Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:23 PM GMT

PDB ID : 1AJR
Title : REFINEMENT AND COMPARISON OF THE CRYSTAL STRUCTURES
OF PIG CYTOSOLIC ASPARTATE AMINOTRANSFERASE AND ITS
COMPLEX WITH 2-METHYLASPARTATE
Authors : Rhee, S.; Silva, M.M.; Hyde, C.C.; Rogers, P.H.; Metzler, C.M.; Metzler, D.E.;
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Deposited on : 1997-05-08
Resolution : 1.74 Å(reported)

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 1.74 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.
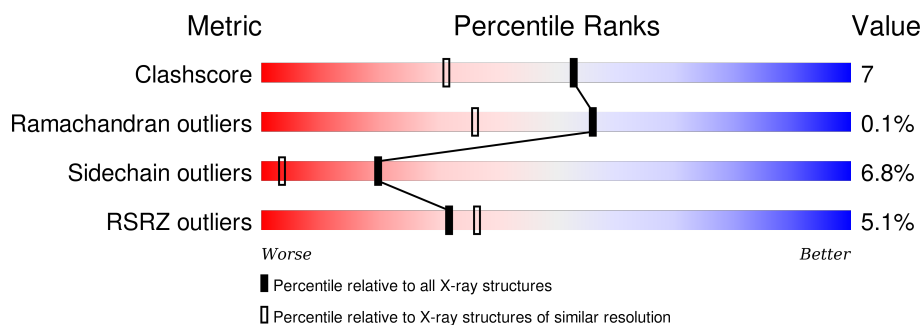
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2570 (1.76-1.72)
Ramachandran outliers	100387	2544 (1.76-1.72)
Sidechain outliers	100360	2544 (1.76-1.72)
RSRZ outliers	91569	2420 (1.76-1.72)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	412	
1	B	412	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6938 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 ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	412	Total 3289	C 2095	N 575	O 607	P 1	S 11	0	0	0
1	B	412	Total 3295	C 2098	N 578	O 607	P 1	S 11	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
A	63	ASN	ASP	CONFLICT	UNP P00503
A	258	LLP	LYS	MODIFIED RESIDUE	UNP P00503
A	288	GLN	GLU	CONFLICT	UNP P00503
A	376	GLN	GLU	CONFLICT	UNP P00503
B	63	ASN	ASP	CONFLICT	UNP P00503
B	258	LLP	LYS	MODIFIED RESIDUE	UNP P00503
B	288	GLN	GLU	CONFLICT	UNP P00503
B	376	GLN	GLU	CONFLICT	UNP P00503

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	150	Total 150	O 150	0	0
2	B	204	Total 204	O 204	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: ASPARTATE AMINOTRANSFERASE
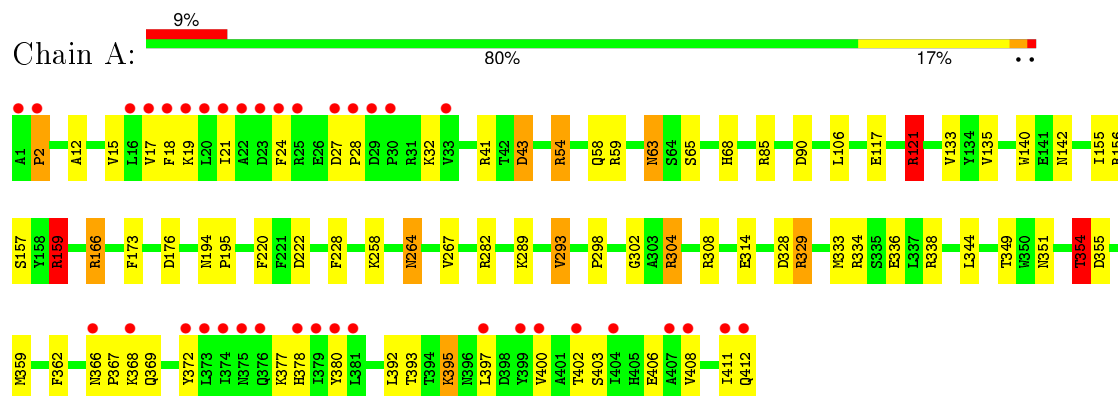
- Molecule 1: ASPARTATE AMINOTRANSFERASE
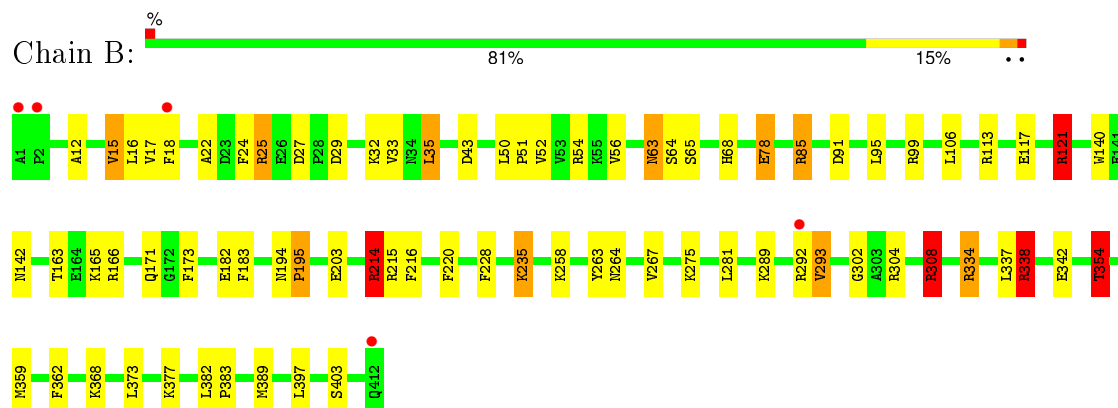
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.00Å 130.80Å 55.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.74 41.62 – 1.74	Depositor EDS
% Data completeness (in resolution range)	95.0 (8.00-1.74) 97.6 (41.62-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$<I/\sigma(I)>$ [1]	1.40 (at 1.74Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.170 , (Not available) 0.162 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	16.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 64.6	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.33$	Xtriage
Outliers	1 of 91696 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6938	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: LLP

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	0.79	0/3348	1.30	23/4548 (0.5%)
1	B	0.83	0/3359	1.33	22/4562 (0.5%)
All	All	0.81	0/6707	1.31	45/9110 (0.5%)

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	3
1	B	0	5
All	All	0	8

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	338	ARG	CD-NE-CZ	22.84	155.58	123.60
1	A	159	ARG	NE-CZ-NH1	15.14	127.87	120.30
1	B	338	ARG	NE-CZ-NH1	14.09	127.34	120.30
1	A	304	ARG	NE-CZ-NH1	13.41	127.00	120.30
1	A	308	ARG	NE-CZ-NH1	12.93	126.76	120.30
1	B	166	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	A	159	ARG	CD-NE-CZ	10.22	137.91	123.60
1	B	334	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	B	214	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	B	214	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	A	41	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	A	282	ARG	NE-CZ-NH2	-8.52	116.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	304	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	41	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	A	159	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	B	308	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	308	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	B	91	ASP	CB-CG-OD1	7.02	124.62	118.30
1	A	156	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	B	293	VAL	CG1-CB-CG2	6.59	121.45	110.90
1	A	328	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	A	334	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	A	293	VAL	N-CA-CB	-6.36	97.51	111.50
1	B	304	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	113	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	293	VAL	CG1-CB-CG2	6.01	120.52	110.90
1	B	215	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	B	338	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	B	121	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	A	334	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	293	VAL	N-CA-CB	-5.66	99.05	111.50
1	B	292[A]	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	292[B]	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	304	ARG	CD-NE-CZ	5.44	131.22	123.60
1	B	166	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	354	THR	N-CA-CB	-5.35	100.14	110.30
1	A	355	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	29	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	59	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	43	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	A	54	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	293	VAL	CA-CB-CG1	5.15	118.62	110.90
1	B	354	THR	N-CA-CB	-5.11	100.59	110.30
1	A	43	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	121	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	ARG	Sidechain
1	A	304	ARG	Sidechain
1	A	329	ARG	Sidechain
1	B	121	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	214	ARG	Sidechain
1	B	308	ARG	Sidechain
1	B	338	ARG	Sidechain
1	B	85	ARG	Sidechain

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	3289	0	3231	51	0
1	B	3295	0	3240	40	0
2	A	150	0	0	2	0
2	B	204	0	0	3	0
All	All	6938	0	6471	86	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 (86) 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:27:ASP:HB3	1:B:32:LYS:HD2	1.56	0.87
1:B:338:ARG:HH21	1:B:354:THR:HG21	1.40	0.86
1:A:15:VAL:HB	1:A:18:PHE:HD2	1.40	0.85
1:B:15:VAL:HG12	1:B:18:PHE:CD2	2.22	0.75
1:B:354:THR:HG23	2:B:597:HOH:O	1.88	0.74
1:A:338:ARG:HH11	1:A:354:THR:HG21	1.57	0.70
1:A:159:ARG:HD3	1:A:176:ASP:OD2	1.92	0.68
1:A:27:ASP:HB3	1:A:32:LYS:HD2	1.76	0.66
1:B:117:GLU:OE1	1:B:121:ARG:NH1	2.29	0.65
1:A:366:ASN:HB2	1:A:367:PRO:HD2	1.79	0.64
1:A:15:VAL:HB	1:A:18:PHE:CD2	2.31	0.62
1:A:333:MET:HE2	1:A:392:LEU:HB3	1.82	0.61
1:B:63:ASN:ND2	1:B:65:SER:H	1.99	0.59
1:A:133:VAL:HB	1:A:155:ILE:HD13	1.85	0.59
1:B:203:GLU:HG3	2:B:511:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ARG:O	1:A:58:GLN:HG2	2.03	0.59
1:B:228:PHE:CE1	1:B:359:MET:HG3	2.38	0.58
1:A:392:LEU:HD21	1:A:400:VAL:HG11	1.86	0.57
1:A:166:ARG:NH1	1:A:349:THR:O	2.37	0.57
1:A:32:LYS:HA	1:A:378:HIS:O	2.04	0.56
1:A:228:PHE:CE1	1:A:359:MET:HG3	2.40	0.56
1:A:372:TYR:HB2	1:A:411:ILE:HD12	1.88	0.56
1:B:228:PHE:HE1	1:B:359:MET:HG3	1.70	0.55
1:B:338:ARG:HH21	1:B:354:THR:CG2	2.18	0.54
1:A:63:ASN:HD22	1:A:65:SER:H	1.55	0.54
1:B:63:ASN:HD22	1:B:63:ASN:C	2.10	0.54
1:A:63:ASN:ND2	1:A:65:SER:H	2.07	0.53
1:A:289:LYS:HD2	1:B:12:ALA:HB1	1.91	0.52
1:B:33:VAL:HG12	1:B:35:LEU:HD13	1.90	0.52
1:A:336:GLU:CB	1:A:397:LEU:HD21	2.40	0.52
1:A:338:ARG:NH1	1:A:354:THR:HG21	2.24	0.51
1:B:214:ARG:HG2	1:B:214:ARG:HH11	1.75	0.51
1:A:43:ASP:OD2	1:A:395:LYS:HE3	2.11	0.51
1:A:228:PHE:HE1	1:A:359:MET:HG3	1.75	0.51
1:B:78:GLU:H	1:B:78:GLU:CD	2.14	0.51
1:A:264:ASN:ND2	1:B:68:HIS:ND1	2.58	0.51
1:A:402:THR:O	1:A:406:GLU:HG3	2.12	0.50
1:B:22:ALA:HA	1:B:25:ARG:NH1	2.25	0.50
1:A:258:LLP:OP4	1:A:258:LLP:H4'2	2.11	0.50
1:B:183:PHE:HA	1:B:216:PHE:O	2.12	0.49
1:B:63:ASN:HD22	1:B:64:SER:N	2.11	0.49
1:A:393:THR:O	1:A:397:LEU:HB2	2.12	0.49
1:A:63:ASN:C	1:A:63:ASN:HD22	2.16	0.48
1:A:372:TYR:HB2	1:A:411:ILE:CD1	2.43	0.48
1:A:333:MET:HE2	1:A:392:LEU:CB	2.44	0.47
1:A:17:VAL:O	1:A:21:ILE:HG12	2.14	0.47
1:B:63:ASN:HD22	1:B:65:SER:H	1.64	0.46
1:A:333:MET:CE	1:A:392:LEU:HB3	2.45	0.46
1:B:140:TRP:CZ3	1:B:142:ASN:HB3	2.51	0.46
1:B:382:LEU:HA	1:B:383:PRO:HD3	1.82	0.45
1:B:338:ARG:HD3	1:B:342:GLU:CD	2.36	0.45
1:A:106:LEU:HD11	1:B:106:LEU:HD11	1.99	0.45
1:A:68:HIS:O	1:B:263:TYR:HB2	2.17	0.45
1:A:368:LYS:HG3	1:A:411:ILE:CG2	2.47	0.45
1:A:333:MET:CE	1:A:397:LEU:HD22	2.46	0.45
1:B:334:ARG:NH1	1:B:389:MET:HE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:VAL:HG22	1:B:302:GLY:HA3	1.99	0.44
1:A:267:VAL:HG22	1:A:302:GLY:HA3	1.99	0.44
1:B:373:LEU:HD23	1:B:377:LYS:HG3	2.00	0.44
1:A:194:ASN:HA	1:A:195:PRO:HA	1.81	0.44
1:A:135:VAL:O	1:A:157:SER:HA	2.17	0.44
1:B:52:VAL:O	1:B:56:VAL:HG23	2.19	0.43
1:B:24:PHE:CE1	1:B:32:LYS:HG2	2.54	0.43
1:B:27:ASP:HB3	1:B:32:LYS:CD	2.38	0.43
1:A:222:ASP:OD2	1:A:258:LLP:N1	2.52	0.43
1:A:24:PHE:HD1	1:A:380:TYR:CD1	2.37	0.43
1:A:85:ARG:HD2	1:A:85:ARG:HH11	1.69	0.43
1:A:27:ASP:OD1	1:A:28:PRO:HD2	2.19	0.42
1:A:377:LYS:HG3	1:A:403:SER:HB3	2.01	0.42
1:B:50:LEU:HA	1:B:51:PRO:HD3	1.89	0.42
1:B:140:TRP:CH2	1:B:142:ASN:HB3	2.54	0.42
1:B:377:LYS:HD3	1:B:403:SER:HB3	2.02	0.42
1:A:12:ALA:HB1	1:B:289:LYS:HD2	2.02	0.42
2:A:436:HOH:O	1:B:258:LLP:H4'1	2.18	0.42
1:B:194:ASN:HA	1:B:195:PRO:HA	1.84	0.42
1:A:338:ARG:HH11	1:A:354:THR:CG2	2.27	0.41
1:B:182:GLU:HG3	2:B:495:HOH:O	2.21	0.41
1:B:235:LYS:HD3	1:B:235:LYS:C	2.40	0.41
1:A:140:TRP:CH2	1:A:142:ASN:HB3	2.56	0.41
1:A:366:ASN:OD1	1:A:369:GLN:HG3	2.20	0.41
1:A:369:GLN:NE2	1:A:412:GLN:OE1	2.54	0.41
1:A:54:ARG:HD2	2:A:424:HOH:O	2.21	0.41
1:B:258:LLP:OP4	1:B:258:LLP:H4'2	2.21	0.41
1:A:377:LYS:O	1:A:378:HIS:HB2	2.21	0.40
1:A:366:ASN:HB2	1:A:367:PRO:CD	2.50	0.40
1:A:117:GLU:OE1	1:A:121:ARG:NH2	2.55	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	409/412 (99%)	396 (97%)	12 (3%)	1 (0%)	52	32
1	B	410/412 (100%)	400 (98%)	10 (2%)	0	100	100
All	All	819/824 (99%)	796 (97%)	22 (3%)	1 (0%)	56	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	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	351/351 (100%)	332 (95%)	19 (5%)	27	6
1	B	352/351 (100%)	323 (92%)	29 (8%)	14	2
All	All	703/702 (100%)	655 (93%)	48 (7%)	20	3

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	19	LYS
1	A	63	ASN
1	A	90	ASP
1	A	121	ARG
1	A	166	ARG
1	A	173	PHE
1	A	220	PHE
1	A	264	ASN
1	A	293	VAL
1	A	298	PRO
1	A	314	GLU

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Mol	Chain	Res	Type
1	A	329	ARG
1	A	344	LEU
1	A	351	ASN
1	A	354	THR
1	A	362	PHE
1	A	395	LYS
1	A	408	VAL
1	B	15	VAL
1	B	16	LEU
1	B	17	VAL
1	B	25	ARG
1	B	35	LEU
1	B	54	ARG
1	B	63	ASN
1	B	78	GLU
1	B	85	ARG
1	B	95	LEU
1	B	99	ARG
1	B	163	THR
1	B	165	LYS
1	B	171	GLN
1	B	173	PHE
1	B	195	PRO
1	B	220	PHE
1	B	235	LYS
1	B	264	ASN
1	B	275	LYS
1	B	281	LEU
1	B	293	VAL
1	B	308	ARG
1	B	337	LEU
1	B	338	ARG
1	B	354	THR
1	B	362	PHE
1	B	368	LYS
1	B	397	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	171	GLN

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Mol	Chain	Res	Type
1	A	264	ASN
1	A	288	GLN
1	A	301	GLN
1	A	405	HIS
1	B	63	ASN
1	B	124	ASN
1	B	171	GLN
1	B	264	ASN
1	B	288	GLN
1	B	301	GLN
1	B	317	HIS
1	B	405	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	#$|Z| > 2$
1	LLP	A	258	1	23,24,25	1.43	3 (13%)	28,32,34	2.04	12 (42%)
1	LLP	B	258	1	23,24,25	1.20	2 (8%)	28,32,34	1.98	8 (28%)

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
1	LLP	A	258	1	-	0/15/17/19	0/1/1/1
1	LLP	B	258	1	-	0/15/17/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	LLP	C4-C5	-4.30	1.36	1.42
1	B	258	LLP	C4-C5	-3.02	1.37	1.42
1	A	258	LLP	O3-C3	-2.76	1.30	1.37
1	B	258	LLP	O3-C3	-2.49	1.31	1.37
1	A	258	LLP	CB-CA	2.51	1.56	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	LLP	C3-C4-C4'	-4.16	114.77	120.16
1	B	258	LLP	C5-C6-N1	-3.20	118.31	123.86
1	A	258	LLP	C5-C6-N1	-2.97	118.71	123.86
1	B	258	LLP	C3-C4-C4'	-2.59	116.81	120.16
1	A	258	LLP	C5'-C5-C6	-2.55	114.45	119.28
1	A	258	LLP	O-C-CA	-2.45	119.11	125.49
1	B	258	LLP	O-C-CA	-2.10	120.01	125.49
1	B	258	LLP	CE-NZ-C4'	2.08	124.98	118.97
1	A	258	LLP	C5'-C5-C4	2.30	125.34	121.47
1	A	258	LLP	CE-NZ-C4'	2.41	125.92	118.97
1	A	258	LLP	C5-C4-C4'	2.45	125.04	121.52
1	A	258	LLP	O3-C3-C2	2.55	122.09	117.66
1	A	258	LLP	C6-N1-C2	2.56	124.51	119.28
1	A	258	LLP	C3-C4-C5	2.76	120.17	118.11
1	B	258	LLP	C6-N1-C2	2.89	125.17	119.28
1	B	258	LLP	C2'-C2-C3	3.28	125.00	121.04
1	A	258	LLP	C2'-C2-C3	3.32	125.04	121.04
1	B	258	LLP	C3-C4-C5	4.05	121.14	118.11
1	A	258	LLP	OP4-C5'-C5	4.10	115.77	108.99
1	B	258	LLP	OP4-C5'-C5	5.31	117.77	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	258	LLP	2	0
1	B	258	LLP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	411/412 (99%)	0.05	37 (9%)	12	13	6, 18, 71, 135	0
1	B	411/412 (99%)	-0.36	5 (1%)	81	87	6, 15, 46, 106	0
All	All	822/824 (99%)	-0.16	42 (5%)	32	36	6, 17, 62, 135	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	412	GLN	7.4
1	A	1	ALA	6.9
1	B	1	ALA	6.8
1	A	2	PRO	5.2
1	A	21	ILE	4.9
1	A	20	LEU	4.7
1	A	24	PHE	4.1
1	A	33	VAL	4.0
1	A	408	VAL	3.9
1	A	411	ILE	3.8
1	A	379	ILE	3.7
1	A	22	ALA	3.7
1	A	375	ASN	3.7
1	A	18	PHE	3.6
1	A	372	TYR	3.6
1	A	376	GLN	3.6
1	A	380	TYR	3.5
1	A	404	ILE	3.4
1	A	28	PRO	3.4
1	A	27	ASP	3.3
1	A	17	VAL	3.3
1	A	25	ARG	3.3
1	A	399	TYR	3.1
1	A	373	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	374	ILE	2.9
1	A	378	HIS	2.9
1	A	16	LEU	2.8
1	A	29	ASP	2.8
1	B	292[A]	ARG	2.8
1	B	18	PHE	2.7
1	A	30	PRO	2.6
1	A	368	LYS	2.5
1	A	407	ALA	2.5
1	A	366	ASN	2.5
1	B	2	PRO	2.5
1	A	23	ASP	2.3
1	A	381	LEU	2.3
1	B	412	GLN	2.3
1	A	19	LYS	2.2
1	A	400	VAL	2.2
1	A	397	LEU	2.2
1	A	402	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
1	LLP	B	258	24/25	0.94	0.11	-	5,9,14,24	0
1	LLP	A	258	24/25	0.93	0.12	-	9,12,19,28	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.