:PRO:HD3	2.03	0.41
1:A:149:ALA:O	1:A:152:LYS:HB2	2.21	0.41
1:C:180:TYR:CE1	1:C:197:LEU:HB2	2.55	0.41
1:D:95:ALA:O	1:D:96:LYS:C	2.59	0.41
1:D:221:MET:HE2	1:D:229:MET:HE3	2.03	0.41
1:C:390:ALA:HB1	1:C:408:LEU:HD13	2.01	0.41
1:B:17:GLU:CB	1:B:60:ARG:HG2	2.51	0.41
1:B:340:LEU:HD13	1:B:397:MET:HE1	2.02	0.41
1:C:78:ALA:HA	1:C:99:ILE:CG2	2.43	0.41
1:A:209:LEU:C	1:A:210:HIS:CG	2.94	0.41
1:B:214:ASN:O	1:B:217:THR:HG22	2.21	0.41
1:D:92:ASP:C	1:D:94:ALA:N	2.71	0.41
1:B:43:ASP:CG	1:B:46:GLN:OE1	2.60	0.41
1:B:318:ASN:OD1	1:B:320:SER:HB2	2.21	0.41
1:B:355:ASN:HD21	1:C:351:LEU:HD13	1.84	0.41
1:D:20:HIS:CD2	1:D:22:LYS:HB2	2.52	0.41
1:D:20:HIS:CD2	1:D:22:LYS:H	2.39	0.41
1:D:60:ARG:O	1:D:88:GLN:NE2	2.54	0.41
1:D:217:THR:HG23	1:D:243:VAL:HG22	2.03	0.41
1:D:287:VAL:CG1	1:D:289:LEU:HD13	2.49	0.41
1:A:38:HIS:HD2	1:A:42:LEU:CD2	2.33	0.41
1:B:387:GLU:O	1:B:391:GLU:HG3	2.21	0.41
1:C:43:ASP:OD1	1:C:46:GLN:HB2	2.21	0.41
1:C:394:LEU:HG	1:C:394:LEU:O	2.21	0.41
1:A:121:LEU:HD23	1:A:121:LEU:HA	1.94	0.40
1:A:331:SER:O	1:A:369:TYR:CD2	2.74	0.40
1:A:368:GLN:HE21	1:A:381:ILE:HG12	1.85	0.40
1:A:291:PRO:HD2	1:A:293:ILE:CG1	2.41	0.40
1:D:84:ILE:O	1:D:84:ILE:HG12	2.22	0.40
1:A:184:ASN:N	1:A:184:ASN:HD22	2.18	0.40
1:A:211:VAL:O	3:A:508:NAI:H4D	2.22	0.40
1:B:173:LEU:HD12	1:B:173:LEU:HA	1.83	0.40
1:C:147:PHE:CD2	1:C:147:PHE:N	2.89	0.40
1:C:407:ARG:HD3	1:C:407:ARG:HA	1.96	0.40
1:B:78:ALA:HA	1:B:99:ILE:CG2	2.51	0.40
1:C:290:THR:O	1:C:292:HIS:N	2.48	0.40
1:A:79:ILE:HB	1:A:101:VAL:HG22	2.04	0.40
1:B:346:ASN:HD21	1:B:372:THR:CG2	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:VAL:HG21	1:C:220:MET:HE1	2.03	0.40
1:C:351:LEU:HA	1:C:351:LEU:HD23	1.88	0.40
1:D:360:GLU:C	1:D:362:GLY:H	2.25	0.40
1:D:366:ALA:N	1:D:382:ASP:O	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	404/410 (98%)	365 (90%)	33 (8%)	6 (2%)	10	21
1	B	402/410 (98%)	363 (90%)	37 (9%)	2 (0%)	29	52
1	C	404/410 (98%)	373 (92%)	26 (6%)	5 (1%)	13	27
1	D	401/410 (98%)	374 (93%)	25 (6%)	2 (0%)	29	52
All	All	1611/1640 (98%)	1475 (92%)	121 (8%)	15 (1%)	17	35

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	374	ALA
1	B	224	LYS
1	A	44	ASP
1	A	336	VAL
1	B	182	ILE
1	C	323	SER
1	C	73	ALA
1	D	30	ALA
1	A	47	LEU
1	A	48	LYS

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Mol	Chain	Res	Type
1	C	18	GLY
1	C	336	VAL
1	D	219	ASN
1	C	214	ASN

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	325/328 (99%)	286 (88%)	39 (12%)	5	9
1	B	323/328 (98%)	290 (90%)	33 (10%)	7	14
1	C	325/328 (99%)	288 (89%)	37 (11%)	5	10
1	D	322/328 (98%)	283 (88%)	39 (12%)	5	9
All	All	1295/1312 (99%)	1147 (89%)	148 (11%)	5	10

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	8	LYS
1	A	11	ILE
1	A	12	LYS
1	A	15	LEU
1	A	24	LEU
1	A	44	ASP
1	A	57	ILE
1	A	64	HIS
1	A	75	LYS
1	A	87	ASN
1	A	99	ILE
1	A	108	ASN
1	A	141	LYS
1	A	142	LEU
1	A	150	ARG
1	A	183	GLU

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Mol	Chain	Res	Type
1	A	184	ASN
1	A	200	LEU
1	A	220	MET
1	A	224	LYS
1	A	256	LYS
1	A	258	LEU
1	A	268	THR
1	A	274	SER
1	A	283	GLU
1	A	293	ILE
1	A	307	GLU
1	A	312	LEU
1	A	318	ASN
1	A	335	HIS
1	A	338	ARG
1	A	352	THR
1	A	354	LEU
1	A	356	LYS
1	A	368	GLN
1	A	369	TYR
1	A	405	ARG
1	A	407	ARG
1	B	16	VAL
1	B	48	LYS
1	B	52	ARG
1	B	59	LEU
1	B	60	ARG
1	B	61	SER
1	B	62	ARG
1	B	67	GLU
1	B	88	GLN
1	B	103	ASN
1	B	124	LEU
1	B	141	LYS
1	B	142	LEU
1	B	150	ARG
1	B	173	LEU
1	B	186	LEU
1	B	188	LEU
1	B	220	MET
1	B	245	ASP
1	B	246	ILE

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Mol	Chain	Res	Type
1	B	253	LEU
1	B	278	THR
1	B	289	LEU
1	B	293	ILE
1	B	327	PHE
1	B	331	SER
1	B	334	LEU
1	B	338	ARG
1	B	341	MET
1	B	347	ARG
1	B	351	LEU
1	B	369	TYR
1	B	407	ARG
1	C	24	LEU
1	C	33	THR
1	C	34	ASN
1	C	39	LYS
1	C	42	LEU
1	C	46	GLN
1	C	48	LYS
1	C	49	GLU
1	C	51	ILE
1	C	52	ARG
1	C	55	HIS
1	C	57	ILE
1	C	59	LEU
1	C	67	GLU
1	C	68	ASP
1	C	77	VAL
1	C	140	ASN
1	C	142	LEU
1	C	154	LEU
1	C	185	LYS
1	C	202	ASN
1	C	221	MET
1	C	274	SER
1	C	290	THR
1	C	322	LEU
1	C	338	ARG
1	C	341	MET
1	C	354	LEU
1	C	355	ASN

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Mol	Chain	Res	Type
1	C	360	GLU
1	C	364	ASN
1	C	369	TYR
1	C	370	LEU
1	C	384	GLU
1	C	387	GLU
1	C	388	ASP
1	C	394	LEU
1	D	8	LYS
1	D	10	LYS
1	D	22	LYS
1	D	36	GLU
1	D	48	LYS
1	D	51	ILE
1	D	57	ILE
1	D	59	LEU
1	D	106	PHE
1	D	150	ARG
1	D	164	THR
1	D	165	GLN
1	D	172	SER
1	D	184	ASN
1	D	195	GLN
1	D	202	ASN
1	D	217	THR
1	D	224	LYS
1	D	235	LEU
1	D	246	ILE
1	D	274	SER
1	D	283	GLU
1	D	289	LEU
1	D	299	GLU
1	D	322	LEU
1	D	327	PHE
1	D	334	LEU
1	D	339	ARG
1	D	341	MET
1	D	354	LEU
1	D	356	LYS
1	D	361	GLN
1	D	369	TYR
1	D	370	LEU

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Mol	Chain	Res	Type
1	D	375	GLN
1	D	384	GLU
1	D	391	GLU
1	D	392	LYS
1	D	395	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	135	HIS
1	A	184	ASN
1	A	273	ASN
1	A	292	HIS
1	A	303	ASN
1	A	318	ASN
1	A	335	HIS
1	A	342	HIS
1	A	344	HIS
1	A	364	ASN
1	A	368	GLN
1	B	20	HIS
1	B	88	GLN
1	B	103	ASN
1	B	108	ASN
1	B	161	HIS
1	B	190	ASN
1	B	219	ASN
1	B	344	HIS
1	B	346	ASN
1	B	355	ASN
1	C	20	HIS
1	C	34	ASN
1	C	46	GLN
1	C	55	HIS
1	C	71	ASN
1	C	135	HIS
1	C	140	ASN
1	C	190	ASN
1	C	301	GLN
1	C	303	ASN
1	C	342	HIS

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Mol	Chain	Res	Type
1	C	344	HIS
1	D	20	HIS
1	D	38	HIS
1	D	55	HIS
1	D	87	ASN
1	D	135	HIS
1	D	140	ASN
1	D	184	ASN
1	D	190	ASN
1	D	237	ASN
1	D	273	ASN
1	D	318	ASN
1	D	342	HIS
1	D	344	HIS
1	D	346	ASN
1	D	355	ASN
1	D	368	GLN
1	D	395	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	PO4	D	505	-	4,4,4	1.06	0	6,6,6	0.82	0
2	PO4	C	502	-	4,4,4	0.83	0	6,6,6	1.31	1 (16%)
2	PO4	A	500	-	4,4,4	1.49	1 (25%)	6,6,6	1.02	0
4	CIT	D	513	-	3,12,12	1.51	0	3,17,17	5.23	2 (66%)
2	PO4	B	499	-	4,4,4	0.79	0	6,6,6	1.15	0
4	CIT	A	514	-	3,12,12	1.15	0	3,17,17	2.33	2 (66%)
4	CIT	A	518	-	3,12,12	1.19	0	3,17,17	5.12	3 (100%)
2	PO4	C	501	-	4,4,4	1.25	0	6,6,6	0.83	0
5	SO4	C	506	-	4,4,4	0.36	0	6,6,6	0.58	0
2	PO4	B	503	-	4,4,4	1.33	0	6,6,6	0.52	0
3	NAI	B	509	-	42,48,48	1.94	8 (19%)	47,73,73	1.75	8 (17%)
4	CIT	C	515	-	3,12,12	1.39	0	3,17,17	3.90	2 (66%)
3	NAI	C	510	-	42,48,48	1.91	8 (19%)	47,73,73	1.58	8 (17%)
3	NAI	A	508	-	42,48,48	1.91	6 (14%)	47,73,73	1.53	10 (21%)
4	CIT	B	516	-	3,12,12	1.66	1 (33%)	3,17,17	2.89	1 (33%)
4	CIT	C	517	-	3,12,12	1.93	1 (33%)	3,17,17	3.71	1 (33%)
2	PO4	D	507	-	4,4,4	0.67	0	6,6,6	1.20	1 (16%)
3	NAI	D	511	-	42,48,48	1.89	6 (14%)	47,73,73	1.73	10 (21%)
2	PO4	A	504	-	4,4,4	0.86	0	6,6,6	1.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	B	516	-	-	0/6/16/16	-
4	CIT	A	514	-	-	3/6/16/16	-
4	CIT	A	518	-	-	1/6/16/16	-
4	CIT	C	517	-	-	2/6/16/16	-
3	NAI	B	509	-	-	7/25/72/72	0/5/5/5
4	CIT	C	515	-	-	0/6/16/16	-
3	NAI	A	508	-	-	4/25/72/72	0/5/5/5
3	NAI	C	510	-	-	7/25/72/72	0/5/5/5
3	NAI	D	511	-	-	7/25/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	D	513	-	-	3/6/16/16	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	511	NAI	O7N-C7N	7.22	1.41	1.24
3	B	509	NAI	O7N-C7N	6.83	1.40	1.24
3	A	508	NAI	O7N-C7N	6.67	1.40	1.24
3	C	510	NAI	O7N-C7N	6.41	1.39	1.24
3	A	508	NAI	C4N-C3N	-5.73	1.38	1.49
3	C	510	NAI	C4N-C3N	-5.48	1.39	1.49
3	B	509	NAI	C4N-C3N	-5.43	1.39	1.49
3	D	511	NAI	C4N-C3N	-5.38	1.39	1.49
3	A	508	NAI	C2A-N3A	4.47	1.39	1.32
3	C	510	NAI	C2A-N3A	3.91	1.38	1.32
3	C	510	NAI	C6N-C5N	3.79	1.40	1.33
3	D	511	NAI	C4N-C5N	-3.74	1.39	1.48
3	B	509	NAI	C2A-N3A	3.74	1.38	1.32
3	C	510	NAI	C4N-C5N	-3.69	1.39	1.48
3	D	511	NAI	C2A-N3A	3.69	1.38	1.32
3	A	508	NAI	C4N-C5N	-3.66	1.39	1.48
3	B	509	NAI	C6N-C5N	3.48	1.39	1.33
3	D	511	NAI	C6N-C5N	3.47	1.39	1.33
3	B	509	NAI	C4N-C5N	-3.34	1.40	1.48
3	A	508	NAI	C6N-C5N	3.26	1.39	1.33
3	B	509	NAI	C2B-C1B	-3.14	1.49	1.53
3	A	508	NAI	C2A-N1A	2.70	1.38	1.33
3	C	510	NAI	C2A-N1A	2.59	1.38	1.33
3	B	509	NAI	C2A-N1A	2.50	1.38	1.33
2	A	500	PO4	P-O4	-2.50	1.47	1.54
3	B	509	NAI	C2N-C3N	2.35	1.41	1.34
3	D	511	NAI	C2A-N1A	2.22	1.38	1.33
4	C	517	CIT	C4-C3	-2.13	1.51	1.54
4	B	516	CIT	C4-C3	-2.07	1.52	1.54
3	C	510	NAI	C2B-C1B	-2.05	1.50	1.53
3	C	510	NAI	PN-O1N	-2.02	1.45	1.55

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	513	CIT	C3-C4-C5	-7.04	103.71	114.98
4	A	518	CIT	C3-C4-C5	-6.84	104.03	114.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	517	CIT	C3-C4-C5	-6.37	104.78	114.98
4	D	513	CIT	C3-C2-C1	-5.68	105.89	114.98
3	D	511	NAI	N3A-C2A-N1A	-5.39	120.25	128.68
3	B	509	NAI	N3A-C2A-N1A	-5.28	120.42	128.68
3	C	510	NAI	N3A-C2A-N1A	-5.28	120.42	128.68
4	C	515	CIT	C3-C2-C1	-4.92	107.11	114.98
4	B	516	CIT	C3-C4-C5	-4.80	107.30	114.98
3	B	509	NAI	O4D-C1D-N1N	4.79	117.42	108.06
3	D	511	NAI	C1B-N9A-C4A	-4.77	118.26	126.64
3	B	509	NAI	C5A-C6A-N6A	-4.65	113.29	120.35
3	C	510	NAI	O7N-C7N-C3N	-4.60	112.24	120.90
4	A	518	CIT	C3-C2-C1	-4.51	107.76	114.98
4	C	515	CIT	C3-C4-C5	-4.46	107.83	114.98
3	A	508	NAI	O7N-C7N-C3N	-3.87	113.61	120.90
3	A	508	NAI	N3A-C2A-N1A	-3.76	122.81	128.68
3	A	508	NAI	C3N-C2N-N1N	-3.65	117.88	123.10
3	C	510	NAI	C3N-C7N-N7N	3.63	124.12	117.67
3	D	511	NAI	C2D-C1D-N1N	-3.41	104.76	113.30
4	A	518	CIT	C4-C3-C2	3.38	118.37	109.33
3	D	511	NAI	O3D-C3D-C2D	-3.21	101.45	111.82
3	C	510	NAI	O3D-C3D-C2D	-2.92	102.36	111.82
3	A	508	NAI	O4D-C1D-N1N	2.84	113.60	108.06
4	A	514	CIT	C3-C4-C5	-2.81	110.48	114.98
2	C	502	PO4	O4-P-O3	2.71	116.67	107.97
3	B	509	NAI	C3N-C2N-N1N	-2.67	119.29	123.10
4	A	514	CIT	C3-C2-C1	-2.62	110.79	114.98
3	C	510	NAI	PN-O3-PA	-2.56	124.06	132.83
3	D	511	NAI	C2B-C3B-C4B	2.50	107.51	102.64
3	A	508	NAI	O4B-C1B-C2B	-2.50	103.28	106.93
3	D	511	NAI	C3N-C2N-N1N	-2.46	119.59	123.10
3	D	511	NAI	O4D-C1D-C2D	-2.45	101.29	106.64
3	C	510	NAI	C3N-C2N-N1N	-2.44	119.61	123.10
2	D	507	PO4	O4-P-O2	2.42	115.74	107.97
3	A	508	NAI	C3B-C2B-C1B	2.36	104.54	100.98
3	D	511	NAI	C4A-C5A-N7A	-2.34	106.96	109.40
3	B	509	NAI	PN-O3-PA	-2.28	125.01	132.83
3	A	508	NAI	C4A-C5A-N7A	-2.23	107.07	109.40
3	C	510	NAI	O3D-C3D-C4D	-2.19	104.72	111.05
3	A	508	NAI	C2D-C1D-N1N	-2.17	107.86	113.30
3	B	509	NAI	C2B-C3B-C4B	2.17	106.86	102.64
3	B	509	NAI	C3D-C2D-C1D	-2.16	97.33	101.43
3	A	508	NAI	C3N-C7N-N7N	2.13	121.46	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	510	NAI	O4D-C1D-N1N	2.13	112.21	108.06
3	A	508	NAI	O3B-C3B-C4B	-2.07	105.06	111.05
3	B	509	NAI	O4B-C4B-C5B	2.05	116.12	109.37
3	D	511	NAI	PN-O3-PA	-2.05	125.80	132.83
3	D	511	NAI	O4D-C1D-N1N	2.04	112.05	108.06

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	509	NAI	C5D-O5D-PN-O3
3	B	509	NAI	C5D-O5D-PN-O2N
4	A	514	CIT	C6-C3-C4-C5
4	D	513	CIT	C2-C3-C4-C5
4	D	513	CIT	O7-C3-C4-C5
4	D	513	CIT	C6-C3-C4-C5
3	A	508	NAI	O4B-C4B-C5B-O5B
3	D	511	NAI	O4B-C4B-C5B-O5B
4	A	514	CIT	O7-C3-C4-C5
3	C	510	NAI	O4B-C4B-C5B-O5B
3	C	510	NAI	C3B-C4B-C5B-O5B
4	A	514	CIT	C2-C3-C4-C5
3	D	511	NAI	C3B-C4B-C5B-O5B
3	C	510	NAI	C2D-C1D-N1N-C2N
3	C	510	NAI	C2D-C1D-N1N-C6N
4	A	518	CIT	C1-C2-C3-C6
4	C	517	CIT	C1-C2-C3-C6
4	C	517	CIT	C6-C3-C4-C5
3	C	510	NAI	O4D-C1D-N1N-C2N
3	A	508	NAI	O4D-C1D-N1N-C2N
3	D	511	NAI	PN-O3-PA-O1A
3	A	508	NAI	C3B-C4B-C5B-O5B
3	B	509	NAI	O4D-C1D-N1N-C2N
3	D	511	NAI	O4D-C1D-N1N-C2N
3	D	511	NAI	C2D-C1D-N1N-C2N
3	B	509	NAI	O4B-C4B-C5B-O5B
3	C	510	NAI	O4D-C1D-N1N-C6N
3	A	508	NAI	C2D-C1D-N1N-C2N
3	B	509	NAI	PN-O3-PA-O1A
3	C	510	NAI	PN-O3-PA-O1A
3	D	511	NAI	PN-O3-PA-O2A
3	B	509	NAI	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
3	D	511	NAI	C2D-C1D-N1N-C6N
3	B	509	NAI	C3D-C4D-C5D-O5D

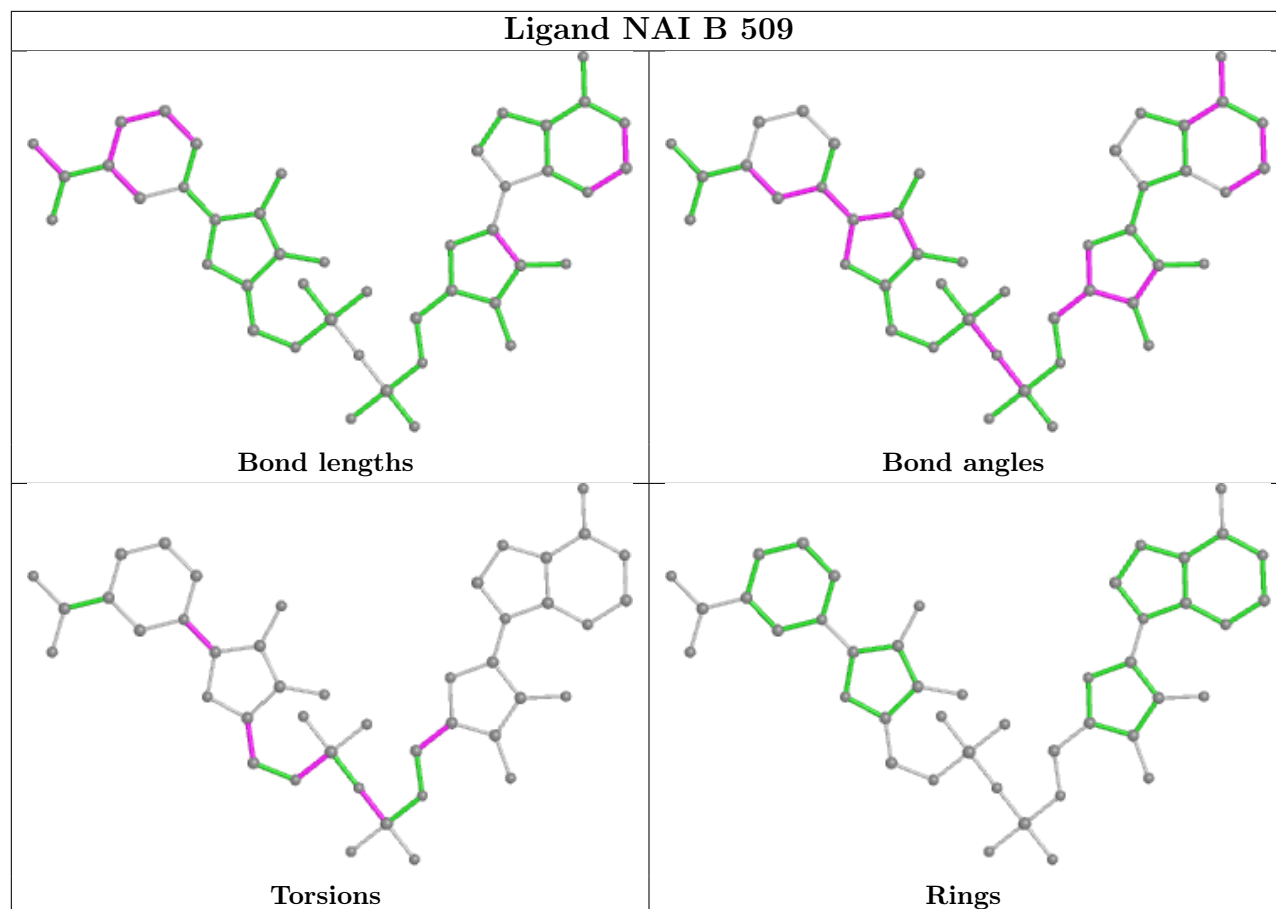
There are no ring outliers.

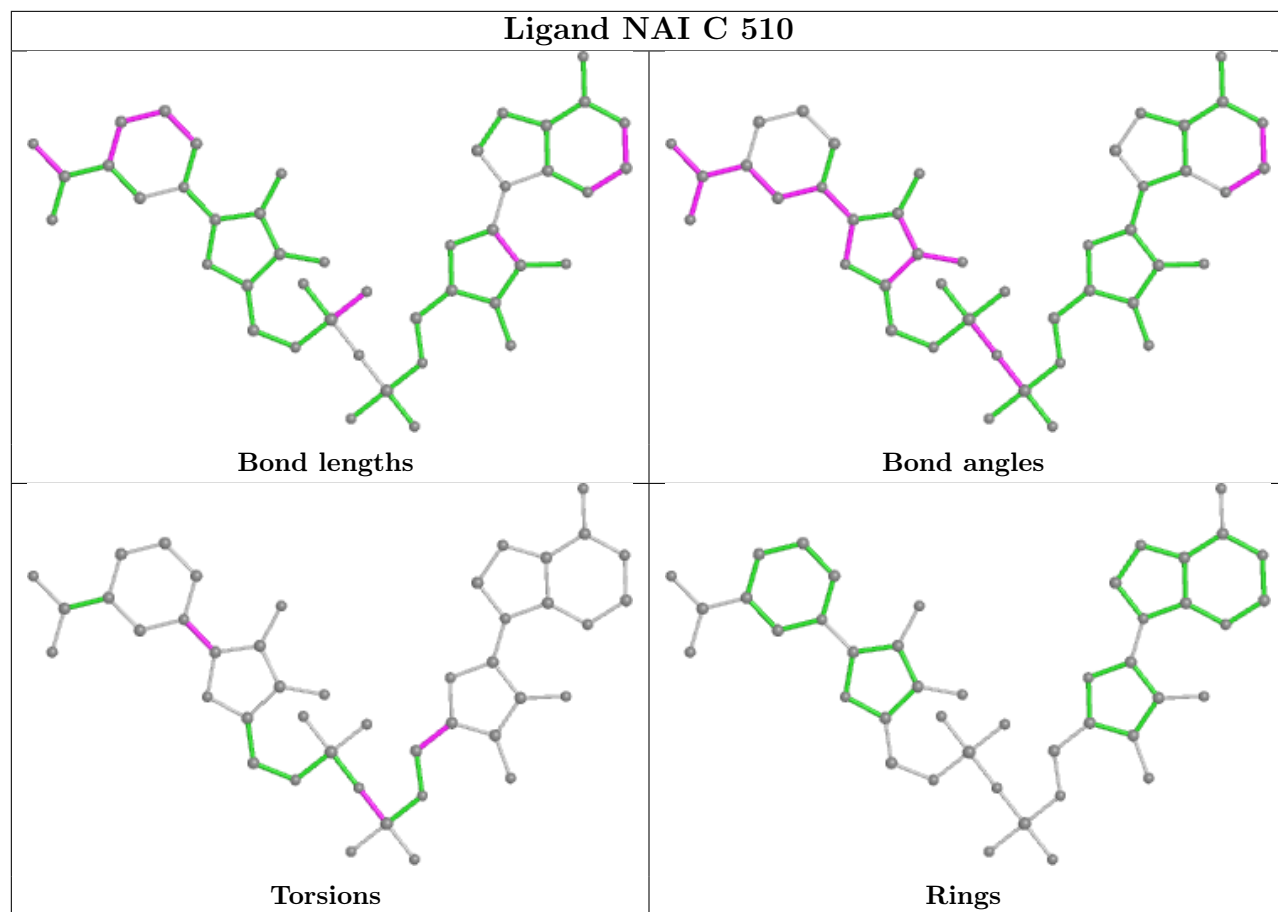
11 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	513	CIT	3	0
2	B	499	PO4	3	0
4	A	514	CIT	5	0
4	A	518	CIT	2	0
5	C	506	SO4	1	0
3	B	509	NAI	4	0
4	C	515	CIT	2	0
3	A	508	NAI	2	0
4	B	516	CIT	3	0
4	C	517	CIT	4	0
3	D	511	NAI	1	0

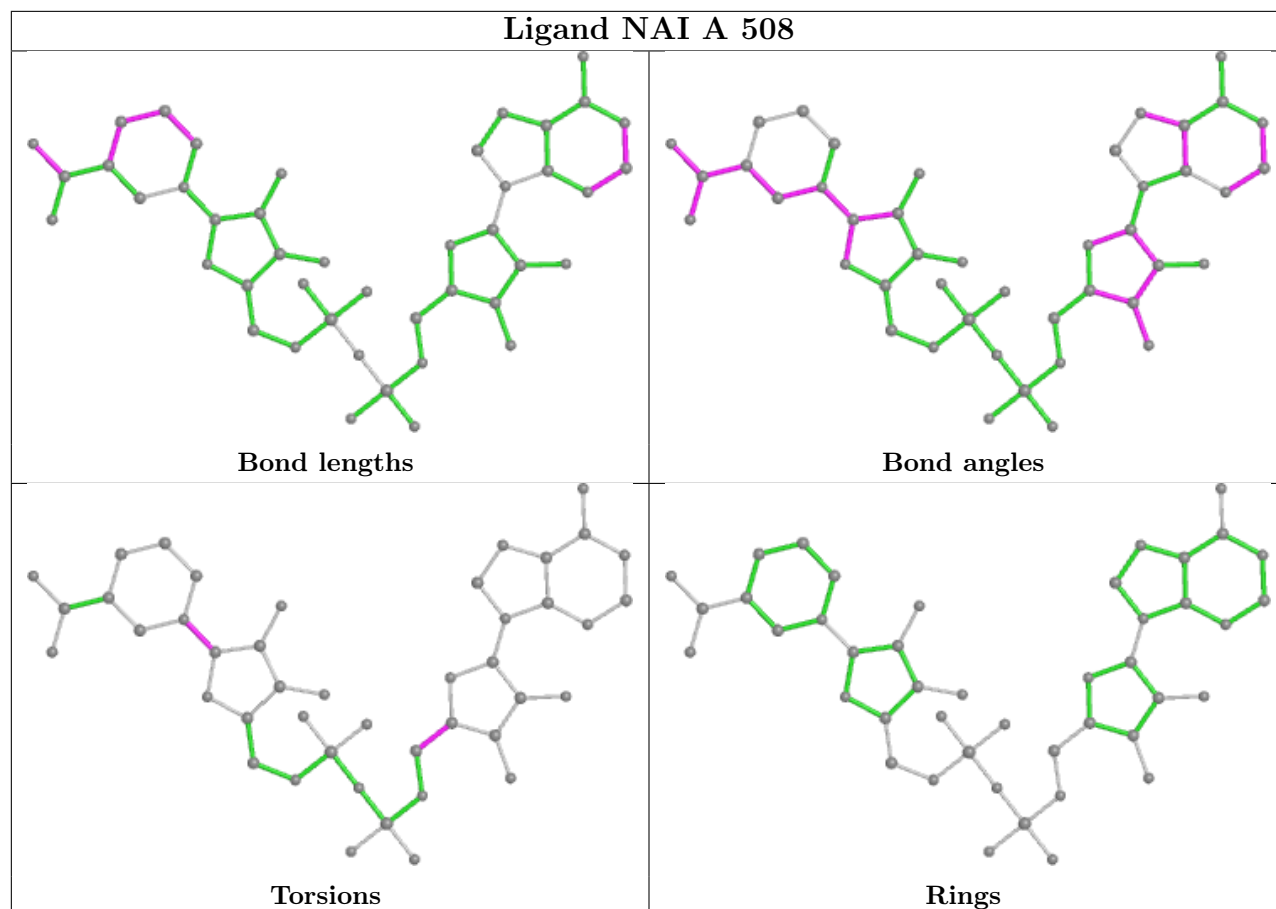
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

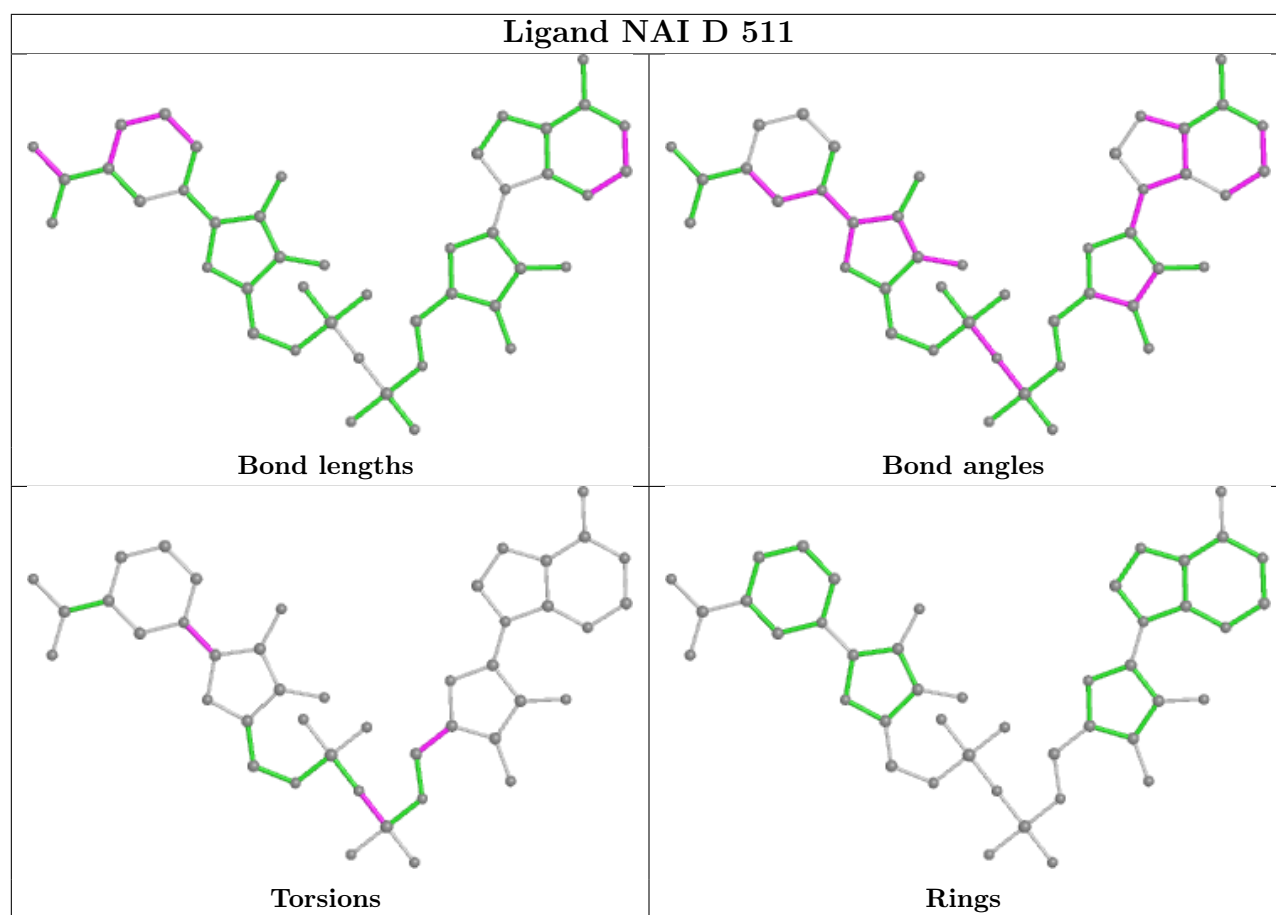
Ligand NAI B 509





Ligand NAI A 508





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	406/410 (99%)	-0.31	0	100 100	20, 38, 66, 87	3 (0%)
1	B	404/410 (98%)	-0.36	1 (0%)	95 95	17, 37, 59, 73	3 (0%)
1	C	406/410 (99%)	-0.34	2 (0%)	91 89	21, 37, 64, 92	8 (1%)
1	D	403/410 (98%)	-0.34	1 (0%)	95 95	16, 36, 69, 87	6 (1%)
All	All	1619/1640 (98%)	-0.34	4 (0%)	95 95	16, 37, 65, 92	20 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	6	LEU	4.7
1	B	45	GLU	3.5
1	D	65	LEU	2.2
1	C	335	HIS	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](#)

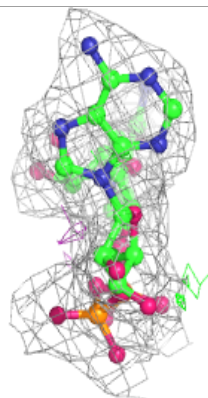
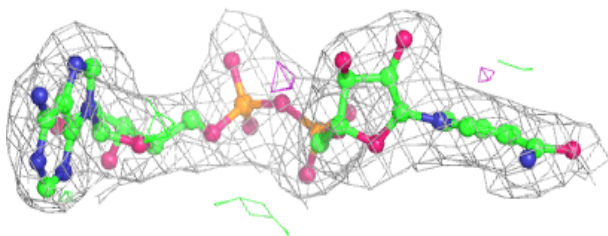
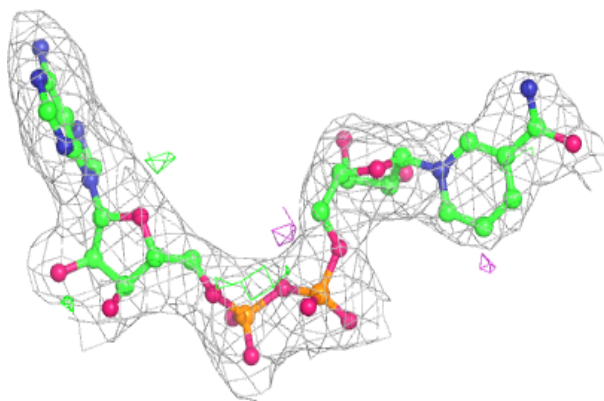
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CIT	A	518	13/13	0.81	0.31	59,68,81,96	0
4	CIT	B	516	13/13	0.82	0.23	29,53,60,66	0
4	CIT	A	514	13/13	0.86	0.26	58,72,97,102	0
4	CIT	C	515	13/13	0.87	0.24	44,62,73,81	0
4	CIT	C	517	13/13	0.89	0.32	61,71,82,89	0
4	CIT	D	513	13/13	0.89	0.28	49,69,77,85	0
2	PO4	B	499	5/5	0.92	0.11	62,62,75,76	0
2	PO4	A	504	5/5	0.93	0.20	61,67,69,79	0
5	SO4	C	506	5/5	0.93	0.11	56,57,70,72	0
2	PO4	D	505	5/5	0.96	0.13	51,61,71,71	0
3	NAI	D	511	44/44	0.97	0.13	27,39,49,53	0
2	PO4	B	503	5/5	0.97	0.15	35,39,45,48	0
2	PO4	D	507	5/5	0.97	0.13	54,56,59,64	0
3	NAI	B	509	44/44	0.97	0.12	26,45,51,59	0
3	NAI	A	508	44/44	0.98	0.15	18,37,48,51	0
3	NAI	C	510	44/44	0.98	0.14	21,41,49,53	0
2	PO4	C	501	5/5	0.99	0.15	28,32,36,41	0
2	PO4	C	502	5/5	0.99	0.12	25,28,35,37	0
2	PO4	A	500	5/5	0.99	0.15	16,25,29,30	0

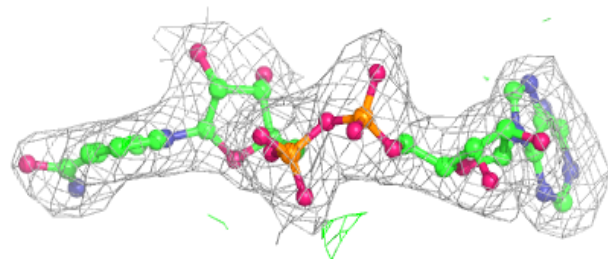
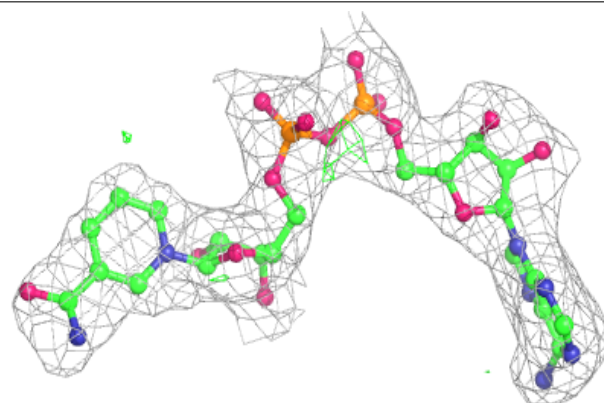
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI D 511:

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

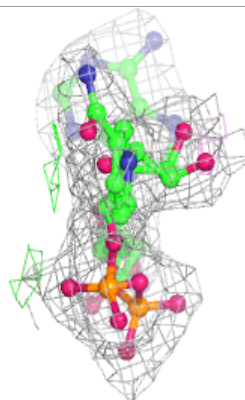
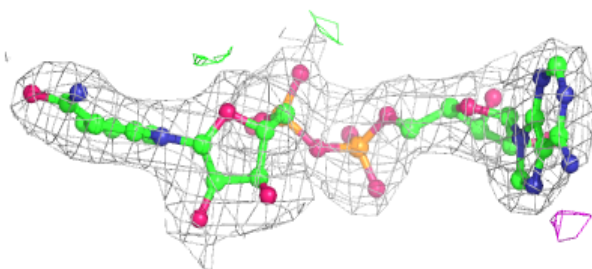
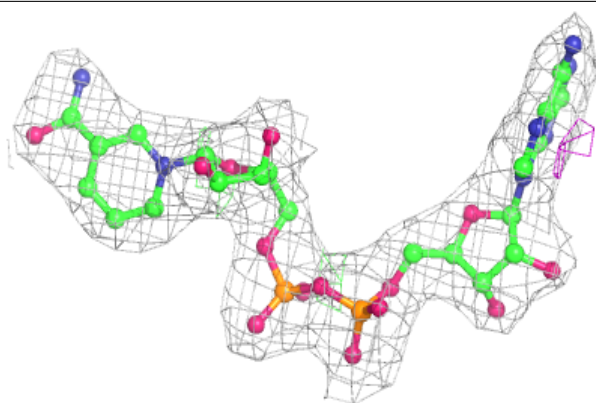
**Electron density around NAI B 509:**

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

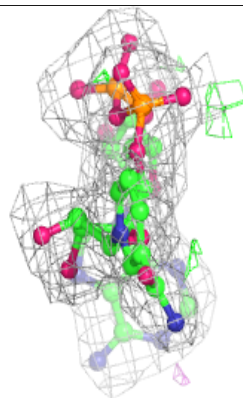
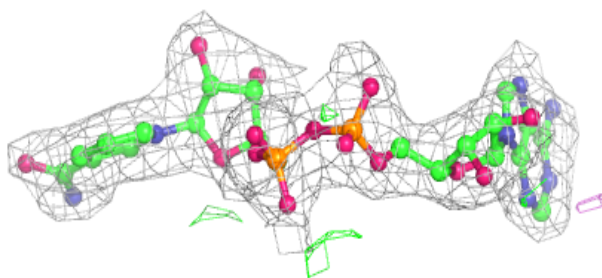
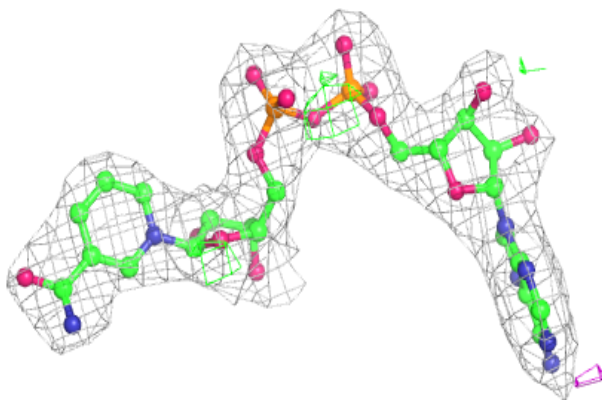


Electron density around NAI A 508:

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

**Electron density around NAI C 510:**

$2mF_o-DF_c$ (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.