



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 10:59 PM BST

PDB ID : 5ZIE
Title : Crystal structure of Legionella pneumophila aminopeptidase A in complex with aspartic acid
Authors : Marapaka, A.K.; Addlagatta, A.
Deposited on : 2018-03-14
Resolution : 2.00 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 : 2.14.4.dev1
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) : 2.14.4.dev1

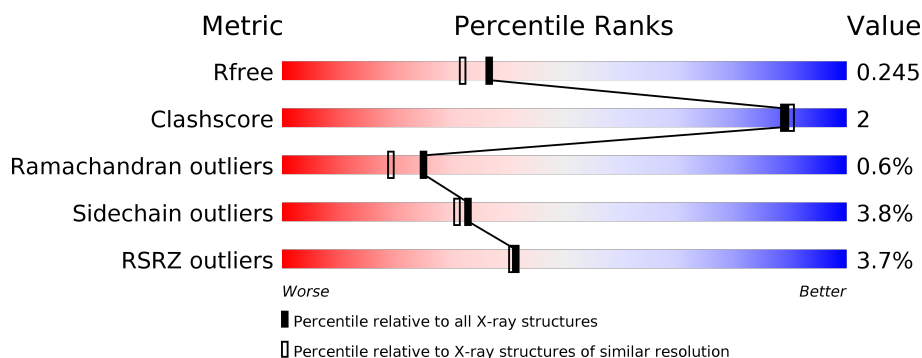
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	921	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>8%</div> </div> </div>
1	B	921	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13907 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	850	Total	C	N	O	S	0	5	0
			6836	4384	1117	1307	28			
1	B	850	Total	C	N	O	S	0	4	0
			6828	4380	1113	1308	27			

There are 42 discrepancies between the modelled and reference sequences:

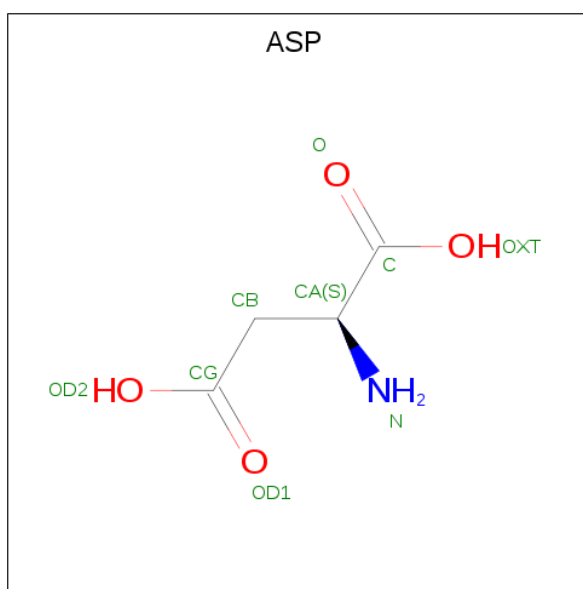
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q5ZVE3
A	-19	GLY	-	expression tag	UNP Q5ZVE3
A	-18	SER	-	expression tag	UNP Q5ZVE3
A	-17	SER	-	expression tag	UNP Q5ZVE3
A	-16	HIS	-	expression tag	UNP Q5ZVE3
A	-15	HIS	-	expression tag	UNP Q5ZVE3
A	-14	HIS	-	expression tag	UNP Q5ZVE3
A	-13	HIS	-	expression tag	UNP Q5ZVE3
A	-12	HIS	-	expression tag	UNP Q5ZVE3
A	-11	HIS	-	expression tag	UNP Q5ZVE3
A	-10	SER	-	expression tag	UNP Q5ZVE3
A	-9	SER	-	expression tag	UNP Q5ZVE3
A	-8	GLY	-	expression tag	UNP Q5ZVE3
A	-7	LEU	-	expression tag	UNP Q5ZVE3
A	-6	VAL	-	expression tag	UNP Q5ZVE3
A	-5	PRO	-	expression tag	UNP Q5ZVE3
A	-4	ARG	-	expression tag	UNP Q5ZVE3
A	-3	GLY	-	expression tag	UNP Q5ZVE3
A	-2	SER	-	expression tag	UNP Q5ZVE3
A	-1	HIS	-	expression tag	UNP Q5ZVE3
A	0	MET	-	expression tag	UNP Q5ZVE3
B	-20	MET	-	initiating methionine	UNP Q5ZVE3
B	-19	GLY	-	expression tag	UNP Q5ZVE3
B	-18	SER	-	expression tag	UNP Q5ZVE3
B	-17	SER	-	expression tag	UNP Q5ZVE3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP Q5ZVE3
B	-15	HIS	-	expression tag	UNP Q5ZVE3
B	-14	HIS	-	expression tag	UNP Q5ZVE3
B	-13	HIS	-	expression tag	UNP Q5ZVE3
B	-12	HIS	-	expression tag	UNP Q5ZVE3
B	-11	HIS	-	expression tag	UNP Q5ZVE3
B	-10	SER	-	expression tag	UNP Q5ZVE3
B	-9	SER	-	expression tag	UNP Q5ZVE3
B	-8	GLY	-	expression tag	UNP Q5ZVE3
B	-7	LEU	-	expression tag	UNP Q5ZVE3
B	-6	VAL	-	expression tag	UNP Q5ZVE3
B	-5	PRO	-	expression tag	UNP Q5ZVE3
B	-4	ARG	-	expression tag	UNP Q5ZVE3
B	-3	GLY	-	expression tag	UNP Q5ZVE3
B	-2	SER	-	expression tag	UNP Q5ZVE3
B	-1	HIS	-	expression tag	UNP Q5ZVE3
B	0	MET	-	expression tag	UNP Q5ZVE3

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	1	4		
2	B	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	103	Total 103	O 103	0	0
3	B	122	Total 122	O 122	0	0

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.

[illegible]

Chain B:

2% 7% 8%

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET MET VAL VAL LYS GLN GLY VAL PHE MET LYS THR ASP GLN S13 K16 K22 P52 S58 L75 L82 K33 E84 D85 T90 K91 D92 S93 I99 N102 T106

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.95Å 102.51Å 111.24Å 90.00° 90.52° 90.00°	Depositor
Resolution (Å)	33.89 – 2.00 33.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (33.89-2.00) 99.4 (33.89-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.178 , 0.240 0.186 , 0.245	Depositor DCC
R_{free} test set	5473 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13907	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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

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	0.83	2/6987 (0.0%)	0.92	22/9459 (0.2%)
1	B	0.86	0/6979	0.94	20/9449 (0.2%)
All	All	0.85	2/13966 (0.0%)	0.93	42/18908 (0.2%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	741	TRP	CB-CG	-5.71	1.40	1.50
1	A	136	GLU	CD-OE1	-5.11	1.20	1.25

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	668	ARG	NE-CZ-NH2	-14.62	112.99	120.30
1	A	668	ARG	NE-CZ-NH2	-13.50	113.55	120.30
1	A	668	ARG	NE-CZ-NH1	11.30	125.95	120.30
1	B	668	ARG	NE-CZ-NH1	11.21	125.91	120.30
1	B	624	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	B	624	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	B	344	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	344	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	A	344	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	624	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	393	MET	CG-SD-CE	6.74	110.99	100.20
1	B	252	ARG	NE-CZ-NH2	6.74	123.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	B	565	ASP	CB-CG-OD1	6.55	124.20	118.30
1	A	756	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	A	756	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	A	485	ASP	CB-CG-OD1	6.24	123.91	118.30
1	B	668	ARG	CG-CD-NE	-6.15	98.89	111.80
1	B	414	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	767	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	A	624	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	B	612	GLN	N-CA-C	6.00	127.19	111.00
1	B	756	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	466	LYS	CD-CE-NZ	5.68	124.77	111.70
1	A	767	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	252	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	414	ASP	CB-CG-OD1	5.56	123.30	118.30
1	B	756	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	A	351	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	762	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	661	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	852	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	251	GLU	OE1-CD-OE2	-5.34	116.90	123.30
1	A	320	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	514	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	717	CYS	CA-CB-SG	5.21	123.37	114.00
1	B	624	ARG	CG-CD-NE	-5.17	100.95	111.80
1	B	494	ASP	CB-CG-OD1	5.14	122.92	118.30
1	B	713	CYS	CA-CB-SG	-5.12	104.79	114.00
1	A	709	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	762	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	B	414	ASP	CB-CG-OD2	-5.05	113.76	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	229	PRO	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	6836	0	6825	29	0
1	B	6828	0	6814	23	0
2	A	9	0	3	0	0
2	B	9	0	3	1	0
3	A	103	0	0	0	0
3	B	122	0	0	0	0
All	All	13907	0	13645	51	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 2.

All (51) 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:535:TYR:OH	1:B:565:ASP:OD2	1.96	0.82
1:A:466:LYS:HE2	1:A:466:LYS:O	1.98	0.64
1:B:571:LYS:O	1:B:573:GLU:N	2.33	0.62
1:B:212:THR:HG21	1:B:244:LYS:HZ3	1.71	0.55
1:A:75:LEU:HD21	1:A:96:ILE:HD12	1.90	0.54
1:A:427:ILE:HD12	1:A:435:LEU:HD12	1.91	0.53
1:B:501:GLN:OE1	1:B:502:GLU:N	2.42	0.52
1:A:568:ILE:HD11	1:A:570:LYS:HE2	1.91	0.52
1:A:840:LYS:O	1:A:844:SER:OG	2.25	0.50
1:A:101:GLN:O	1:A:103:THR:HG22	2.12	0.50
1:A:174:LEU:HD11	1:A:187:VAL:HG22	1.95	0.49
1:A:466:LYS:HE2	1:A:466:LYS:C	2.32	0.49
1:B:75:LEU:HG	1:B:82:LEU:HD12	1.94	0.49
1:B:566:PHE:HB2	1:B:572:ILE:CG1	2.43	0.48
1:A:824:TRP:CZ2	1:A:862:VAL:HG12	2.49	0.48
1:B:798:LEU:HD23	1:B:798:LEU:C	2.35	0.47
1:B:119:LEU:HD21	1:B:270:LYS:HE3	1.97	0.47
1:B:355:LEU:HD13	1:B:598:GLU:HG2	1.96	0.46
1:B:277:GLU:OE1	2:B:911:ASP:N	2.48	0.46
1:B:90:THR:HG22	1:B:93:SER:H	1.81	0.46
1:A:450:LEU:HD11	1:A:477:ILE:HD13	1.97	0.46
1:B:612:GLN:HB3	1:B:615:PRO:HB3	1.98	0.46
1:B:511:ILE:HG21	1:B:515:PRO:HG3	1.97	0.46
1:A:174:LEU:CD1	1:A:187:VAL:HG22	2.46	0.46
1:A:75:LEU:HD21	1:A:96:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:PRO:O	1:B:624:ARG:HD2	2.17	0.45
1:A:220:ARG:NH1	1:A:257:GLU:OE1	2.47	0.45
1:A:782:ILE:HA	1:A:788:PHE:HB2	1.98	0.44
1:A:824:TRP:CE3	1:A:836:ILE:HD11	2.52	0.44
1:B:212:THR:HG22	1:B:213:TYR:H	1.81	0.44
1:A:747:LEU:HG	1:A:780:SER:HB3	2.00	0.44
1:A:202:LEU:HD23	1:A:202:LEU:C	2.39	0.43
1:A:411:LYS:CE	1:B:490:GLU:O	2.67	0.43
1:A:372:THR:HG21	1:A:853:THR:HG21	2.01	0.42
1:A:798:LEU:C	1:A:798:LEU:HD23	2.40	0.42
1:B:566:PHE:HB2	1:B:572:ILE:HG13	2.01	0.42
1:A:67:GLY:HA3	1:A:143:TYR:CD2	2.55	0.42
1:A:614:LYS:HA	1:A:828:ASP:N	2.35	0.42
1:A:837:SER:O	1:A:841:ILE:HG12	2.20	0.42
1:B:609:ILE:O	1:B:826:LYS:NZ	2.45	0.42
1:B:52:PRO:HG3	1:B:102:ASN:HA	2.03	0.41
1:A:839:LEU:HB3	1:A:859:LEU:HD21	2.02	0.41
1:A:516:ILE:N	1:A:516:ILE:HD12	2.35	0.41
1:B:212:THR:HG21	1:B:244:LYS:NZ	2.36	0.41
1:B:577:GLN:O	1:B:581:VAL:HG23	2.20	0.41
1:A:364:ARG:NH1	1:A:819:GLU:OE2	2.53	0.41
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.90	0.41
1:A:603:PRO:O	1:A:624:ARG:HD2	2.21	0.40
1:B:16:LYS:O	1:B:370:ALA:HA	2.21	0.40
1:A:652:ASP:O	1:A:654:LYS:N	2.55	0.40
1:B:305:LEU:CD2	1:B:344:ARG:HG2	2.52	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	853/921 (93%)	824 (97%)	26 (3%)	3 (0%)	34	30
1	B	852/921 (92%)	820 (96%)	25 (3%)	7 (1%)	19	13
All	All	1705/1842 (93%)	1644 (96%)	51 (3%)	10 (1%)	25	19

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	653	ASP
1	B	572	ILE
1	B	612	GLN
1	B	613	ASP
1	A	55	ASN
1	B	286	THR
1	B	573	GLU
1	B	611	ASN
1	A	277	GLU
1	B	277	GLU

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	759/816 (93%)	730 (96%)	29 (4%)	33	31
1	B	758/816 (93%)	729 (96%)	29 (4%)	33	31
All	All	1517/1632 (93%)	1459 (96%)	58 (4%)	33	31

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	93	SER
1	A	103	THR
1	A	106	THR
1	A	113	LEU
1	A	119	LEU

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Mol	Chain	Res	Type
1	A	130	LEU
1	A	185	HIS
1	A	187	VAL
1	A	256	LEU
1	A	286	THR
1	A	461	LYS
1	A	462	GLN
1	A	495	LYS
1	A	502	GLU
1	A	529	MET
1	A	532	GLU
1	A	571	LYS
1	A	591	LEU
1	A	654	LYS
1	A	721	ASP
1	A	740	ASN
1	A	790	SER
1	A	817	LEU
1	A	826	LYS
1	A	844	SER
1	A	847	THR
1	A	850	ASP
1	A	856	LYS
1	B	22	LYS
1	B	58	SER
1	B	83	LYS
1	B	90	THR
1	B	91	LYS
1	B	99	ILE
1	B	106	THR
1	B	109	MET
1	B	113	LEU
1	B	179	GLU
1	B	185	HIS
1	B	187	VAL
1	B	257	GLU
1	B	261	ARG
1	B	286	THR
1	B	404	GLU
1	B	411	LYS
1	B	461	LYS
1	B	529	MET

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Mol	Chain	Res	Type
1	B	591	LEU
1	B	610	GLU
1	B	614	LYS
1	B	658	LYS
1	B	717	CYS
1	B	718	GLU
1	B	732	LYS
1	B	817	LEU
1	B	826	LYS
1	B	850	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ASP	A	911	-	2,8,8	0.42	0	1,10,10	1.53	0
2	ASP	B	911	-	2,8,8	0.66	0	1,10,10	2.64	1 (100%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ASP	A	911	-	-	1/2/8/8	-
2	ASP	B	911	-	-	1/2/8/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	911	ASP	CB-CA-C	2.64	114.96	110.69

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	911	ASP	N-CA-CB-CG
2	B	911	ASP	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	911	ASP	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	850/921 (92%)	0.14	41 (4%) 30 29	26, 41, 71, 121	0
1	B	850/921 (92%)	-0.05	22 (2%) 56 54	27, 38, 64, 111	0
All	All	1700/1842 (92%)	0.04	63 (3%) 41 41	26, 40, 69, 121	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	VAL	7.7
1	A	651	ASP	6.9
1	A	55	ASN	6.2
1	B	653	ASP	6.2
1	B	650	GLY	4.9
1	A	614	LYS	4.7
1	A	57	ASP	4.6
1	B	567	CYS	4.5
1	A	824	TRP	4.2
1	A	652	ASP	3.9
1	A	234	SER	3.8
1	B	570	LYS	3.8
1	A	61	ASN	3.8
1	A	232	ALA	3.6
1	B	566	PHE	3.5
1	A	459	ASP	3.4
1	A	180	LEU	3.3
1	A	58	SER	3.3
1	B	652	ASP	3.2
1	A	233	THR	3.1
1	A	231	SER	3.1
1	B	568	ILE	3.0
1	A	862	VAL	3.0
1	A	653	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	182	LEU	3.0
1	B	85	ASN	3.0
1	A	179	GLU	3.0
1	A	829	VAL	2.9
1	B	654	LYS	2.9
1	A	83	LYS	2.9
1	A	54	LEU	2.9
1	B	651	ASP	2.9
1	A	53	ASN	2.9
1	A	59	HIS	2.9
1	B	658	LYS	2.8
1	B	459	ASP	2.7
1	A	658	LYS	2.7
1	B	571	LYS	2.6
1	A	183	GLY	2.6
1	A	611	ASN	2.6
1	A	230	PRO	2.6
1	B	13	SER	2.5
1	B	83	LYS	2.5
1	B	573	GLU	2.5
1	A	464	PHE	2.4
1	A	612	GLN	2.4
1	A	617	PHE	2.3
1	A	97	LYS	2.3
1	A	613	ASP	2.3
1	B	572	ILE	2.3
1	B	721	ASP	2.2
1	A	858	GLY	2.2
1	B	218	SER	2.2
1	A	184	LEU	2.1
1	A	199	LEU	2.1
1	B	219	GLY	2.1
1	A	133	ALA	2.1
1	A	84	GLU	2.1
1	B	611	ASN	2.1
1	A	178	LYS	2.1
1	A	198	TYR	2.1
1	B	217	LYS	2.1
1	A	654	LYS	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
2	ASP	A	911	9/9	0.94	0.23	37,46,50,52	0
2	ASP	B	911	9/9	0.94	0.26	33,42,46,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.