



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:54 AM UTC

PDB ID : 2DNS / pdb_00002dns
Title : The crystal structure of D-amino acid amidase from Ochrobactrum anthropi SV3 complexed with D-Phenylalanine
Authors : Okazaki, S.; Suzuki, A.; Komeda, H.; Asano, Y.; Yamane, T.
Deposited on : 2006-04-26
Resolution : 2.40 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

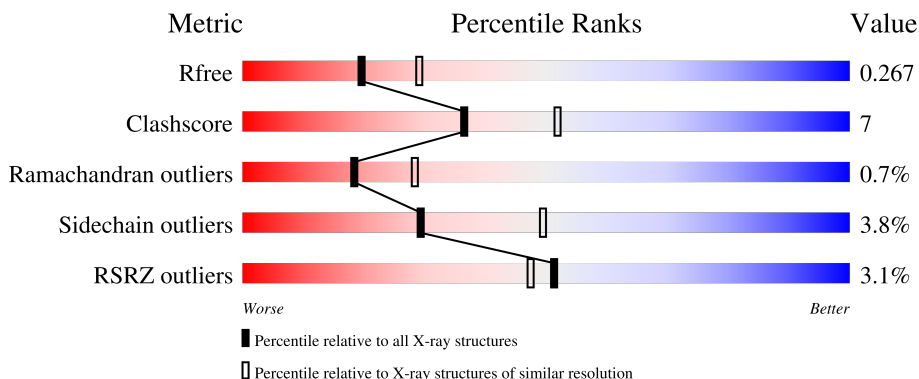
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



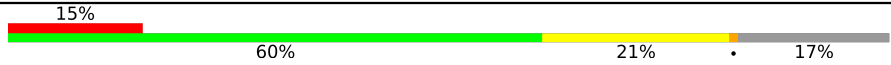
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	363	83% 15% .
1	B	363	87% 12% .
1	C	363	85% 12% ..
1	D	363	86% 11% ..
1	E	363	75% 18% ...

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Mol	Chain	Length	Quality of chain
1	F	363	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '15%', a green segment labeled '60%', a yellow segment labeled '21%', and a grey segment on the right labeled '17%'. A small black dot is located on the boundary between the yellow and grey segments.</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17094 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.

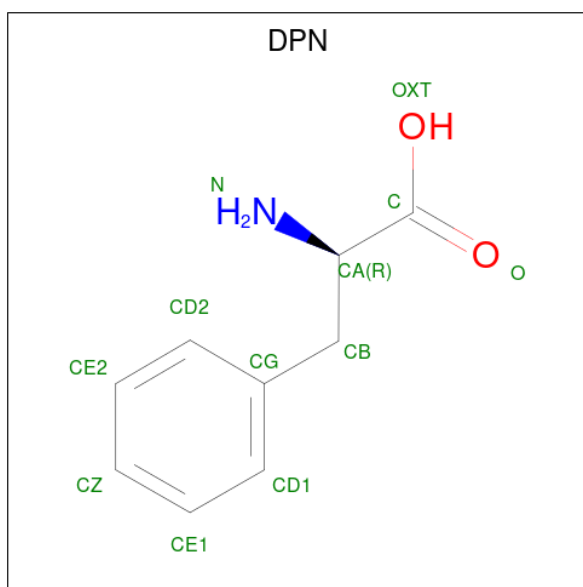
- Molecule 1 is a protein called D-amino acid amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	362	2811	1775	486	534	16	0	0	0
1	B	362	2841	1791	496	538	16	0	3	0
1	C	360	2799	1769	484	530	16	0	0	0
1	D	355	2772	1756	479	519	18	0	2	0
1	E	349	2709	1715	467	511	16	0	0	0
1	F	300	2342	1483	405	439	15	0	0	0

- Molecule 2 is BARIUM ION (CCD ID: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Ba	0	0
			5	5		
2	B	2	Total	Ba	0	0
			2	2		
2	C	4	Total	Ba	0	0
			4	4		
2	D	4	Total	Ba	0	0
			4	4		
2	E	2	Total	Ba	0	0
			2	2		
2	F	3	Total	Ba	0	0
			3	3		

- Molecule 3 is D-PHENYLALANINE (CCD ID: DPN) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	11	9	1	1	0	0
3	B	1	11	9	1	1	0	0
3	C	1	11	9	1	1	0	0
3	D	1	11	9	1	1	0	0
3	E	1	11	9	1	1	0	0

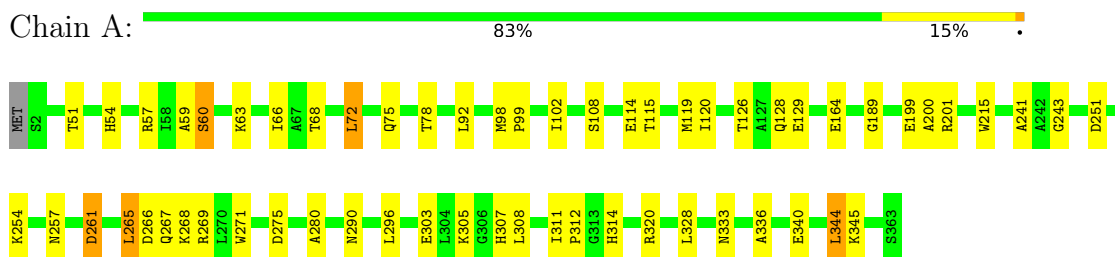
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	125	125	125	0	0
4	B	164	164	164	0	0
4	C	158	158	158	0	0
4	D	138	138	138	0	0
4	E	70	70	70	0	0
4	F	90	90	90	0	0

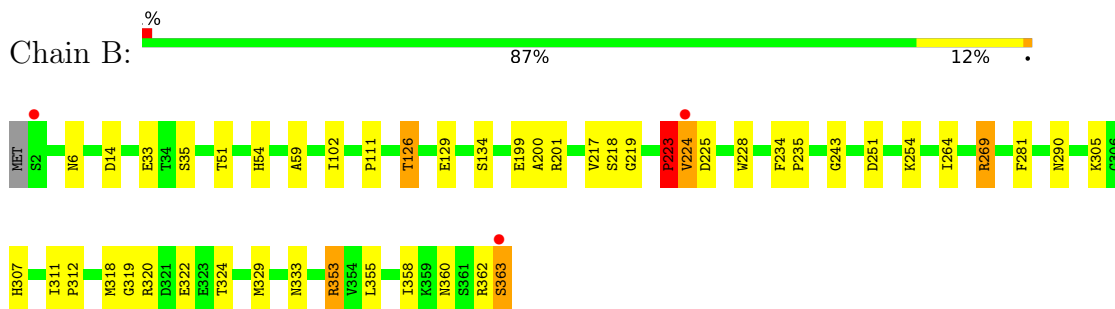
3 Residue-property plots i

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

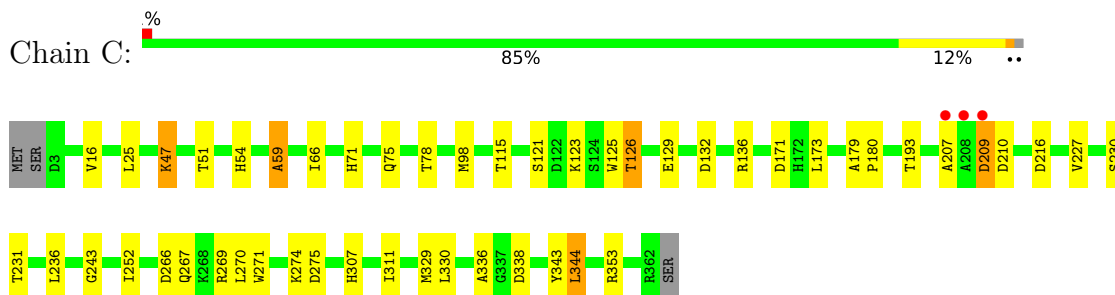
- Molecule 1: D-amino acid amidase



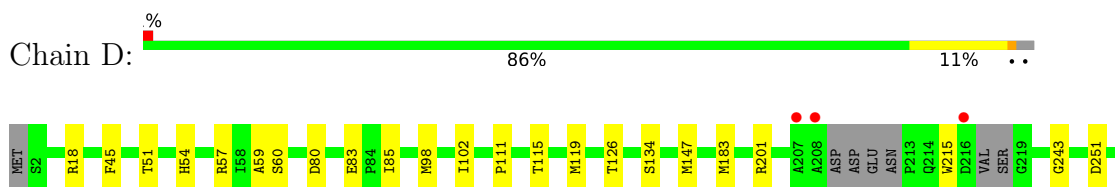
- Molecule 1: D-amino acid amidase



- Molecule 1: D-amino acid amidase

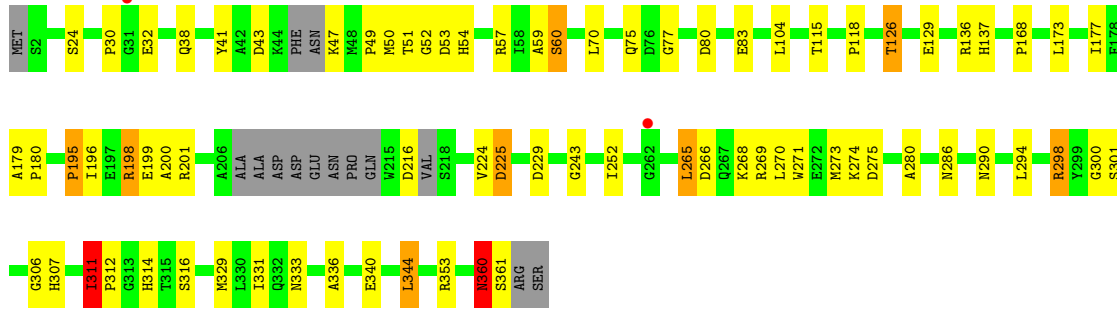
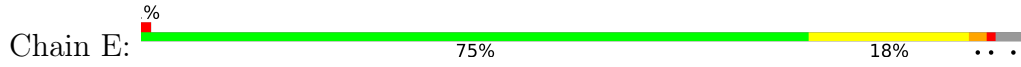


- Molecule 1: D-amino acid amidase

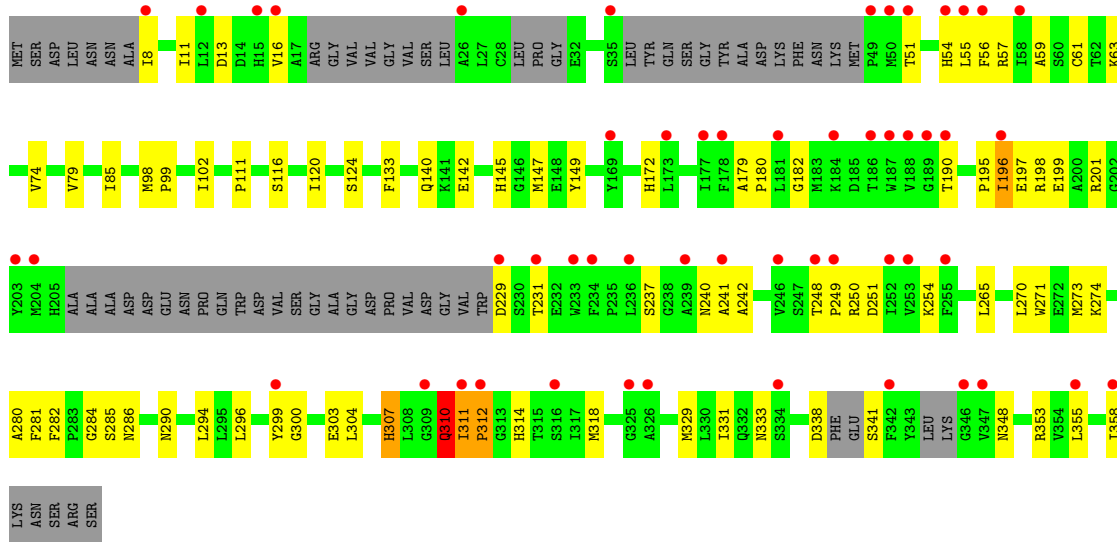




● Molecule 1: D-amino acid amidase



● Molecule 1: D-amino acid amidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.07Å 123.70Å 116.05Å 90.00° 104.44° 90.00°	Depositor
Resolution (Å)	19.87 – 2.40 19.87 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.87-2.40) 99.5 (19.87-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.41Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.269 0.195 , 0.267	Depositor DCC
R_{free} test set	4106 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtrriage
Anisotropy	0.070	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17094	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: BA, DPN

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	0.60	0/2883	0.92	7/3910 (0.2%)
1	B	0.63	0/2913	0.98	11/3949 (0.3%)
1	C	0.62	0/2871	0.87	1/3894 (0.0%)
1	D	0.62	0/2845	0.96	4/3853 (0.1%)
1	E	0.57	0/2776	0.91	3/3759 (0.1%)
1	F	0.63	0/2397	0.90	1/3239 (0.0%)
All	All	0.61	0/16685	0.92	27/22604 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	59	ALA	CA-C-N	15.13	144.99	120.63
1	D	59	ALA	C-N-CA	15.13	144.99	120.63
1	B	59	ALA	CA-C-N	10.77	141.02	120.99
1	B	59	ALA	C-N-CA	10.77	141.02	120.99
1	D	59	ALA	O-C-N	-10.65	108.43	122.59
1	B	224	VAL	N-CA-C	9.81	122.56	109.21
1	A	60	SER	O-C-N	-9.48	109.38	122.46
1	A	59	ALA	O-C-N	-8.48	107.92	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	59	ALA	O-C-N	-8.45	111.35	122.59
1	A	60	SER	CA-C-N	8.02	132.09	120.38
1	A	60	SER	C-N-CA	8.02	132.09	120.38
1	A	59	ALA	CA-C-N	7.79	136.60	121.18
1	A	59	ALA	C-N-CA	7.79	136.60	121.18
1	B	59	ALA	O-C-N	-7.30	109.45	121.20
1	E	311	ILE	CB-CA-C	7.02	116.21	109.33
1	E	311	ILE	N-CA-C	-6.18	104.12	109.19
1	F	307	HIS	N-CA-C	6.17	118.34	109.14
1	D	60	SER	O-C-N	-6.14	114.35	122.33
1	E	60	SER	O-C-N	-6.09	112.67	122.41
1	B	223	PRO	CA-C-N	5.97	130.67	121.71
1	B	223	PRO	C-N-CA	5.97	130.67	121.71
1	B	224	VAL	N-CA-CB	-5.82	102.28	110.26
1	B	223	PRO	N-CA-C	-5.81	101.97	111.21
1	A	189	GLY	N-CA-C	5.19	118.92	112.64
1	B	319	GLY	N-CA-C	5.14	118.08	110.63
1	B	264	ILE	CB-CA-C	-5.14	107.34	111.71
1	B	217	VAL	N-CA-C	5.09	117.07	111.77

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	223	PRO	Peptide
1	E	60	SER	Mainchain

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2811	0	2709	40	0
1	B	2841	0	2739	27	0
1	C	2799	0	2700	35	0
1	D	2772	0	2687	24	0
1	E	2709	0	2620	43	0
1	F	2342	0	2266	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	2	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	2	0	0	0	0
2	F	3	0	0	0	0
3	A	11	0	10	1	0
3	B	11	0	10	0	0
3	C	11	0	10	1	0
3	D	11	0	10	1	0
3	E	11	0	10	0	0
4	A	125	0	0	4	0
4	B	164	0	0	3	0
4	C	158	0	0	9	0
4	D	138	0	0	2	0
4	E	70	0	0	2	0
4	F	90	0	0	9	0
All	All	17094	0	15771	227	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 7.

All (227) 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:A:102:ILE:HG21	4:A:3140:HOH:O	1.35	1.25
1:F:331:ILE:HG23	4:F:3090:HOH:O	1.52	1.06
1:A:267:GLN:NE2	1:F:284:GLY:H	1.60	0.98
1:A:51:THR:H	1:A:54:HIS:HD2	0.98	0.97
1:D:119[A]:MET:HE2	1:D:215:TRP:HB2	1.46	0.94
1:E:75:GLN:HE22	1:E:265:LEU:HA	1.32	0.91
1:A:267:GLN:HE22	1:F:284:GLY:H	0.94	0.91
1:A:51:THR:H	1:A:54:HIS:CD2	1.87	0.91
1:A:98:MET:HB3	1:A:102:ILE:HD11	1.52	0.91
1:C:75:GLN:HE22	1:C:266:ASP:H	1.19	0.89
1:C:126:THR:HG22	1:C:129:GLU:H	1.39	0.88
1:C:75:GLN:HG2	1:C:269:ARG:HD3	1.57	0.87
1:A:267:GLN:HE22	1:F:284:GLY:N	1.75	0.84
1:A:72:LEU:HD13	1:A:265:LEU:HD12	1.58	0.84
1:B:269:ARG:HD2	1:B:269:ARG:N	1.97	0.80
1:F:237:SER:HB3	4:F:3042:HOH:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:PRO:HB2	1:E:198:ARG:HG3	1.62	0.79
1:B:51:THR:H	1:B:54:HIS:HD2	1.28	0.79
1:C:126:THR:HG21	4:C:3091:HOH:O	1.82	0.78
1:E:51:THR:H	1:E:54:HIS:HD2	1.33	0.76
1:C:51:THR:H	1:C:54:HIS:HD2	1.30	0.75
1:F:240:ASN:CG	1:F:241:ALA:H	1.93	0.75
1:D:57:ARG:H	1:D:314:HIS:HD2	1.32	0.75
1:D:51:THR:H	1:D:54:HIS:HD2	1.34	0.75
1:C:209:ASP:CB	4:C:3141:HOH:O	2.36	0.73
1:B:223:PRO:HD3	1:B:228:TRP:CZ2	2.24	0.72
1:B:51:THR:H	1:B:54:HIS:CD2	2.07	0.71
1:C:75:GLN:HE22	1:C:266:ASP:N	1.88	0.71
1:F:300:GLY:O	4:F:3089:HOH:O	2.08	0.71
1:E:126:THR:HG22	1:E:129:GLU:H	1.56	0.70
1:C:75:GLN:NE2	1:C:266:ASP:H	1.89	0.70
1:D:85:ILE:HD11	1:D:98:MET:HE2	1.72	0.70
1:A:257:ASN:O	1:A:261:ASP:HB2	1.90	0.70
1:F:282:PHE:O	1:F:285:SER:OG	2.09	0.69
1:F:57:ARG:H	1:F:314:HIS:HD2	1.40	0.69
1:F:59:ALA:HB2	1:F:311:ILE:HD13	1.74	0.69
1:C:336:ALA:H	1:C:344:LEU:HD13	1.56	0.69
1:E:80:ASP:O	1:E:83:GLU:HG2	1.92	0.68
1:C:209:ASP:HB3	4:C:3141:HOH:O	1.92	0.67
1:E:24:SER:HB2	1:E:50:MET:HE2	1.75	0.67
1:F:270:LEU:O	1:F:274:LYS:HG2	1.94	0.67
1:B:14:ASP:HB2	1:B:353[B]:ARG:HH22	1.59	0.66
1:A:75:GLN:NE2	1:A:266:ASP:H	1.93	0.66
1:A:126:THR:HB	1:A:129:GLU:HB2	1.79	0.64
1:E:75:GLN:NE2	1:E:266:ASP:H	1.94	0.64
1:B:126:THR:HG22	1:B:129:GLU:H	1.62	0.64
1:E:118:PRO:HA	1:E:216:ASP:HB3	1.78	0.63
1:A:72:LEU:HD13	1:A:265:LEU:CD1	2.28	0.63
1:C:171:ASP:HB3	4:C:3160:HOH:O	1.99	0.62
1:F:111:PRO:HG3	1:F:140:GLN:HB2	1.81	0.62
1:F:195:PRO:HB2	1:F:198:ARG:HG3	1.82	0.62
1:F:51:THR:H	1:F:54:HIS:CD2	2.18	0.61
1:F:190:THR:HB	4:F:3087:HOH:O	1.99	0.61
1:C:209:ASP:HB2	4:C:3141:HOH:O	1.99	0.60
3:A:1060:DPN:C	4:A:3043:HOH:O	2.49	0.60
1:F:172:HIS:HA	4:F:3094:HOH:O	2.01	0.60
1:F:341:SER:N	4:F:3102:HOH:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:PRO:HB2	4:B:3121:HOH:O	2.02	0.60
1:F:51:THR:H	1:F:54:HIS:HD2	1.49	0.60
1:F:314:HIS:HB2	4:F:3073:HOH:O	2.03	0.59
1:F:280:ALA:HB2	1:F:290:ASN:OD1	2.03	0.59
1:B:224:VAL:HG23	1:B:225:ASP:HB3	1.84	0.59
1:E:201:ARG:O	1:E:333:ASN:HB2	2.03	0.59
1:F:355:LEU:O	1:F:358:ILE:HG22	2.04	0.58
1:A:99:PRO:O	1:A:102:ILE:HG13	2.04	0.58
1:F:61:CYS:HB3	1:F:318:MET:SD	2.43	0.58
1:D:119[A]:MET:CE	1:D:215:TRP:HB2	2.28	0.57
1:B:269:ARG:HD2	1:B:269:ARG:H	1.70	0.56
1:B:126:THR:HG23	4:B:3058:HOH:O	2.04	0.56
1:F:286:ASN:ND2	1:F:299:TYR:CD1	2.74	0.56
1:D:119[B]:MET:HE1	3:D:1060:DPN:HE2	1.88	0.56
1:A:126:THR:HG22	1:A:128:GLN:H	1.71	0.55
1:C:71:HIS:O	1:C:75:GLN:HG3	2.07	0.55
1:A:75:GLN:HE22	1:A:266:ASP:H	1.54	0.55
1:B:224:VAL:HG23	1:B:225:ASP:OD1	2.07	0.55
1:C:210:ASP:HA	1:C:338:ASP:HB2	1.89	0.55
1:D:305:LYS:HE3	1:D:322:GLU:OE1	2.06	0.55
1:F:147:MET:HE3	1:F:280:ALA:HB1	1.88	0.54
1:D:45:PHE:HD1	4:D:3114:HOH:O	1.88	0.54
1:D:353:ARG:NH1	1:D:356:GLU:OE1	2.40	0.54
1:E:38:GLN:NE2	1:E:52:GLY:HA2	2.22	0.54
1:E:316:SER:HB3	1:E:331:ILE:HG23	1.89	0.54
1:F:273:MET:HE2	1:F:294:LEU:HG	1.90	0.54
1:A:75:GLN:HE22	1:A:265:LEU:HA	1.73	0.54
1:E:50:MET:HE1	1:E:54:HIS:HB2	1.90	0.54
1:F:133:PHE:HD1	4:F:3037:HOH:O	1.91	0.53
1:F:240:ASN:CG	1:F:241:ALA:N	2.64	0.53
1:E:252:ILE:HG21	1:E:329:MET:HE2	1.90	0.53
1:D:201:ARG:O	1:D:333:ASN:HB2	2.08	0.53
1:C:179:ALA:HB3	1:C:180:PRO:HD3	1.89	0.53
1:B:111:PRO:O	1:B:134:SER:HB3	2.09	0.53
1:C:123:LYS:HD3	1:C:125:TRP:CE2	2.44	0.52
1:A:268:LYS:HD3	1:F:281:PHE:CD2	2.44	0.52
1:E:77:GLY:HA2	4:E:3040:HOH:O	2.09	0.52
1:B:320:ARG:HD3	4:B:3086:HOH:O	2.10	0.52
1:E:51:THR:H	1:E:54:HIS:CD2	2.21	0.52
1:E:75:GLN:NE2	1:E:265:LEU:HA	2.13	0.52
1:A:271:TRP:CD1	1:A:275:ASP:HB2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:ARG:H	1:F:314:HIS:CD2	2.26	0.52
1:B:201:ARG:O	1:B:333:ASN:HB2	2.09	0.52
1:B:305:LYS:HE3	1:B:322:GLU:OE1	2.10	0.52
1:E:59:ALA:HB2	1:E:311:ILE:HB	1.90	0.52
1:F:59:ALA:CB	1:F:310:GLN:H	2.23	0.52
1:F:59:ALA:HB3	1:F:310:GLN:H	1.75	0.52
1:F:201:ARG:HB3	1:F:229:ASP:OD2	2.11	0.51
1:C:132:ASP:O	1:C:136:ARG:HG3	2.09	0.51
1:A:126:THR:HG22	1:A:128:GLN:N	2.26	0.51
1:E:224:VAL:O	1:E:225:ASP:HB2	2.11	0.51
1:B:33:GLU:HB2	1:C:209:ASP:OD1	2.10	0.51
1:F:54:HIS:O	1:F:248:THR:HG22	2.11	0.51
1:D:119[A]:MET:HG3	1:D:215:TRP:HB3	1.94	0.51
1:D:183:MET:HE3	1:D:251:ASP:O	2.11	0.51
1:A:340:GLU:OE2	4:A:3142:HOH:O	2.19	0.50
1:F:355:LEU:HG	4:F:3026:HOH:O	2.10	0.50
1:F:13:ASP:HA	1:F:16:VAL:HG22	1.93	0.50
1:F:285:SER:HA	1:F:348:ASN:HD21	1.76	0.50
1:F:251:ASP:HA	1:F:254:LYS:HD2	1.93	0.50
1:E:271:TRP:CD1	1:E:275:ASP:HB2	2.46	0.50
3:C:1060:DPN:C	4:C:3074:HOH:O	2.59	0.50
1:E:201:ARG:HD3	1:E:229:ASP:OD2	2.12	0.50
1:C:266:ASP:OD1	1:C:269:ARG:HD2	2.12	0.49
1:D:310:GLN:NE2	1:D:344:LEU:HG	2.27	0.49
1:F:63:LYS:HD2	1:F:149:TYR:OH	2.12	0.49
1:E:75:GLN:HE22	1:E:265:LEU:CA	2.15	0.49
1:C:59:ALA:HB2	1:C:311:ILE:HB	1.94	0.49
1:B:324:THR:HG22	1:B:362:ARG:HH12	1.78	0.49
1:C:98:MET:HE2	4:C:3012:HOH:O	2.11	0.49
1:B:225:ASP:O	1:B:225:ASP:OD2	2.31	0.48
1:E:280:ALA:HB2	1:E:290:ASN:OD1	2.13	0.48
1:A:57:ARG:H	1:A:314:HIS:HD2	1.60	0.48
1:F:142:GLU:O	1:F:145:HIS:HB3	2.14	0.48
1:A:68:THR:HG23	1:A:265:LEU:HD13	1.96	0.48
1:D:111:PRO:O	1:D:134:SER:HB3	2.13	0.48
1:B:360:ASN:HA	1:B:363:SER:HB2	1.96	0.48
1:D:274:LYS:HD2	1:D:322:GLU:OE2	2.14	0.48
1:F:85:ILE:HG12	1:F:98:MET:HB2	1.95	0.48
1:A:78:THR:OG1	1:A:164:GLU:OE1	2.32	0.47
1:A:280:ALA:HB2	1:A:290:ASN:OD1	2.15	0.47
1:D:85:ILE:CD1	1:D:98:MET:HE2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:LEU:O	1:E:274:LYS:HG2	2.13	0.47
1:A:201:ARG:O	1:A:333:ASN:HB2	2.14	0.47
1:A:257:ASN:HA	1:A:320:ARG:HH21	1.79	0.47
1:D:273:MET:HE2	1:D:294:LEU:HG	1.97	0.47
1:C:66:ILE:HD13	1:C:173:LEU:HD11	1.97	0.46
1:F:299:TYR:HE2	1:F:304:LEU:HD12	1.81	0.46
1:D:80:ASP:O	1:D:83:GLU:HG2	2.14	0.46
1:E:173:LEU:O	1:E:177:ILE:HB	2.16	0.46
1:F:56:PHE:HE1	1:F:333:ASN:OD1	1.99	0.46
4:C:3144:HOH:O	1:E:300:GLY:HA2	2.16	0.46
1:E:126:THR:HG21	4:E:3074:HOH:O	2.15	0.46
1:B:199:GLU:HG2	1:B:200:ALA:O	2.16	0.46
1:A:251:ASP:O	1:A:254:LYS:HB2	2.15	0.45
1:F:249:PRO:HB3	1:F:329:MET:O	2.15	0.45
1:F:311:ILE:HB	1:F:312:PRO:HD2	1.98	0.45
1:E:360:ASN:O	1:E:361:SER:HB2	2.17	0.45
1:F:251:ASP:O	1:F:254:LYS:HB2	2.17	0.45
1:F:98:MET:HB3	1:F:102:ILE:HG21	1.98	0.44
1:A:66:ILE:HG13	1:A:241:ALA:HB1	1.99	0.44
1:F:179:ALA:N	1:F:180:PRO:HD2	2.32	0.44
1:F:63:LYS:NZ	1:F:242:ALA:O	2.50	0.44
1:E:199:GLU:HG2	1:E:200:ALA:O	2.17	0.44
1:A:336:ALA:H	1:A:344:LEU:HD13	1.82	0.44
1:E:57:ARG:H	1:E:314:HIS:HD2	1.66	0.44
1:E:43:ASP:O	1:E:47:LYS:HA	2.17	0.43
1:F:8:ILE:HA	1:F:11:ILE:HD12	2.00	0.43
1:F:55:LEU:H	1:F:199:GLU:HA	1.82	0.43
1:B:355:LEU:HA	1:B:358:ILE:HD12	1.99	0.43
1:A:102:ILE:O	1:A:108:SER:HB3	2.18	0.43
1:E:41:TYR:HA	1:E:49:PRO:HA	2.00	0.43
1:E:57:ARG:H	1:E:314:HIS:CD2	2.36	0.43
1:C:98:MET:CE	4:C:3012:HOH:O	2.65	0.43
1:E:179:ALA:HB3	1:E:180:PRO:HD3	2.00	0.43
1:F:296:LEU:HD11	1:F:303:GLU:HB2	2.01	0.43
1:D:283:PRO:HA	1:D:284:GLY:HA2	1.84	0.43
1:F:57:ARG:N	1:F:314:HIS:HD2	2.10	0.43
1:F:286:ASN:ND2	1:F:299:TYR:CE1	2.86	0.43
1:C:230:SER:O	1:C:231:THR:C	2.62	0.43
1:F:250:ARG:HG2	1:F:254:LYS:HE3	2.00	0.43
1:A:311:ILE:O	1:A:312:PRO:C	2.62	0.42
1:C:123:LYS:HD3	1:C:125:TRP:CZ2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:LYS:O	1:D:305:LYS:NZ	2.52	0.42
1:E:273:MET:HE2	1:E:294:LEU:HG	2.00	0.42
1:D:57:ARG:N	1:D:314:HIS:HD2	2.09	0.42
1:C:207:ALA:O	1:C:343:TYR:CE2	2.72	0.42
1:C:252:ILE:HG13	1:C:329:MET:HE2	2.01	0.42
1:A:119:MET:HG3	1:A:215:TRP:HB3	2.02	0.42
1:E:286:ASN:HB3	1:E:298:ARG:O	2.19	0.42
1:F:338:ASP:O	1:F:341:SER:HB3	2.19	0.42
1:A:296:LEU:HD13	1:A:305:LYS:HG2	2.01	0.42
1:F:56:PHE:CE1	1:F:333:ASN:OD1	2.73	0.42
1:F:56:PHE:CG	1:F:331:ILE:HG21	2.54	0.42
1:B:234:PHE:HA	1:B:235:PRO:HD3	1.93	0.41
1:B:251:ASP:O	1:B:254:LYS:HB3	2.20	0.41
1:A:75:GLN:HE21	1:A:269:ARG:HB2	1.84	0.41
1:A:199:GLU:HG2	1:A:200:ALA:O	2.19	0.41
1:E:136:ARG:HG2	1:E:137:HIS:CE1	2.55	0.41
1:C:25:LEU:HD13	1:C:330:LEU:HD12	2.02	0.41
1:C:271:TRP:CD1	1:C:275:ASP:HB2	2.55	0.41
1:D:147:MET:HE3	1:D:280:ALA:HB1	2.03	0.41
1:E:118:PRO:HA	1:E:216:ASP:CB	2.46	0.41
1:A:60:SER:O	1:A:63:LYS:HB2	2.20	0.41
1:E:265:LEU:HG	1:E:269:ARG:HB3	2.02	0.41
1:F:63:LYS:HD2	1:F:149:TYR:HH	1.85	0.41
1:E:70:LEU:HD23	1:E:104:LEU:HD11	2.03	0.41
1:A:114:GLU:HG2	4:A:3051:HOH:O	2.20	0.41
1:A:296:LEU:HD11	1:A:303:GLU:OE2	2.21	0.41
1:A:308:LEU:C	1:A:308:LEU:HD12	2.46	0.41
1:D:335:GLY:HA3	4:D:3081:HOH:O	2.20	0.41
1:E:38:GLN:HE21	1:E:52:GLY:HA2	1.84	0.41
1:E:336:ALA:H	1:E:344:LEU:HD13	1.86	0.41
1:F:282:PHE:C	1:F:282:PHE:CD2	2.99	0.41
1:B:318:MET:HB3	1:B:329:MET:SD	2.61	0.41
1:C:47:LYS:HA	1:C:47:LYS:HD3	1.91	0.41
1:F:74:VAL:HA	1:F:79:VAL:O	2.21	0.41
1:B:311:ILE:O	1:B:312:PRO:C	2.64	0.40
1:C:51:THR:H	1:C:54:HIS:CD2	2.22	0.40
1:C:75:GLN:HE21	1:C:269:ARG:HB2	1.86	0.40
1:E:294:LEU:HD22	1:E:306:GLY:HA2	2.02	0.40
1:F:99:PRO:O	1:F:102:ILE:HG22	2.21	0.40
1:A:265:LEU:HG	1:A:269:ARG:HB3	2.02	0.40
1:B:218:SER:HA	1:B:219:GLY:HA2	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:ARG:HA	1:C:353:ARG:HD3	1.97	0.40
1:D:18:ARG:NH1	1:D:349:GLU:OE1	2.55	0.40
1:C:216:ASP:OD1	1:C:216:ASP:C	2.64	0.40
1:B:281:PHE:HB2	1:F:271:TRP:CE2	2.56	0.40
1:C:270:LEU:HG	1:C:274:LYS:HE3	2.04	0.40
1:E:30:PRO:C	1:E:32:GLU:H	2.29	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	360/363 (99%)	349 (97%)	10 (3%)	1 (0%)	36	50
1	B	363/363 (100%)	346 (95%)	16 (4%)	1 (0%)	36	50
1	C	358/363 (99%)	341 (95%)	15 (4%)	2 (1%)	21	32
1	D	351/363 (97%)	338 (96%)	12 (3%)	1 (0%)	36	50
1	E	341/363 (94%)	322 (94%)	14 (4%)	5 (2%)	8	12
1	F	286/363 (79%)	264 (92%)	17 (6%)	5 (2%)	7	10
All	All	2059/2178 (94%)	1960 (95%)	84 (4%)	15 (1%)	18	28

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	310	GLN
1	E	360	ASN
1	F	182	GLY
1	A	243	GLY
1	E	243	GLY
1	F	312	PRO

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Mol	Chain	Res	Type
1	B	243	GLY
1	C	47	LYS
1	C	243	GLY
1	F	197	GLU
1	F	196	ILE
1	D	243	GLY
1	E	168	PRO
1	E	195	PRO
1	E	312	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/301 (100%)	290 (97%)	10 (3%)	33	55
1	B	303/301 (101%)	293 (97%)	10 (3%)	33	55
1	C	298/301 (99%)	286 (96%)	12 (4%)	28	47
1	D	295/301 (98%)	287 (97%)	8 (3%)	39	62
1	E	289/301 (96%)	273 (94%)	16 (6%)	19	34
1	F	251/301 (83%)	241 (96%)	10 (4%)	28	47
All	All	1736/1806 (96%)	1670 (96%)	66 (4%)	29	49

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	92	LEU
1	A	115	THR
1	A	120	ILE
1	A	261	ASP
1	A	265	LEU
1	A	307	HIS
1	A	328	LEU
1	A	344	LEU

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Mol	Chain	Res	Type
1	A	345	LYS
1	B	6	ASN
1	B	35	SER
1	B	102	ILE
1	B	126	THR
1	B	269	ARG
1	B	290	ASN
1	B	307	HIS
1	B	353[A]	ARG
1	B	353[B]	ARG
1	B	363	SER
1	C	16	VAL
1	C	78	THR
1	C	115	THR
1	C	121	SER
1	C	126	THR
1	C	193	THR
1	C	209	ASP
1	C	227	VAL
1	C	236	LEU
1	C	267	GLN
1	C	307	HIS
1	C	344	LEU
1	D	102	ILE
1	D	115	THR
1	D	126	THR
1	D	290	ASN
1	D	307	HIS
1	D	320	ARG
1	D	344	LEU
1	D	353	ARG
1	E	53	ASP
1	E	115	THR
1	E	126	THR
1	E	196	ILE
1	E	198	ARG
1	E	225	ASP
1	E	265	LEU
1	E	268	LYS
1	E	298	ARG
1	E	301	SER
1	E	307	HIS

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Mol	Chain	Res	Type
1	E	311	ILE
1	E	340	GLU
1	E	344	LEU
1	E	353	ARG
1	E	360	ASN
1	F	116	SER
1	F	120	ILE
1	F	124	SER
1	F	196	ILE
1	F	231	THR
1	F	265	LEU
1	F	307	HIS
1	F	310	GLN
1	F	311	ILE
1	F	353	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	46	ASN
1	A	54	HIS
1	A	75	GLN
1	A	137	HIS
1	A	205	HIS
1	A	267	GLN
1	B	54	HIS
1	B	163	HIS
1	B	267	GLN
1	B	360	ASN
1	C	5	ASN
1	C	6	ASN
1	C	54	HIS
1	C	75	GLN
1	C	97	GLN
1	C	137	HIS
1	C	163	HIS
1	C	267	GLN
1	C	348	ASN
1	C	360	ASN
1	D	54	HIS
1	D	163	HIS

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Mol	Chain	Res	Type
1	D	314	HIS
1	D	360	ASN
1	E	5	ASN
1	E	54	HIS
1	E	75	GLN
1	E	205	HIS
1	E	310	GLN
1	E	314	HIS
1	F	9	GLN
1	F	54	HIS
1	F	75	GLN
1	F	137	HIS
1	F	163	HIS
1	F	191	HIS
1	F	205	HIS
1	F	257	ASN
1	F	314	HIS
1	F	348	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 20 are monoatomic - leaving 5 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	DPN	A	1060	1	10,11,12	0.78	0	8,13,15	0.73	0
3	DPN	E	1060	1	10,11,12	0.65	0	8,13,15	0.91	0
3	DPN	C	1060	1	10,11,12	0.44	0	8,13,15	0.73	0
3	DPN	B	1060	1	10,11,12	0.59	0	8,13,15	0.74	0
3	DPN	D	1060	1	10,11,12	0.62	0	8,13,15	0.57	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
3	DPN	A	1060	1	-	1/5/6/8	0/1/1/1
3	DPN	E	1060	1	-	0/5/6/8	0/1/1/1
3	DPN	C	1060	1	-	0/5/6/8	0/1/1/1
3	DPN	B	1060	1	-	1/5/6/8	0/1/1/1
3	DPN	D	1060	1	-	1/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1060	DPN	O-C-CA-CB
3	D	1060	DPN	O-C-CA-CB
3	B	1060	DPN	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1060	DPN	1	0
3	C	1060	DPN	1	0
3	D	1060	DPN	1	0

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	362/363 (99%)	-0.33	0 100 100	14, 29, 40, 55	0
1	B	362/363 (99%)	-0.46	3 (0%) 82 80	9, 23, 41, 56	3 (0%)
1	C	360/363 (99%)	-0.47	3 (0%) 82 80	13, 24, 42, 49	0
1	D	355/363 (97%)	-0.48	3 (0%) 82 80	12, 23, 40, 61	2 (0%)
1	E	349/363 (96%)	0.01	2 (0%) 85 83	18, 37, 58, 74	0
1	F	300/363 (82%)	1.01	53 (17%) 4 3	22, 53, 70, 72	0
All	All	2088/2178 (95%)	-0.15	64 (3%) 51 47	9, 28, 59, 74	5 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	208	ALA	4.1
1	F	239	ALA	4.0
1	F	189	GLY	4.0
1	F	347	VAL	4.0
1	F	55	LEU	3.3
1	F	248	THR	3.3
1	F	233	TRP	3.1
1	F	326	ALA	3.1
1	F	49	PRO	3.1
1	F	358	ILE	3.0
1	F	334	SER	3.0
1	F	246	VAL	3.0
1	F	253	VAL	3.0
1	F	241	ALA	3.0
1	D	208	ALA	2.9
1	F	12	LEU	2.9
1	F	249	PRO	2.9
1	F	196	ILE	2.9
1	F	188	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	207	ALA	2.8
1	D	207	ALA	2.8
1	C	209	ASP	2.8
1	B	224	VAL	2.8
1	F	231	THR	2.8
1	F	342	PHE	2.8
1	F	309	GLY	2.7
1	F	355	LEU	2.6
1	F	169	TYR	2.6
1	F	16	VAL	2.6
1	E	31	GLY	2.6
1	F	181	LEU	2.6
1	F	178	PHE	2.5
1	F	58	ILE	2.5
1	F	26	ALA	2.5
1	F	190	THR	2.4
1	F	50	MET	2.4
1	F	229	ASP	2.3
1	B	363	SER	2.3
1	F	186	THR	2.3
1	F	35	SER	2.3
1	F	173	LEU	2.3
1	F	56	PHE	2.3
1	F	252	ILE	2.2
1	F	325	GLY	2.2
1	D	216	ASP	2.2
1	F	187	TRP	2.2
1	F	204	MET	2.2
1	F	236	LEU	2.2
1	F	15	HIS	2.2
1	F	8	ILE	2.2
1	F	312	PRO	2.2
1	E	262	GLY	2.1
1	F	311	ILE	2.1
1	F	54	HIS	2.1
1	F	51	THR	2.1
1	F	177	ILE	2.1
1	F	255	PHE	2.1
1	F	203	TYR	2.1
1	F	234	PHE	2.0
1	F	184	LYS	2.0
1	F	346	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	2	SER	2.0
1	F	299	TYR	2.0
1	F	316	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BA	F	3008	1/1	0.73	0.19	49,49,49,49	1
2	BA	D	3012	1/1	0.74	0.33	61,61,61,61	1
2	BA	B	3019	1/1	0.76	0.11	59,59,59,59	1
2	BA	A	3020	1/1	0.81	0.17	66,66,66,66	1
2	BA	A	3018	1/1	0.84	0.14	57,57,57,57	1
2	BA	D	3017	1/1	0.85	0.18	58,58,58,58	1
2	BA	E	3010	1/1	0.87	0.15	73,73,73,73	1
3	DPN	E	1060	11/12	0.87	0.09	28,31,32,32	0
3	DPN	A	1060	11/12	0.88	0.10	22,23,24,26	0
3	DPN	D	1060	11/12	0.90	0.08	29,31,33,34	0
2	BA	C	3009	1/1	0.90	0.30	71,71,71,71	1
2	BA	A	3007	1/1	0.93	0.19	59,59,59,59	1
2	BA	F	3006	1/1	0.94	0.08	51,51,51,51	1
3	DPN	B	1060	11/12	0.94	0.07	23,26,27,27	0
2	BA	F	3014	1/1	0.95	0.08	44,44,44,44	1
2	BA	C	3011	1/1	0.96	0.11	53,53,53,53	1
3	DPN	C	1060	11/12	0.96	0.06	13,16,19,19	0
2	BA	A	3004	1/1	0.97	0.06	41,41,41,41	1
2	BA	D	3013	1/1	0.97	0.06	59,59,59,59	1
2	BA	E	3016	1/1	0.98	0.10	36,36,36,36	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BA	D	3015	1/1	0.99	0.06	29,29,29,29	1
2	BA	B	3002	1/1	1.00	0.01	28,28,28,28	1
2	BA	A	3003	1/1	1.00	0.03	28,28,28,28	1
2	BA	C	3001	1/1	1.00	0.01	29,29,29,29	0
2	BA	C	3005	1/1	1.00	0.01	37,37,37,37	1

6.5 Other polymers [i](#)

There are no such residues in this entry.