



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:22 PM GMT

PDB ID : 4A2Q
Title : Structure of duck RIG-I tandem CARDS and helicase domain
Authors : Kowalinski, E.; Lunardi, T.; Mccarthy, A.A.; Cusack, S.
Deposited on : 2011-09-28
Resolution : 3.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

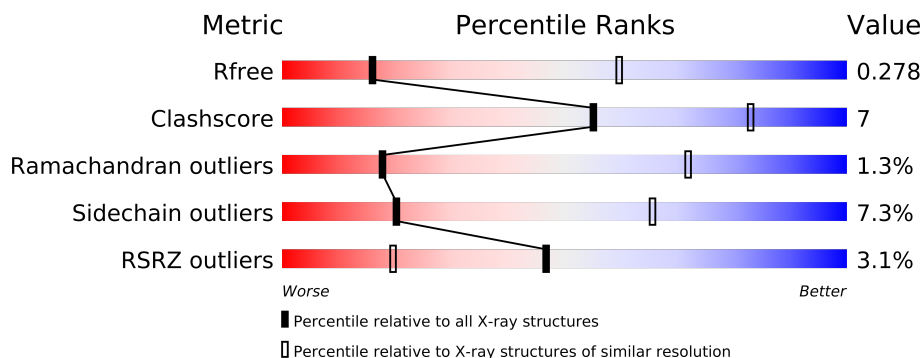
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.40 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}	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	797	
1	B	797	
1	D	797	
1	E	797	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21661 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RETINOIC ACID INDUCIBLE PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	0	0
			5425	3430	933	1028	34			
1	B	675	Total	C	N	O	S	0	0	0
			5436	3436	937	1029	34			
1	D	671	Total	C	N	O	S	0	0	0
			5404	3417	930	1024	33			
1	E	670	Total	C	N	O	S	0	0	0
			5396	3413	929	1021	33			

There are 12 discrepancies between the modelled and reference sequences:

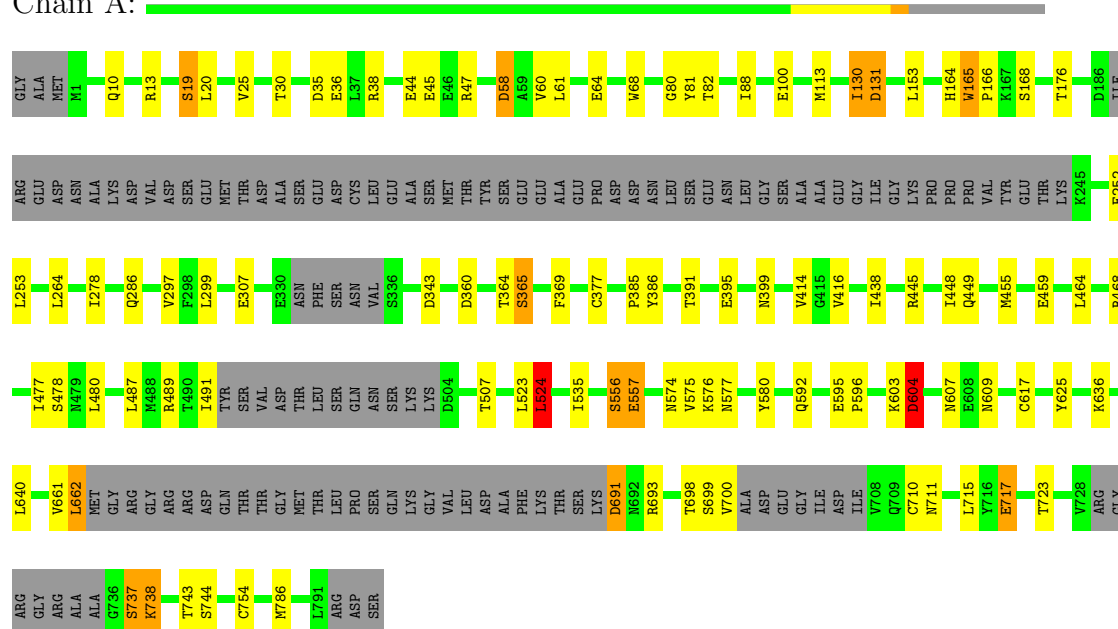
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP D3TI84
A	-1	ALA	-	EXPRESSION TAG	UNP D3TI84
A	0	MET	-	EXPRESSION TAG	UNP D3TI84
B	-2	GLY	-	EXPRESSION TAG	UNP D3TI84
B	-1	ALA	-	EXPRESSION TAG	UNP D3TI84
B	0	MET	-	EXPRESSION TAG	UNP D3TI84
D	-2	GLY	-	EXPRESSION TAG	UNP D3TI84
D	-1	ALA	-	EXPRESSION TAG	UNP D3TI84
D	0	MET	-	EXPRESSION TAG	UNP D3TI84
E	-2	GLY	-	EXPRESSION TAG	UNP D3TI84
E	-1	ALA	-	EXPRESSION TAG	UNP D3TI84
E	0	MET	-	EXPRESSION TAG	UNP D3TI84

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.

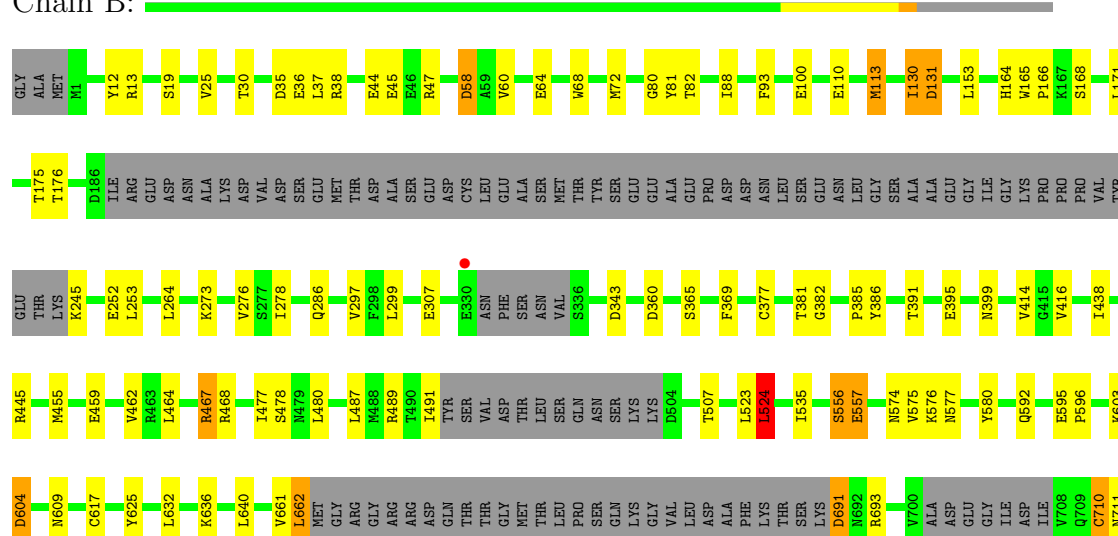
• Molecule 1: RETINOIC ACID INDUCIBLE PROTEIN I

Chain A:



• Molecule 1: RETINOIC ACID INDUCIBLE PROTEIN I

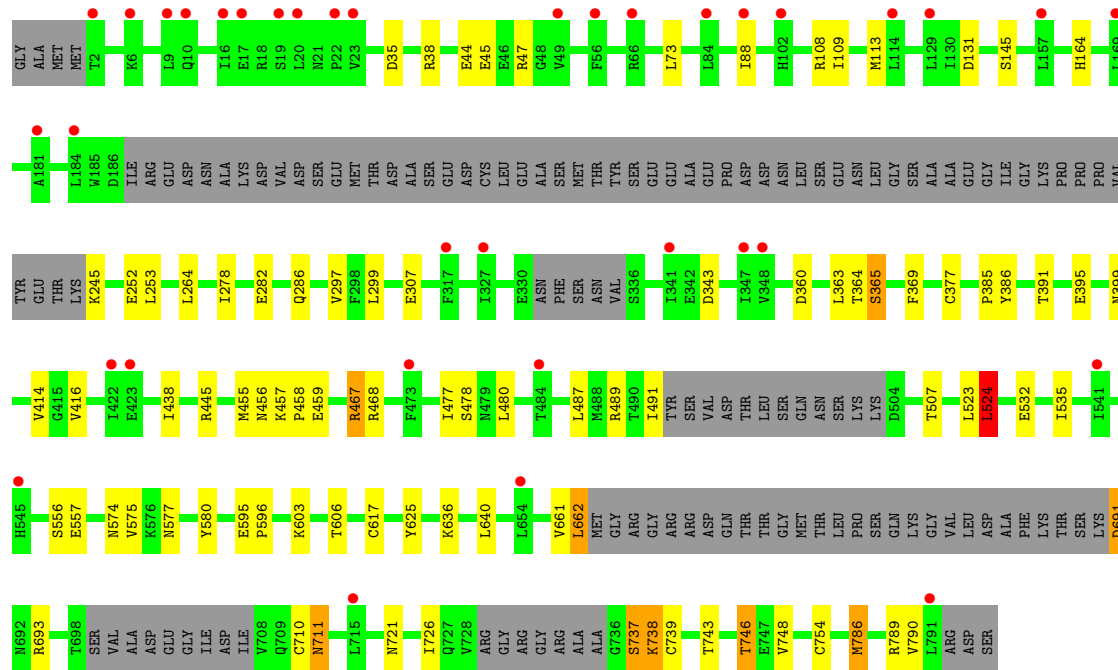
Chain B:





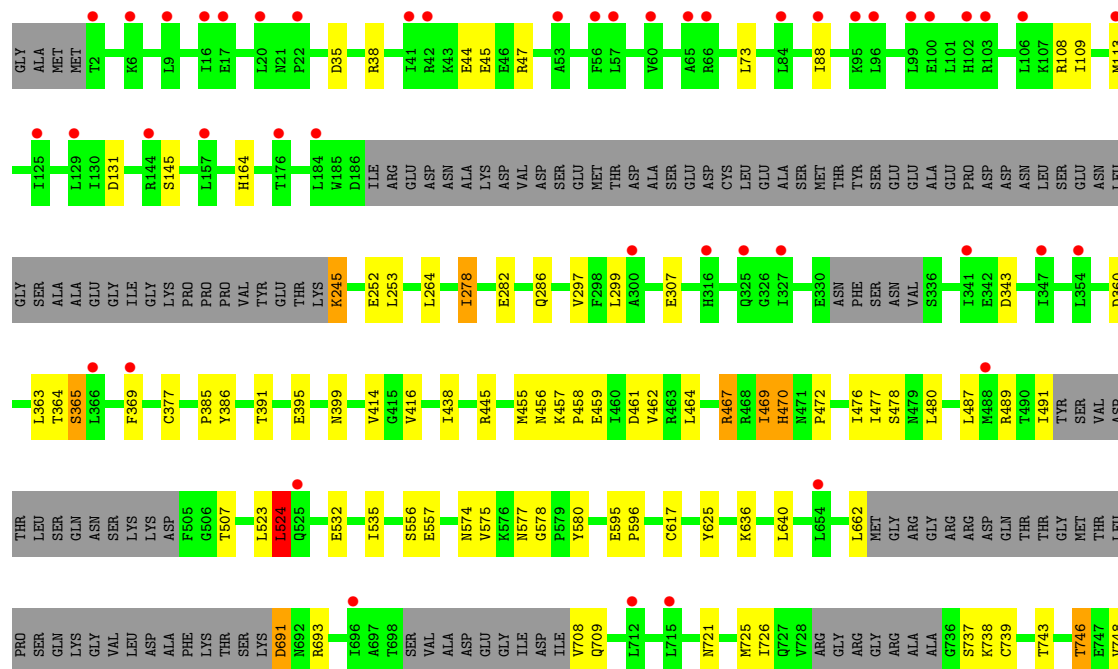
• Molecule 1: RETINOIC ACID INDUCIBLE PROTEIN I

Chain D:



• Molecule 1: RETINOIC ACID INDUCIBLE PROTEIN I

Chain E:





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	314.97Å 134.49Å 102.26Å 90.00° 92.17° 90.00°	Depositor
Resolution (Å)	157.37 – 3.40 48.06 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.6 (157.37-3.40) 97.6 (48.06-3.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.239 , 0.276 0.243 , 0.278	Depositor DCC
R_{free} test set	2904 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	97.2	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 93.7	EDS
Estimated twinning fraction	0.054 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	6 of 57367 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21661	wwPDB-VP
Average B, all atoms (Å ²)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.49	1/5510 (0.0%)	0.63	0/7434
1	B	0.49	0/5521	0.64	0/7448
1	D	0.42	0/5489	0.55	0/7406
1	E	0.43	0/5481	0.56	0/7395
All	All	0.46	1/22001 (0.0%)	0.60	0/29683

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	TRP	CD2-CE2	5.06	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5425	0	0	38	0
1	B	5436	0	0	46	0
1	D	5404	0	0	33	0
1	E	5396	0	0	33	0
All	All	21661	0	0	146	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (146) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:13:ARG:NH2	1:A:58:ASP:OD1	2.15	0.79
1:B:13:ARG:NH2	1:B:58:ASP:OD1	2.18	0.77
1:A:592:GLN:OE1	1:B:592:GLN:OE1	2.10	0.68
1:A:44:GLU:OE2	1:A:47:ARG:NH1	2.32	0.62
1:D:108:ARG:NH2	1:D:532:GLU:OE2	2.32	0.62
1:B:44:GLU:OE2	1:B:47:ARG:NH1	2.34	0.61
1:A:595:GLU:OE1	1:B:576:LYS:NZ	2.34	0.60
1:B:717:GLU:OE2	1:B:744:SER:OG	2.18	0.60
1:E:416:VAL:CG1	1:E:416:VAL:O	2.50	0.59
1:A:165:TRP:O	1:A:166:PRO:C	2.40	0.59
1:B:165:TRP:O	1:B:166:PRO:C	2.38	0.58
1:E:469:ILE:O	1:E:470:HIS:CG	2.56	0.58
1:D:416:VAL:CG1	1:D:416:VAL:O	2.51	0.58
1:A:576:LYS:NZ	1:B:595:GLU:OE1	2.37	0.58
1:A:416:VAL:CG1	1:A:416:VAL:O	2.53	0.57
1:E:108:ARG:NH2	1:E:532:GLU:OE2	2.37	0.57
1:A:603:LYS:O	1:A:604:ASP:C	2.42	0.56
1:A:35:ASP:OD1	1:A:38:ARG:NH2	2.38	0.55
1:A:698:THR:O	1:A:700:VAL:N	2.40	0.55
1:B:130:ILE:O	1:B:131:ASP:C	2.45	0.54
1:B:477:ILE:O	1:B:480:LEU:N	2.40	0.54
1:B:35:ASP:OD1	1:B:38:ARG:NH2	2.41	0.54
1:B:416:VAL:O	1:B:416:VAL:CG1	2.55	0.54
1:D:710:CYS:SG	1:D:711:ASN:N	2.82	0.52
1:A:130:ILE:O	1:A:131:ASP:C	2.47	0.52
1:B:557:GLU:O	1:B:609:ASN:ND2	2.43	0.51
1:B:297:VAL:CG1	1:B:299:LEU:CD2	2.88	0.51
1:A:477:ILE:O	1:A:480:LEU:N	2.44	0.51
1:A:80:GLY:O	1:A:82:THR:N	2.45	0.50
1:D:726:ILE:CD1	1:D:739:CYS:SG	3.00	0.49
1:A:297:VAL:CG1	1:A:299:LEU:CD2	2.90	0.49
1:D:603:LYS:NZ	1:E:578:GLY:O	2.46	0.49
1:D:477:ILE:O	1:D:480:LEU:N	2.46	0.48
1:B:595:GLU:N	1:B:596:PRO:CD	2.76	0.48
1:A:557:GLU:O	1:A:609:ASN:ND2	2.46	0.48
1:E:691:ASP:OD2	1:E:691:ASP:N	2.47	0.48
1:A:60:VAL:CG1	1:A:68:TRP:CZ3	2.96	0.48
1:B:603:LYS:O	1:B:604:ASP:C	2.52	0.47
1:D:746:THR:O	1:D:748:VAL:N	2.46	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:523:LEU:O	1:B:524:LEU:C	2.53	0.47
1:A:487:LEU:O	1:A:491:ILE:CD1	2.63	0.47
1:D:574:ASN:O	1:D:577:ASN:N	2.48	0.47
1:D:297:VAL:CG1	1:D:299:LEU:CD2	2.93	0.47
1:A:523:LEU:O	1:A:524:LEU:C	2.53	0.47
1:B:395:GLU:O	1:B:399:ASN:N	2.48	0.47
1:B:722:VAL:O	1:B:723:THR:C	2.53	0.47
1:B:477:ILE:O	1:B:478:SER:C	2.52	0.47
1:A:691:ASP:OD2	1:A:691:ASP:N	2.48	0.47
1:E:746:THR:O	1:E:748:VAL:N	2.48	0.46
1:B:252:GLU:OE2	1:B:445:ARG:N	2.48	0.46
1:B:80:GLY:O	1:B:82:THR:N	2.47	0.46
1:E:297:VAL:CG1	1:E:299:LEU:CD2	2.93	0.46
1:E:395:GLU:O	1:E:399:ASN:N	2.49	0.46
1:E:477:ILE:O	1:E:480:LEU:N	2.48	0.46
1:D:691:ASP:N	1:D:691:ASP:OD2	2.48	0.46
1:D:44:GLU:OE2	1:D:47:ARG:NH1	2.48	0.46
1:B:691:ASP:N	1:B:691:ASP:OD2	2.49	0.46
1:D:35:ASP:OD1	1:D:38:ARG:NH2	2.49	0.46
1:E:708:VAL:CG1	1:E:709:GLN:N	2.79	0.46
1:E:523:LEU:O	1:E:524:LEU:C	2.55	0.46
1:B:60:VAL:CG1	1:B:68:TRP:CZ3	2.99	0.46
1:A:595:GLU:N	1:A:596:PRO:CD	2.78	0.45
1:E:297:VAL:CG2	1:E:369:PHE:CE2	3.00	0.45
1:A:395:GLU:O	1:A:399:ASN:N	2.49	0.45
1:D:109:ILE:O	1:D:109:ILE:CG2	2.64	0.45
1:B:165:TRP:O	1:B:168:SER:N	2.50	0.45
1:B:467:ARG:NH1	1:B:557:GLU:OE2	2.50	0.45
1:D:790:VAL:CG1	1:D:790:VAL:O	2.64	0.45
1:B:574:ASN:O	1:B:575:VAL:C	2.55	0.45
1:B:574:ASN:O	1:B:577:ASN:N	2.50	0.45
1:B:790:VAL:O	1:B:790:VAL:CG1	2.65	0.45
1:E:109:ILE:CG2	1:E:109:ILE:O	2.64	0.45
1:A:264:LEU:CD1	1:A:377:CYS:SG	3.04	0.45
1:A:574:ASN:O	1:A:577:ASN:N	2.50	0.45
1:D:395:GLU:O	1:D:399:ASN:N	2.50	0.45
1:E:574:ASN:O	1:E:577:ASN:N	2.49	0.45
1:E:245:LYS:NZ	1:E:282:GLU:OE1	2.51	0.44
1:E:44:GLU:OE2	1:E:47:ARG:NH1	2.50	0.44
1:E:35:ASP:OD1	1:E:38:ARG:NH2	2.50	0.44
1:D:297:VAL:CG2	1:D:369:PHE:CE2	3.01	0.44
1:D:264:LEU:CD1	1:D:377:CYS:SG	3.06	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:385:PRO:O	1:B:386:TYR:C	2.54	0.44
1:B:737:SER:O	1:B:738:LYS:CB	2.66	0.44
1:E:252:GLU:OE2	1:E:445:ARG:N	2.51	0.43
1:A:252:GLU:OE2	1:A:445:ARG:N	2.51	0.43
1:E:595:GLU:N	1:E:596:PRO:CD	2.81	0.43
1:A:385:PRO:O	1:A:386:TYR:C	2.56	0.43
1:E:469:ILE:O	1:E:470:HIS:CB	2.65	0.43
1:A:477:ILE:O	1:A:478:SER:C	2.57	0.43
1:D:73:LEU:CD2	1:D:88:ILE:CD1	2.97	0.43
1:D:523:LEU:O	1:D:524:LEU:C	2.56	0.43
1:B:297:VAL:CG2	1:B:369:PHE:CE2	3.02	0.43
1:E:264:LEU:CD1	1:E:377:CYS:SG	3.06	0.43
1:A:297:VAL:CG2	1:A:369:PHE:CE2	3.02	0.43
1:E:487:LEU:O	1:E:491:ILE:CD1	2.67	0.43
1:B:747:GLU:O	1:B:751:ASN:CB	2.67	0.43
1:B:110:GLU:O	1:B:113:MET:N	2.51	0.43
1:B:468:ARG:NH1	1:B:556:SER:O	2.52	0.43
1:A:737:SER:O	1:A:738:LYS:CB	2.67	0.43
1:D:245:LYS:NZ	1:D:282:GLU:OE1	2.51	0.43
1:D:468:ARG:NH1	1:D:606:THR:O	2.52	0.42
1:D:595:GLU:N	1:D:596:PRO:CD	2.82	0.42
1:A:468:ARG:NH1	1:A:556:SER:O	2.52	0.42
1:D:456:ASN:O	1:D:458:PRO:N	2.53	0.42
1:E:726:ILE:CD1	1:E:739:CYS:SG	3.07	0.42
1:D:574:ASN:O	1:D:575:VAL:C	2.56	0.42
1:E:477:ILE:O	1:E:478:SER:C	2.57	0.42
1:B:632:LEU:CB	1:B:710:CYS:SG	3.08	0.42
1:A:661:VAL:CG1	1:A:662:LEU:N	2.83	0.42
1:B:60:VAL:CG1	1:B:72:MET:CE	2.97	0.42
1:A:10:GLN:OE1	1:A:61:LEU:CD1	2.68	0.42
1:A:165:TRP:O	1:A:168:SER:N	2.52	0.42
1:E:472:PRO:O	1:E:476:ILE:CD1	2.67	0.42
1:D:786:MET:SD	1:D:789:ARG:NH1	2.93	0.42
1:D:737:SER:O	1:D:738:LYS:CB	2.68	0.42
1:A:574:ASN:O	1:A:575:VAL:C	2.58	0.41
1:D:385:PRO:O	1:D:386:TYR:C	2.58	0.41
1:B:273:LYS:O	1:B:276:VAL:N	2.53	0.41
1:E:364:THR:O	1:E:365:SER:OG	2.38	0.41
1:B:661:VAL:CG1	1:B:662:LEU:N	2.83	0.41
1:A:364:THR:O	1:A:365:SER:OG	2.38	0.41
1:E:574:ASN:O	1:E:575:VAL:C	2.58	0.41
1:A:448:ILE:O	1:A:449:GLN:C	2.59	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:264:LEU:CD1	1:B:377:CYS:SG	3.08	0.41
1:E:73:LEU:CD2	1:E:88:ILE:CD1	2.98	0.41
1:E:297:VAL:CG2	1:E:369:PHE:CD2	3.04	0.41
1:B:171:LEU:O	1:B:175:THR:OG1	2.38	0.41
1:D:487:LEU:O	1:D:491:ILE:CD1	2.68	0.41
1:B:12:TYR:CG	1:B:93:PHE:CE2	3.09	0.41
1:D:252:GLU:OE2	1:D:445:ARG:N	2.53	0.41
1:B:722:VAL:O	1:B:725:MET:N	2.54	0.41
1:A:19:SER:OG	1:A:20:LEU:N	2.54	0.41
1:D:477:ILE:O	1:D:478:SER:C	2.58	0.41
1:B:487:LEU:O	1:B:491:ILE:CD1	2.68	0.41
1:D:297:VAL:CG2	1:D:369:PHE:CD2	3.04	0.41
1:B:153:LEU:C	1:B:153:LEU:CD2	2.88	0.41
1:E:278:ILE:C	1:E:278:ILE:CD1	2.89	0.41
1:E:790:VAL:CG1	1:E:790:VAL:O	2.68	0.41
1:D:364:THR:O	1:D:365:SER:OG	2.39	0.41
1:D:661:VAL:CG1	1:D:662:LEU:N	2.84	0.41
1:B:381:THR:CG2	1:B:382:GLY:N	2.84	0.40
1:A:717:GLU:OE2	1:A:744:SER:OG	2.39	0.40
1:B:37:LEU:O	1:B:38:ARG:C	2.59	0.40
1:A:153:LEU:CD2	1:A:153:LEU:C	2.89	0.40
1:E:456:ASN:O	1:E:458:PRO:N	2.54	0.40
1:E:385:PRO:O	1:E:386:TYR:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	660/797 (83%)	586 (89%)	64 (10%)	10 (2%)	15 68
1	B	661/797 (83%)	587 (89%)	65 (10%)	9 (1%)	16 69
1	D	657/797 (82%)	590 (90%)	60 (9%)	7 (1%)	21 76
1	E	656/797 (82%)	589 (90%)	59 (9%)	8 (1%)	19 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2634/3188 (83%)	2352 (89%)	248 (9%)	34 (1%)	18	72

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	LEU
1	A	699	SER
1	B	524	LEU
1	D	524	LEU
1	D	746	THR
1	E	470	HIS
1	E	524	LEU
1	A	81	TYR
1	A	131	ASP
1	A	604	ASP
1	A	717	GLU
1	A	738	LYS
1	B	81	TYR
1	B	131	ASP
1	B	717	GLU
1	B	738	LYS
1	D	738	LYS
1	E	738	LYS
1	E	746	THR
1	A	365	SER
1	A	723	THR
1	B	365	SER
1	B	723	THR
1	B	747	GLU
1	D	365	SER
1	E	365	SER
1	A	607	ASN
1	D	131	ASP
1	E	131	ASP
1	E	467	ARG
1	B	711	ASN
1	D	467	ARG
1	D	457	LYS
1	E	457	LYS

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	603/704 (86%)	556 (92%)	47 (8%)	18	62
1	B	604/704 (86%)	554 (92%)	50 (8%)	16	59
1	D	600/704 (85%)	563 (94%)	37 (6%)	26	72
1	E	599/704 (85%)	557 (93%)	42 (7%)	21	68
All	All	2406/2816 (85%)	2230 (93%)	176 (7%)	20	65

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	25	VAL
1	A	30	THR
1	A	36	GLU
1	A	45	GLU
1	A	58	ASP
1	A	64	GLU
1	A	88	ILE
1	A	100	GLU
1	A	113	MET
1	A	130	ILE
1	A	164	HIS
1	A	176	THR
1	A	253	LEU
1	A	278	ILE
1	A	286	GLN
1	A	307	GLU
1	A	343	ASP
1	A	360	ASP
1	A	391	THR
1	A	414	VAL
1	A	438	ILE
1	A	455	MET
1	A	459	GLU
1	A	464	LEU
1	A	489	ARG

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Mol	Chain	Res	Type
1	A	507	THR
1	A	524	LEU
1	A	535	ILE
1	A	556	SER
1	A	557	GLU
1	A	580	TYR
1	A	604	ASP
1	A	617	CYS
1	A	625	TYR
1	A	636	LYS
1	A	640	LEU
1	A	662	LEU
1	A	691	ASP
1	A	693	ARG
1	A	710	CYS
1	A	711	ASN
1	A	715	LEU
1	A	737	SER
1	A	743	THR
1	A	754	CYS
1	A	786	MET
1	B	19	SER
1	B	25	VAL
1	B	30	THR
1	B	36	GLU
1	B	45	GLU
1	B	58	ASP
1	B	64	GLU
1	B	88	ILE
1	B	100	GLU
1	B	113	MET
1	B	130	ILE
1	B	164	HIS
1	B	176	THR
1	B	245	LYS
1	B	253	LEU
1	B	278	ILE
1	B	286	GLN
1	B	307	GLU
1	B	343	ASP
1	B	360	ASP
1	B	391	THR

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Mol	Chain	Res	Type
1	B	414	VAL
1	B	438	ILE
1	B	455	MET
1	B	459	GLU
1	B	462	VAL
1	B	464	LEU
1	B	467	ARG
1	B	489	ARG
1	B	507	THR
1	B	524	LEU
1	B	535	ILE
1	B	556	SER
1	B	557	GLU
1	B	580	TYR
1	B	604	ASP
1	B	617	CYS
1	B	625	TYR
1	B	636	LYS
1	B	640	LEU
1	B	662	LEU
1	B	691	ASP
1	B	693	ARG
1	B	710	CYS
1	B	715	LEU
1	B	721	ASN
1	B	737	SER
1	B	743	THR
1	B	754	CYS
1	B	786	MET
1	D	45	GLU
1	D	113	MET
1	D	145	SER
1	D	164	HIS
1	D	253	LEU
1	D	278	ILE
1	D	286	GLN
1	D	307	GLU
1	D	343	ASP
1	D	360	ASP
1	D	363	LEU
1	D	391	THR
1	D	414	VAL

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Mol	Chain	Res	Type
1	D	438	ILE
1	D	455	MET
1	D	459	GLU
1	D	467	ARG
1	D	489	ARG
1	D	507	THR
1	D	524	LEU
1	D	535	ILE
1	D	556	SER
1	D	557	GLU
1	D	580	TYR
1	D	617	CYS
1	D	625	TYR
1	D	636	LYS
1	D	640	LEU
1	D	662	LEU
1	D	691	ASP
1	D	693	ARG
1	D	711	ASN
1	D	721	ASN
1	D	737	SER
1	D	743	THR
1	D	754	CYS
1	D	786	MET
1	E	45	GLU
1	E	113	MET
1	E	145	SER
1	E	164	HIS
1	E	245	LYS
1	E	253	LEU
1	E	278	ILE
1	E	286	GLN
1	E	307	GLU
1	E	343	ASP
1	E	360	ASP
1	E	363	LEU
1	E	391	THR
1	E	414	VAL
1	E	438	ILE
1	E	455	MET
1	E	459	GLU
1	E	461	ASP

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Mol	Chain	Res	Type
1	E	462	VAL
1	E	464	LEU
1	E	467	ARG
1	E	469	ILE
1	E	489	ARG
1	E	507	THR
1	E	524	LEU
1	E	535	ILE
1	E	556	SER
1	E	557	GLU
1	E	580	TYR
1	E	617	CYS
1	E	625	TYR
1	E	636	LYS
1	E	640	LEU
1	E	662	LEU
1	E	691	ASP
1	E	693	ARG
1	E	721	ASN
1	E	725	MET
1	E	737	SER
1	E	743	THR
1	E	754	CYS
1	E	786	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	674/797 (84%)	0.08	0 100 100	52, 97, 153, 210	0
1	B	675/797 (84%)	0.09	1 (0%) 93 82	53, 96, 155, 220	0
1	D	671/797 (84%)	0.47	36 (5%) 25 9	109, 192, 271, 320	0
1	E	670/797 (84%)	0.57	47 (7%) 16 6	104, 199, 293, 359	0
All	All	2690/3188 (84%)	0.30	84 (3%) 47 19	52, 145, 273, 359	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	17	GLU	8.2
1	E	56	PHE	6.4
1	E	60	VAL	6.3
1	D	16	ILE	5.0
1	E	53	ALA	4.8
1	E	16	ILE	4.5
1	D	56	PHE	4.3
1	E	17	GLU	4.3
1	E	157	LEU	4.3
1	D	102	HIS	4.2
1	E	9	LEU	4.2
1	E	57	LEU	4.1
1	E	96	LEU	4.1
1	E	42	ARG	4.0
1	E	327	ILE	3.7
1	E	325	GLN	3.6
1	D	423	GLU	3.5
1	E	696	ILE	3.4
1	D	20	LEU	3.4
1	D	88	ILE	3.4
1	E	20	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	327	ILE	3.3
1	D	341	ILE	3.2
1	E	341	ILE	3.2
1	E	102	HIS	3.2
1	E	88	ILE	3.1
1	D	129	LEU	3.0
1	D	22	PRO	2.9
1	D	2	THR	2.9
1	E	84	LEU	2.9
1	D	84	LEU	2.8
1	E	488	MET	2.8
1	E	750	GLU	2.8
1	D	422	ILE	2.8
1	D	10	GLN	2.8
1	D	157	LEU	2.7
1	D	6	LYS	2.7
1	E	366	LEU	2.6
1	E	316	HIS	2.6
1	E	100	GLU	2.6
1	E	715	LEU	2.6
1	E	103	ARG	2.5
1	E	712	LEU	2.5
1	D	9	LEU	2.5
1	E	129	LEU	2.5
1	E	184	LEU	2.5
1	D	347	ILE	2.4
1	E	113	MET	2.4
1	D	541	ILE	2.4
1	E	41	ILE	2.4
1	E	2	THR	2.4
1	E	369	PHE	2.4
1	E	347	ILE	2.4
1	D	473	PHE	2.4
1	D	19	SER	2.3
1	E	300	ALA	2.3
1	E	22	PRO	2.3
1	D	715	LEU	2.3
1	E	66	ARG	2.3
1	D	791	LEU	2.3
1	D	545	HIS	2.3
1	D	317	PHE	2.3
1	E	106	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	65	ALA	2.2
1	D	654	LEU	2.2
1	E	6	LYS	2.2
1	D	181	ALA	2.2
1	B	330	GLU	2.2
1	D	23	VAL	2.2
1	D	114	LEU	2.2
1	D	184	LEU	2.1
1	E	654	LEU	2.1
1	E	525	GLN	2.1
1	D	169	LEU	2.1
1	E	99	LEU	2.1
1	E	144	ARG	2.1
1	E	95	LYS	2.1
1	E	176	THR	2.1
1	E	125	ILE	2.1
1	D	348	VAL	2.0
1	D	484	THR	2.0
1	E	354	LEU	2.0
1	D	49	VAL	2.0
1	D	66	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.