Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 10:29 PM EDT

PDB ID	:	4FFX
Title	:	Structural and Biochemical Characterization of Human Adenylosuccinate Lyase (ADSL) and the R303C ADSL Deficiency Associated Mutation
Authors	:	Deaton, M.K.; Ray, S.P.; Capodagli, G.C.; Calkins, L.A.F.; Sawle, L.; Ghosh, K.; Patterson, D.; Pegan, S.D.
Deposited on	:	2012-06-01
Resolution	:	2.70 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 (i) 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 (1)) were used in the production of this report:

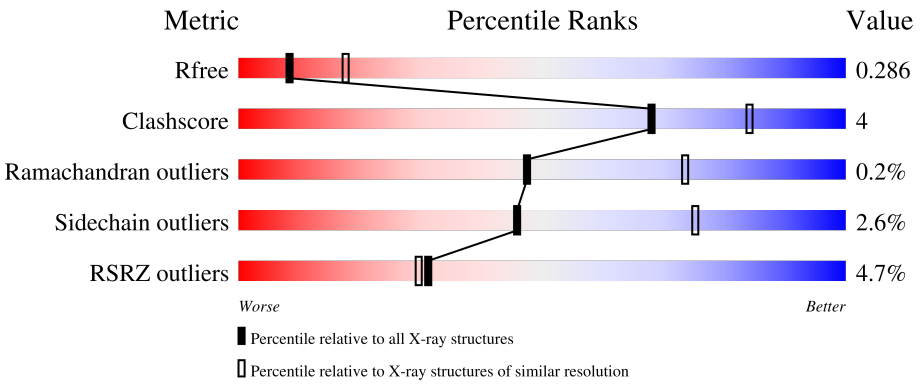
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	487	6%, 84%, 8%, • 6%
1	B	487	3%, 85%, 8%, 6%
1	C	487	5%, 80%, 12%, • 7%
1	D	487	4%, 80%, 13%, 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14819 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 Adenylosuccinate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	457	3662	2306	653	678	25	0	2	0
1	B	456	3661	2306	652	678	25	0	2	0
1	C	451	3619	2282	644	667	26	0	3	0
1	D	456	3663	2310	649	679	25	0	4	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P30566
A	-1	SER	-	expression tag	UNP P30566
A	0	HIS	-	expression tag	UNP P30566
A	63	ARG	GLN	conflict	UNP P30566
B	-2	GLY	-	expression tag	UNP P30566
B	-1	SER	-	expression tag	UNP P30566
B	0	HIS	-	expression tag	UNP P30566
B	63	ARG	GLN	conflict	UNP P30566
C	-2	GLY	-	expression tag	UNP P30566
C	-1	SER	-	expression tag	UNP P30566
C	0	HIS	-	expression tag	UNP P30566
C	63	ARG	GLN	conflict	UNP P30566
D	-2	GLY	-	expression tag	UNP P30566
D	-1	SER	-	expression tag	UNP P30566
D	0	HIS	-	expression tag	UNP P30566
D	63	ARG	GLN	conflict	UNP P30566

- Molecule 2 is water.

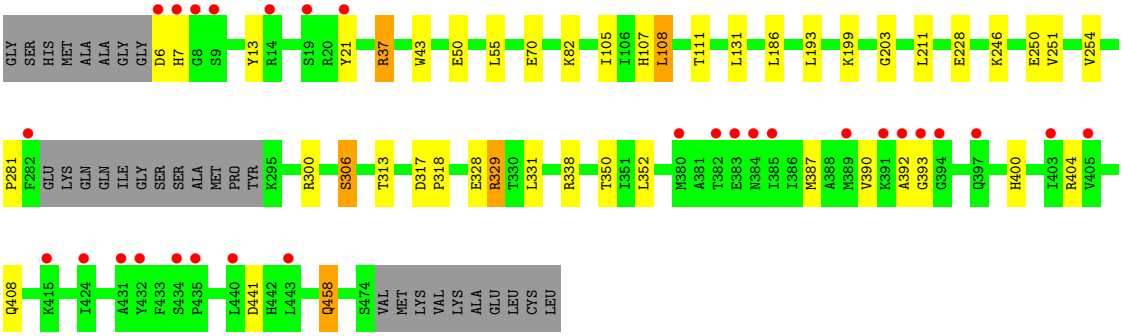
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	67	67	67	0	0
			Total	O		
2	B	45	45	45	0	0
			Total	O		
2	C	38	38	38	0	0
			Total	O		
2	D	64	64	64	0	0

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.

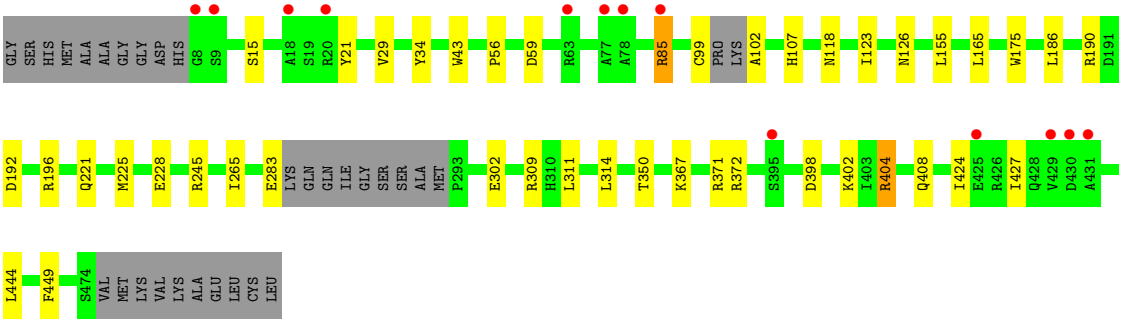
• Molecule 1: Adenylosuccinate lyase

Chain A:



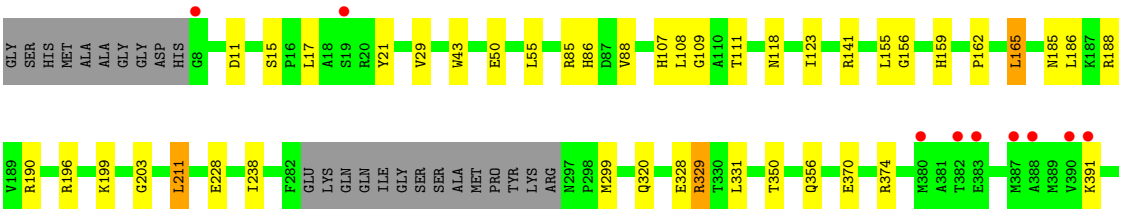
• Molecule 1: Adenylosuccinate lyase

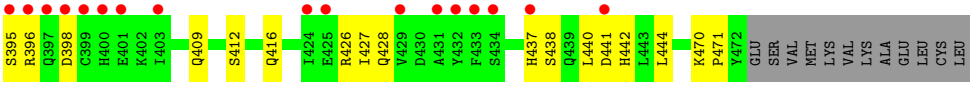
Chain B:



• Molecule 1: Adenylosuccinate lyase

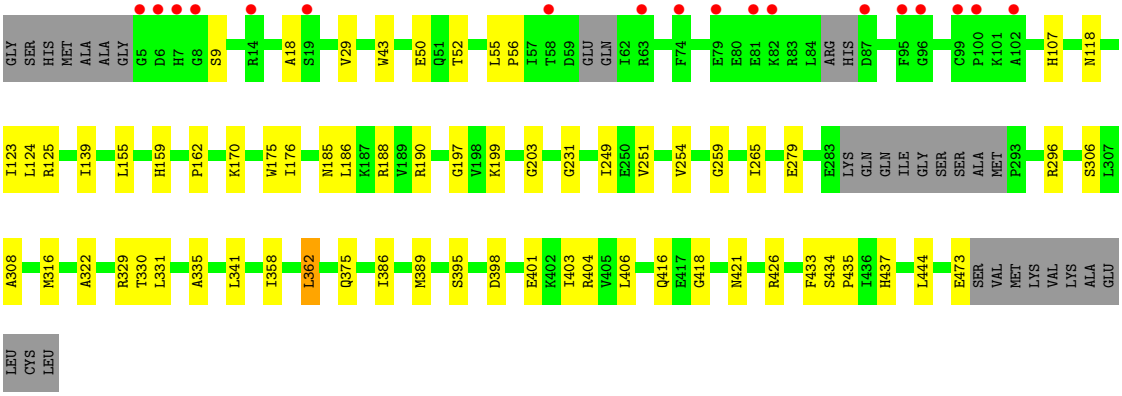
Chain C:





- Molecule 1: Adenylosuccinate lyase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.92Å 105.15Å 214.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 48.75 – 2.70	Depositor EDS
% Data completeness (in resolution range)	86.8 (50.00-2.70) 86.9 (48.75-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.46 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.243 , 0.292 0.239 , 0.286	Depositor DCC
R_{free} test set	2457 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 32.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	14819	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.33	0/3735	0.47	0/5042
1	B	0.33	0/3730	0.47	0/5033
1	C	0.33	0/3691	0.47	0/4983
1	D	0.33	0/3738	0.47	0/5043
All	All	0.33	0/14894	0.47	0/20101

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	3662	0	3681	30	0
1	B	3661	0	3676	25	0
1	C	3619	0	3646	37	0
1	D	3663	0	3681	35	0
2	A	67	0	0	1	0
2	B	45	0	0	0	0
2	C	38	0	0	1	0
2	D	64	0	0	0	0
All	All	14819	0	14684	112	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 4.

All (112) 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:404:ARG:O	1:B:404:ARG:HG3	1.70	0.90
1:C:440:LEU:HB2	1:C:441:ASP:HA	1.56	0.87
1:A:43:TRP:HE1	1:A:107:HIS:HD2	1.27	0.80
1:A:458[B]:GLN:HE21	1:A:458[B]:GLN:HA	1.45	0.78
1:B:15:SER:HB2	1:C:15:SER:HB2	1.67	0.75
1:A:6:ASP:HB2	1:D:9:SER:HB3	1.72	0.72
1:A:43:TRP:HE1	1:A:107:HIS:CD2	2.08	0.72
1:A:328:GLU:O	1:A:329:ARG:HB2	1.93	0.69
1:C:43:TRP:HE1	1:C:107:HIS:CD2	2.12	0.67
1:A:458[B]:GLN:HE21	1:A:458[B]:GLN:CA	2.08	0.66
1:C:43:TRP:HE1	1:C:107:HIS:HD2	1.44	0.65
1:C:165:LEU:H	1:C:165:LEU:HD23	1.61	0.64
1:C:109:GLY:HA3	1:C:211:LEU:HD12	1.80	0.64
1:C:328:GLU:O	1:C:329:ARG:HB2	1.98	0.64
1:A:6:ASP:N	1:D:9:SER:HG	1.95	0.63
1:D:43:TRP:HE1	1:D:107:HIS:CD2	2.18	0.62
1:B:29:VAL:HG12	1:B:123:ILE:HG23	1.80	0.61
1:C:440:LEU:CB	1:C:441:ASP:HA	2.27	0.59
1:C:395:SER:HB3	1:C:398:ASP:HB2	1.86	0.58
1:A:306:SER:HB3	1:D:335:ALA:HB3	1.87	0.57
1:C:111:THR:HG22	2:C:513:HOH:O	2.04	0.57
1:B:85:ARG:NH2	1:C:299[A]:MET:SD	2.78	0.57
1:A:108:LEU:HD12	1:A:211:LEU:HD11	1.87	0.56
1:C:108:LEU:HG	1:C:211:LEU:HD11	1.89	0.55
1:C:185:ASN:HD22	1:C:188[A]:ARG:HH12	1.53	0.55
1:B:43:TRP:HE1	1:B:107:HIS:CD2	2.24	0.55
1:A:458[B]:GLN:HA	1:A:458[B]:GLN:NE2	2.20	0.55
1:A:50:GLU:HB3	1:A:55:LEU:HD12	1.89	0.54
1:C:155:LEU:HD21	1:C:162:PRO:HB3	1.91	0.53
1:D:279:GLU:OE1	1:D:296:ARG:HD3	2.07	0.53
1:A:387:MET:O	1:A:390:VAL:HG22	2.09	0.52
1:D:50:GLU:HB3	1:D:55:LEU:HD12	1.90	0.52
1:C:440:LEU:HA	1:C:442:HIS:H	1.74	0.52
1:A:6:ASP:HB2	1:D:9:SER:CB	2.39	0.51
1:A:199:LYS:HB3	1:A:203:GLY:HA2	1.92	0.51
1:D:125:ARG:HH12	1:D:231:GLY:C	2.13	0.51
1:A:7:HIS:H	1:A:7:HIS:CD2	2.28	0.51
1:C:441:ASP:HB2	1:C:444:LEU:HB2	1.92	0.51
1:D:118:ASN:HD21	1:D:197:GLY:H	1.59	0.50
1:C:470:LYS:HB3	1:C:471:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:VAL:O	1:A:254:VAL:HG22	2.13	0.49
1:A:392:ALA:N	1:A:393:GLY:HA2	2.27	0.49
1:B:398:ASP:O	1:B:402:LYS:HG2	2.13	0.49
1:B:311:LEU:HA	1:B:314:LEU:HD12	1.95	0.48
1:A:246:LYS:O	1:A:250:GLU:HG2	2.14	0.48
1:B:371:ARG:HD2	1:D:418:GLY:O	2.14	0.48
1:C:141:ARG:NH2	1:C:356:GLN:HG2	2.28	0.48
1:A:111:THR:HG22	2:A:520:HOH:O	2.13	0.47
1:B:21:TYR:HB3	1:B:350:THR:HG21	1.96	0.47
1:D:185:ASN:HD22	1:D:188[A]:ARG:HH12	1.63	0.47
1:A:21:TYR:HB3	1:A:350:THR:HG21	1.97	0.47
1:B:309:ARG:HD3	1:C:320:GLN:HB2	1.96	0.46
1:C:412:SER:HA	1:C:416:GLN:HG2	1.96	0.46
1:A:313:THR:HG23	1:D:316:MET:HB2	1.98	0.46
1:B:427:ILE:HG22	1:B:427:ILE:O	2.15	0.46
1:C:156:GLY:H	1:C:165:LEU:HA	1.80	0.46
1:C:185:ASN:ND2	1:C:188[A]:ARG:HH12	2.12	0.46
1:D:175:TRP:HB3	1:D:265:ILE:HG12	1.98	0.46
1:A:400:HIS:O	1:A:404:ARG:HB2	2.16	0.46
1:B:404:ARG:O	1:B:404:ARG:CG	2.54	0.46
1:C:199:LYS:HB3	1:C:203:GLY:HA2	1.98	0.46
1:C:370:GLU:HB3	1:C:374:ARG:NH2	2.30	0.46
1:D:358:ILE:O	1:D:362:LEU:HD13	2.16	0.46
1:B:367:LYS:HG3	1:D:416:GLN:O	2.16	0.46
1:C:118:ASN:ND2	1:C:196:ARG:HB3	2.32	0.45
1:C:50:GLU:HB3	1:C:55:LEU:HD12	1.99	0.45
1:D:406:LEU:HD22	1:D:426:ARG:HB3	1.99	0.45
1:B:175:TRP:HB3	1:B:265:ILE:HG12	1.99	0.45
1:D:199:LYS:HB3	1:D:203:GLY:HA2	1.99	0.44
1:A:131:LEU:HD22	1:A:352:LEU:HD12	2.00	0.44
1:A:281:PRO:O	1:A:300:ARG:NH2	2.50	0.44
1:C:238:ILE:HD12	1:D:170:LYS:HE3	1.99	0.44
1:B:118:ASN:HD21	1:B:196:ARG:HB3	1.82	0.44
1:B:118:ASN:ND2	1:B:196:ARG:HB3	2.32	0.44
1:B:165:LEU:HD12	1:B:449:PHE:HB2	1.99	0.44
1:C:86:HIS:HE1	1:C:88:VAL:HB	1.83	0.44
1:D:375:GLN:HE22	1:D:421:ASN:H	1.66	0.44
1:B:302:GLU:OE1	1:D:159:HIS:HD2	2.00	0.43
1:C:159:HIS:HD2	1:D:331:LEU:HG	1.82	0.43
1:B:221:GLN:O	1:B:225:MET:HG3	2.18	0.43
1:C:17:LEU:HA	1:C:21:TYR:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ASN:HD21	1:C:196:ARG:HB3	1.83	0.43
1:B:99:CYS:HB3	1:B:102:ALA:HB3	1.99	0.43
1:A:37:ARG:HD3	1:A:70:GLU:OE1	2.18	0.43
1:C:29:VAL:HG12	1:C:123:ILE:HG23	2.01	0.43
1:A:21:TYR:HB3	1:A:350:THR:CG2	2.49	0.43
1:B:424:ILE:HD12	1:B:444:LEU:HD11	2.01	0.43
1:D:389:MET:HE1	1:D:433:PHE:HA	2.00	0.43
1:D:29:VAL:HG12	1:D:123:ILE:HG23	2.00	0.42
1:B:155:LEU:HD22	1:B:372:ARG:HG2	2.00	0.42
1:D:249:ILE:HD11	1:D:322:ALA:HB3	2.01	0.42
1:D:434:SER:HA	1:D:437:HIS:ND1	2.35	0.42
1:C:428:GLN:HG3	1:C:437:HIS:HE1	1.84	0.42
1:C:21:TYR:HB3	1:C:350:THR:HG21	2.02	0.42
1:D:124:LEU:HD21	1:D:341:LEU:HD22	2.02	0.42
1:D:43:TRP:HE1	1:D:107:HIS:HD2	1.66	0.41
1:D:259:GLY:O	1:D:308:ALA:HB1	2.20	0.41
1:B:283:GLU:HG3	1:C:85:ARG:HH22	1.86	0.41
1:A:13:TYR:HD2	1:D:18:ALA:HB2	1.86	0.41
1:D:386:ILE:HD11	1:D:403:ILE:HG21	2.03	0.41
1:B:34:TYR:OH	1:B:126:ASN:ND2	2.54	0.41
1:D:139:ILE:HG23	1:D:176:ILE:HG23	2.03	0.41
1:C:409:GLN:HB2	1:C:426:ARG:NH1	2.36	0.41
1:D:251:VAL:O	1:D:254:VAL:HG22	2.21	0.41
1:D:155:LEU:HD21	1:D:162:PRO:HB3	2.03	0.40
1:C:437:HIS:HA	1:C:438:SER:HA	1.74	0.40
1:A:317:ASP:CB	1:A:318:PRO:HD3	2.51	0.40
1:B:245:ARG:HD3	1:B:245:ARG:HA	1.93	0.40
1:D:389:MET:HE1	1:D:435:PRO:HD2	2.04	0.40
1:D:395:SER:HB3	1:D:398:ASP:HB2	2.03	0.40
1:A:105:ILE:HA	1:A:108:LEU:HD23	2.02	0.40
1:A:458[B]:GLN:CA	1:A:458[B]:GLN:NE2	2.80	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	455/487 (93%)	443 (97%)	11 (2%)	1 (0%)	47	73
1	B	452/487 (93%)	433 (96%)	18 (4%)	1 (0%)	47	73
1	C	450/487 (92%)	434 (96%)	15 (3%)	1 (0%)	47	73
1	D	452/487 (93%)	438 (97%)	13 (3%)	1 (0%)	47	73
All	All	1809/1948 (93%)	1748 (97%)	57 (3%)	4 (0%)	47	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ARG
1	C	329	ARG
1	B	56	PRO
1	D	56	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	403/423 (95%)	390 (97%)	13 (3%)	39	68
1	B	402/423 (95%)	394 (98%)	8 (2%)	55	81
1	C	398/423 (94%)	388 (98%)	10 (2%)	47	76
1	D	403/423 (95%)	392 (97%)	11 (3%)	44	74
All	All	1606/1692 (95%)	1564 (97%)	42 (3%)	46	75

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	82	LYS
1	A	108	LEU
1	A	186	LEU

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Mol	Chain	Res	Type
1	A	193	LEU
1	A	228	GLU
1	A	306	SER
1	A	331	LEU
1	A	338	ARG
1	A	408	GLN
1	A	441	ASP
1	A	458[A]	GLN
1	A	458[B]	GLN
1	B	59	ASP
1	B	85	ARG
1	B	186	LEU
1	B	190	ARG
1	B	192	ASP
1	B	228	GLU
1	B	404	ARG
1	B	408	GLN
1	C	11	ASP
1	C	165	LEU
1	C	186	LEU
1	C	190	ARG
1	C	211	LEU
1	C	228	GLU
1	C	331	LEU
1	C	391	LYS
1	C	396	ARG
1	C	427	ILE
1	D	52	THR
1	D	186	LEU
1	D	190	ARG
1	D	306	SER
1	D	329	ARG
1	D	330	THR
1	D	362	LEU
1	D	401	GLU
1	D	404	ARG
1	D	444	LEU
1	D	473	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	68	ASN
1	A	107	HIS
1	A	118	ASN
1	A	126	ASN
1	A	164	GLN
1	A	185	ASN
1	A	408	GLN
1	A	439	GLN
1	B	41	GLN
1	B	107	HIS
1	B	118	ASN
1	B	126	ASN
1	B	177	GLN
1	B	185	ASN
1	C	41	GLN
1	C	107	HIS
1	C	118	ASN
1	C	126	ASN
1	C	177	GLN
1	C	185	ASN
1	C	357	ASN
1	C	437	HIS
1	C	458	GLN
1	D	107	HIS
1	D	118	ASN
1	D	126	ASN
1	D	159	HIS
1	D	164	GLN
1	D	177	GLN
1	D	185	ASN
1	D	356	GLN
1	D	375	GLN
1	D	384	ASN
1	D	408	GLN
1	D	416	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)

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	457/487 (93%)	0.17	29 (6%)	20	19	6, 23, 64, 70	0
1	B	456/487 (93%)	0.13	13 (2%)	51	52	4, 22, 54, 57	0
1	C	451/487 (92%)	0.15	26 (5%)	23	22	6, 23, 69, 71	0
1	D	456/487 (93%)	0.13	18 (3%)	39	38	6, 24, 57, 64	0
All	All	1820/1948 (93%)	0.14	86 (4%)	31	30	4, 23, 62, 71	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	6	ASP	4.9
1	C	8	GLY	4.5
1	D	5	GLY	4.3
1	D	96	GLY	4.1
1	A	392	ALA	4.0
1	A	6	ASP	3.9
1	A	7	HIS	3.9
1	B	18	ALA	3.6
1	C	431	ALA	3.6
1	C	403	ILE	3.6
1	B	8	GLY	3.6
1	B	9	SER	3.5
1	C	383	GLU	3.5
1	D	99	CYS	3.4
1	A	434	SER	3.4
1	B	431	ALA	3.4
1	B	78	ALA	3.4
1	C	401	GLU	3.4
1	D	7	HIS	3.3
1	C	441	ASP	3.3
1	C	424	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	425	GLU	3.2
1	C	437	HIS	3.2
1	B	429	VAL	3.2
1	A	391	LYS	3.2
1	A	19	SER	3.1
1	C	19	SER	3.0
1	A	9	SER	3.0
1	C	429	VAL	3.0
1	C	432	TYR	2.9
1	D	8	GLY	2.9
1	D	79	GLU	2.9
1	D	19[A]	SER	2.9
1	C	433	PHE	2.9
1	A	389	MET	2.9
1	D	63	ARG	2.8
1	B	395	SER	2.8
1	A	415	LYS	2.8
1	D	58	THR	2.8
1	A	431	ALA	2.8
1	B	77	ALA	2.8
1	D	82	LYS	2.8
1	A	394	GLY	2.7
1	C	382	THR	2.6
1	A	14	ARG	2.6
1	B	85	ARG	2.6
1	A	405	VAL	2.6
1	A	424	ILE	2.6
1	A	383	GLU	2.6
1	C	400	HIS	2.6
1	C	390	VAL	2.6
1	D	100	PRO	2.5
1	C	397	GLN	2.5
1	D	81	GLU	2.5
1	A	432	TYR	2.5
1	C	387	MET	2.5
1	C	395	SER	2.5
1	B	63	ARG	2.4
1	D	14	ARG	2.4
1	C	391	LYS	2.4
1	A	21	TYR	2.4
1	A	443	LEU	2.4
1	A	393	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	397	GLN	2.3
1	A	282	PHE	2.3
1	A	440	LEU	2.3
1	A	384	ASN	2.3
1	A	385	ILE	2.3
1	C	388	ALA	2.3
1	D	74	PHE	2.3
1	D	87	ASP	2.3
1	A	382	THR	2.2
1	C	396	ARG	2.2
1	A	8	GLY	2.2
1	A	403	ILE	2.2
1	D	95	PHE	2.2
1	B	20	ARG	2.2
1	B	425	GLU	2.2
1	B	430	ASP	2.2
1	D	102	ALA	2.2
1	C	380	MET	2.2
1	C	399	CYS	2.2
1	C	434	SER	2.1
1	A	380	MET	2.0
1	C	398	ASP	2.0
1	A	435	PRO	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.