Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 04:08 PM EDT

PDB ID	:	6UEW
Title	:	Rubisco / CsoS2 N-peptide complex responsible for alpha-carboxysome cargo loading
Authors	:	Oltrogge, L.M.; Savage, D.F.
Deposited on	:	2019-09-23
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:

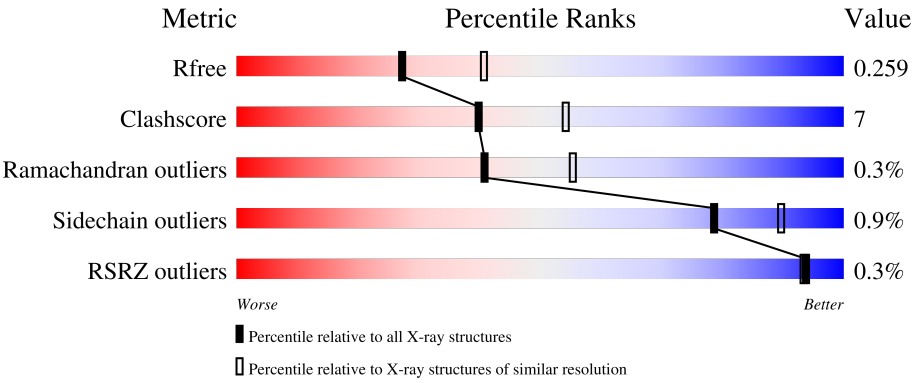
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	506	74% 16% 10%
1	C	506	% 74% 16% 10%
1	E	506	72% 17% • 11%
1	G	506	75% 14% • 10%
2	B	110	75% 19% 5%

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Mol	Chain	Length	Quality of chain
2	D	110	83% 14%
2	F	110	% 82% 13% 5%
2	H	110	78% 14% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18304 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 Ribulose bisphosphate carboxylase large chain, CsoS2 N-peptide fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3550	2248	631	655	16			
1	C	455	Total	C	N	O	S	0	0	0
			3565	2257	634	658	16			
1	E	450	Total	C	N	O	S	0	0	0
			3525	2234	625	650	16			
1	G	454	Total	C	N	O	S	0	0	0
			3553	2249	632	656	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP O85040
A	1	SER	-	cloning artifact	UNP O85040
A	474	SER	-	linker	UNP O85040
A	475	SER	-	linker	UNP O85040
C	0	MET	-	initiating methionine	UNP O85040
C	1	SER	-	cloning artifact	UNP O85040
C	474	SER	-	linker	UNP O85040
C	475	SER	-	linker	UNP O85040
E	0	MET	-	initiating methionine	UNP O85040
E	1	SER	-	cloning artifact	UNP O85040
E	474	SER	-	linker	UNP O85040
E	475	SER	-	linker	UNP O85040
G	0	MET	-	initiating methionine	UNP O85040
G	1	SER	-	cloning artifact	UNP O85040
G	474	SER	-	linker	UNP O85040
G	475	SER	-	linker	UNP O85040

- Molecule 2 is a protein called Ribulose bisphosphate carboxylase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			864	561	143	156	4			
2	D	106	Total	C	N	O	S	0	0	0
			876	568	145	158	5			
2	F	105	Total	C	N	O	S	0	0	0
			872	566	144	157	5			
2	H	101	Total	C	N	O	S	0	0	0
			831	541	136	149	5			

- Molecule 3 is water.

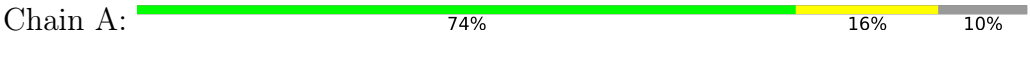
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total	O	0	0
			131	131		
3	B	41	Total	O	0	0
			41	41		
3	C	145	Total	O	0	0
			145	145		
3	D	42	Total	O	0	0
			42	42		
3	E	135	Total	O	0	0
			135	135		
3	F	33	Total	O	0	0
			33	33		
3	G	124	Total	O	0	0
			124	124		
3	H	17	Total	O	0	0
			17	17		

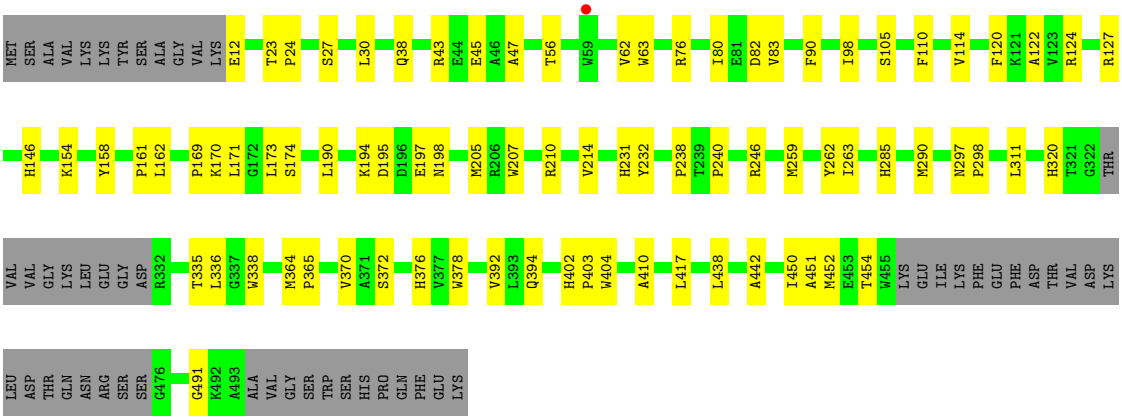
3 Residue-property plots (i)

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: Ribulose bisphosphate carboxylase large chain, CsoS2 N-peptide fusion

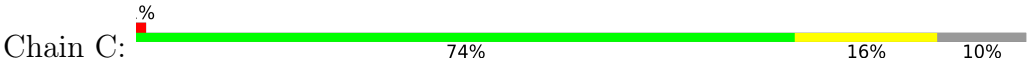
Chain A:

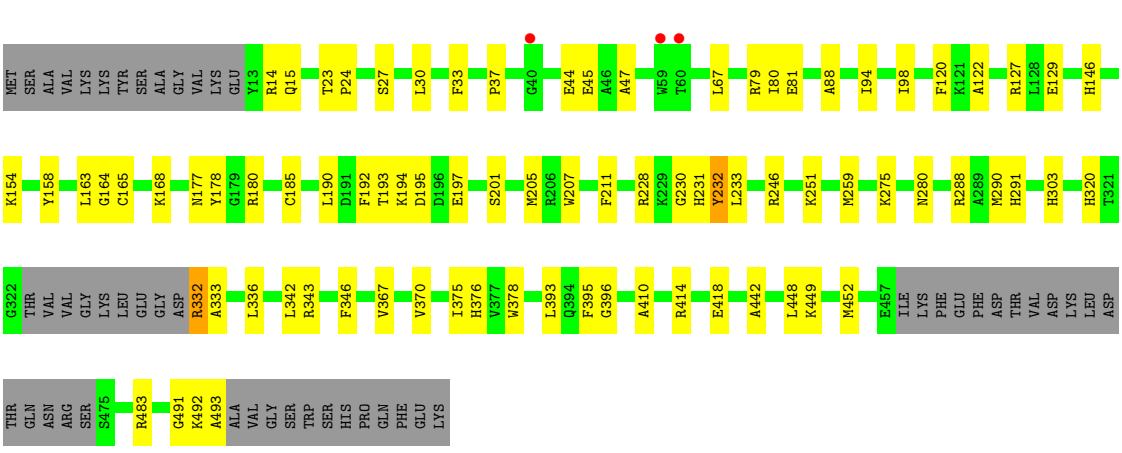




• Molecule 1: Ribulose bisphosphate carboxylase large chain, CsoS2 N-peptide fusion

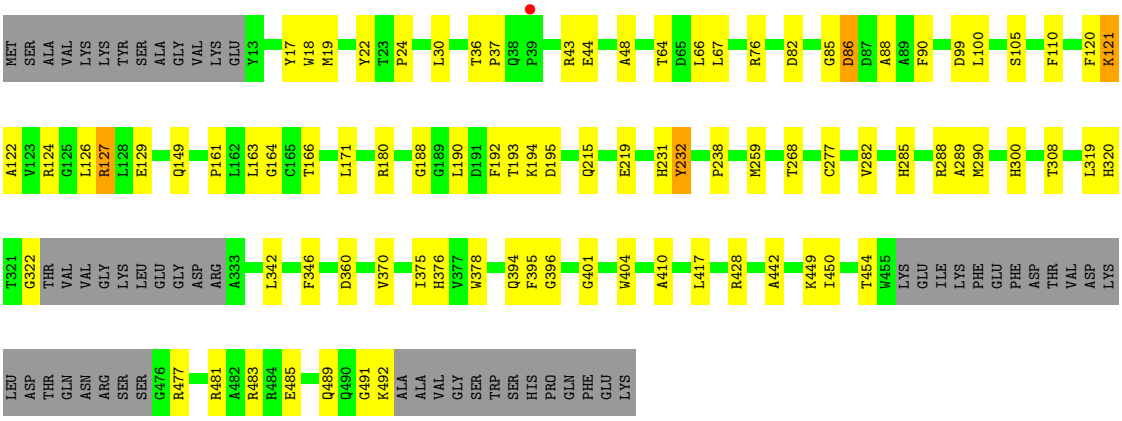
Chain C:





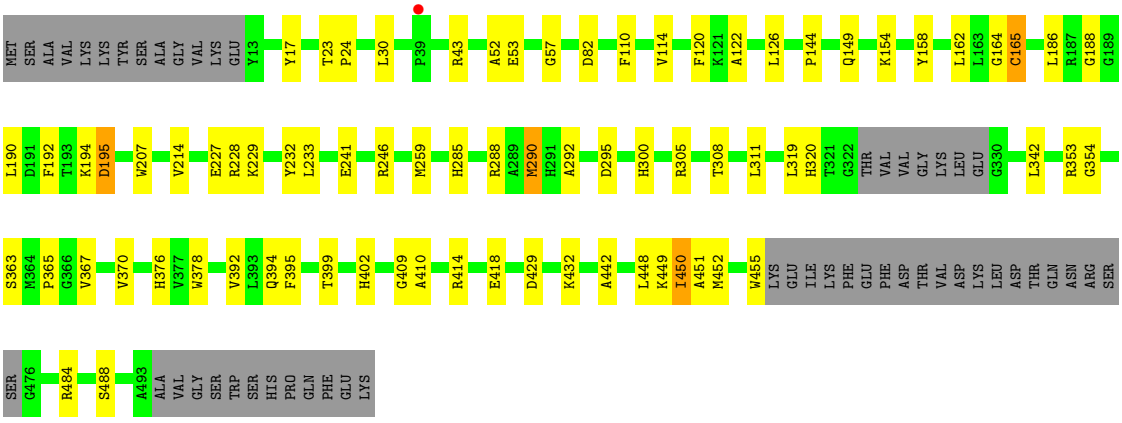
• Molecule 1: Ribulose bisphosphate carboxylase large chain, CsoS2 N-peptide fusion

Chain E:



• Molecule 1: Ribulose bisphosphate carboxylase large chain, CsoS2 N-peptide fusion

Chain G:



• Molecule 2: Ribulose bisphosphate carboxylase small chain

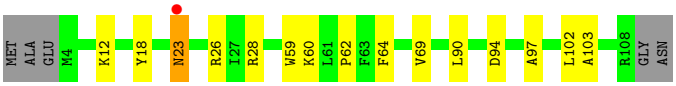
Chain B:

• Molecule 2: Ribulose bisphosphate carboxylase small chain

Chain D:

• Molecule 2: Ribulose bisphosphate carboxylase small chain

Chain F:



• Molecule 2: Ribulose bisphosphate carboxylase small chain

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	171.83Å 153.94Å 108.06Å 90.00° 124.70° 90.00°	Depositor
Resolution (Å)	104.08 – 2.40 104.08 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.9 (104.08-2.40) 85.8 (104.08-2.12)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.50 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.188 , 0.259 0.188 , 0.259	Depositor DCC
R_{free} test set	1429 reflections (1.13%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18304	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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

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	0.42	0/3638	0.56	0/4929
1	C	0.43	0/3653	0.57	1/4948 (0.0%)
1	E	0.43	0/3613	0.56	0/4896
1	G	0.43	0/3641	0.58	2/4933 (0.0%)
2	B	0.41	0/890	0.54	0/1209
2	D	0.46	0/902	0.56	0/1224
2	F	0.44	0/898	0.57	0/1219
2	H	0.38	0/855	0.51	0/1160
All	All	0.43	0/18090	0.56	3/24518 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	168	LYS	CD-CE-NZ	-5.25	99.64	111.70
1	G	450	ILE	CG1-CB-CG2	-5.21	99.94	111.40
1	G	195	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3550	0	3442	59	0
1	C	3565	0	3460	52	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3525	0	3418	61	0
1	G	3553	0	3443	59	0
2	B	864	0	830	12	0
2	D	876	0	842	10	0
2	F	872	0	839	10	0
2	H	831	0	802	13	1
3	A	131	0	0	2	0
3	B	41	0	0	0	0
3	C	145	0	0	3	0
3	D	42	0	0	2	0
3	E	135	0	0	3	0
3	F	33	0	0	2	0
3	G	124	0	0	6	1
3	H	17	0	0	1	0
All	All	18304	0	17076	253	2

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 (253) 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:C:127:ARG:NH2	1:C:303:HIS:HD2	1.57	1.02
1:A:170:LYS:NZ	3:A:601:HOH:O	1.97	0.97
1:C:127:ARG:NH2	1:C:303:HIS:CD2	2.34	0.96
1:C:228:ARG:NH1	3:C:601:HOH:O	2.01	0.93
1:G:450:ILE:HD12	1:G:451:ALA:N	1.86	0.91
1:C:177:ASN:OD1	1:C:180:ARG:NH2	2.09	0.85
2:F:28:ARG:HG3	2:F:69:VAL:HG11	1.63	0.81
1:C:127:ARG:HD3	1:C:129:GLU:OE2	1.81	0.80
1:E:232:TYR:HE2	1:E:394:GLN:HE22	1.30	0.78
1:G:442:ALA:HB1	1:G:449:LYS:HB2	1.70	0.73
1:G:190:LEU:HD11	1:G:399:THR:HG21	1.71	0.72
2:H:80:ARG:HH12	2:H:106:VAL:HG12	1.52	0.72
1:A:194:LYS:HG3	1:A:232:TYR:HD2	1.55	0.71
1:C:79:ARG:NH1	1:C:81:GLU:OE2	2.24	0.71
1:E:19:MET:HG2	1:E:22:TYR:HB2	1.73	0.70
1:E:404:TRP:O	3:E:601:HOH:O	2.09	0.70
1:A:105:SER:HB2	1:E:238:PRO:HG3	1.76	0.68
2:D:58:MET:HE3	1:E:180:ARG:HD2	1.75	0.67
1:E:64:THR:HA	1:E:67:LEU:HD23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HD13	1:E:100:LEU:HD22	1.77	0.67
1:G:402:HIS:NE2	1:G:450:ILE:HD11	2.10	0.66
1:A:56:THR:HG23	1:E:171:LEU:HD12	1.76	0.66
1:G:43:ARG:NH1	1:G:82:ASP:OD1	2.20	0.65
1:G:190:LEU:HG	1:G:410:ALA:HB1	1.78	0.65
1:A:376:HIS:CE1	1:A:378:TRP:HB2	2.32	0.65
1:A:290:MET:HE2	1:E:110:PHE:HE2	1.60	0.65
1:A:372:SER:HB3	1:A:394:GLN:HB2	1.77	0.64
1:E:194:LYS:HB2	1:E:232:TYR:CD2	2.33	0.64
1:C:201:SER:HB2	1:C:207:TRP:HB3	1.80	0.64
1:G:232:TYR:HB3	1:G:259:MET:HB2	1.80	0.64
1:G:241:GLU:OE1	1:G:241:GLU:N	2.30	0.64
2:H:85:THR:OG1	3:H:201:HOH:O	2.15	0.64
1:E:442:ALA:HB1	1:E:449:LYS:HB2	1.80	0.63
1:E:450:ILE:O	1:E:454:THR:HG23	1.98	0.63
2:F:26:ARG:N	3:F:201:HOH:O	2.25	0.63
2:F:23:ASN:OD1	3:F:201:HOH:O	2.16	0.62
1:A:154:LYS:NZ	3:A:605:HOH:O	2.33	0.62
1:A:232:TYR:HB3	1:A:259:MET:HB2	1.82	0.62
1:G:484:ARG:O	1:G:488:SER:OG	2.16	0.62
1:E:163:LEU:HB3	1:E:190:LEU:HD22	1.82	0.61
1:G:376:HIS:CE1	1:G:378:TRP:HB2	2.36	0.60
1:E:161:PRO:HD2	1:E:417:LEU:HD11	1.82	0.60
1:E:477:ARG:NH2	2:F:94:ASP:OD2	2.34	0.60
1:A:238:PRO:HG3	1:E:105:SER:HB2	1.82	0.60
1:G:311:LEU:HG	1:G:319:LEU:HD13	1.82	0.60
1:C:14:ARG:HD2	1:C:44:GLU:HB3	1.82	0.59
1:G:450:ILE:HD12	1:G:450:ILE:C	2.23	0.59
1:A:162:LEU:HB2	1:A:392:VAL:HG22	1.85	0.59
2:D:86:HIS:NE2	3:D:205:HOH:O	2.32	0.58
1:C:127:ARG:CZ	1:C:303:HIS:HD2	2.15	0.57
1:G:402:HIS:CE1	1:G:450:ILE:HD11	2.40	0.57
1:G:24:PRO:HB3	1:G:30:LEU:HD21	1.86	0.56
2:H:68:ASN:OD1	2:H:70:ASP:N	2.37	0.56
1:C:376:HIS:CE1	1:C:378:TRP:HB2	2.41	0.56
1:E:376:HIS:CE1	1:E:378:TRP:HB2	2.41	0.56
1:A:376:HIS:HE1	1:A:378:TRP:HB2	1.70	0.55
1:G:194:LYS:HG2	1:G:195:ASP:O	2.06	0.55
1:A:207:TRP:CD2	1:A:246:ARG:HG2	2.41	0.55
1:E:360:ASP:OD1	3:E:602:HOH:O	2.18	0.55
1:G:158:TYR:CD1	2:H:100:LEU:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LYS:HG3	1:A:232:TYR:CD2	2.41	0.55
1:G:228:ARG:NH2	3:G:606:HOH:O	2.37	0.55
2:B:6:ASP:OD1	2:B:8:LYS:NZ	2.40	0.54
1:E:194:LYS:HG3	1:E:195:ASP:O	2.08	0.54
1:G:402:HIS:HE2	1:G:450:ILE:HD11	1.72	0.53
1:G:120:PHE:CE2	1:G:122:ALA:HB3	2.44	0.53
1:A:262:TYR:CD1	1:A:311:LEU:HD23	2.44	0.53
1:E:215:GLN:O	1:E:219:GLU:HG3	2.09	0.53
2:B:12:LYS:HD2	2:B:18:TYR:CE1	2.44	0.53
1:C:120:PHE:CE1	1:C:122:ALA:HB3	2.44	0.53
1:G:342:LEU:HG	1:G:367:VAL:HB	1.91	0.53
2:H:31:ILE:HD11	2:H:72:VAL:HB	1.91	0.53
1:G:288:ARG:HD3	1:G:320:HIS:O	2.09	0.53
1:E:121:LYS:H	1:E:121:LYS:HE2	1.74	0.53
1:C:164:GLY:HA2	1:C:192:PHE:O	2.08	0.52
1:C:251:LYS:HD2	1:C:280:ASN:HB3	1.91	0.52
1:G:320:HIS:HA	1:G:370:VAL:HB	1.91	0.52
2:H:31:ILE:CD1	2:H:72:VAL:HB	2.39	0.52
1:A:110:PHE:HE2	1:E:290:MET:SD	2.33	0.52
1:G:414:ARG:O	1:G:418:GLU:HG3	2.08	0.52
1:C:158:TYR:CD1	2:D:100:LEU:HB2	2.45	0.52
2:D:13:TYR:HB3	2:D:105:VAL:HG21	1.89	0.52
1:C:375:ILE:HG13	1:C:395:PHE:CD2	2.44	0.52
1:C:442:ALA:HB1	1:C:449:LYS:HB2	1.90	0.52
1:A:43:ARG:NH1	1:A:82:ASP:OD1	2.28	0.52
1:C:165:CYS:HB2	1:C:190:LEU:HD13	1.92	0.52
1:G:162:LEU:HB2	1:G:392:VAL:HG22	1.92	0.52
1:G:188:GLY:HA3	1:G:410:ALA:HB3	1.93	0.51
1:C:185:CYS:HB3	1:C:190:LEU:HD12	1.92	0.51
1:A:297:ASN:HD22	1:A:298:PRO:HD2	1.76	0.51
1:A:120:PHE:CE2	1:A:122:ALA:HB3	2.45	0.51
1:C:127:ARG:HH22	1:C:303:HIS:CD2	2.24	0.51
1:A:161:PRO:HD2	1:A:417:LEU:HD11	1.93	0.50
1:G:149:GLN:HG2	2:H:97:ALA:O	2.11	0.50
1:C:320:HIS:HA	1:C:370:VAL:HB	1.93	0.50
1:G:429:ASP:HB3	1:G:432:LYS:NZ	2.27	0.50
1:C:33:PHE:HD2	1:C:94:ILE:HD12	1.76	0.50
1:G:126:LEU:O	1:G:300:HIS:HA	2.12	0.50
1:G:448:LEU:HG	1:G:452:MET:HE3	1.93	0.50
2:D:28:ARG:HG3	2:D:69:VAL:HG11	1.94	0.49
1:A:320:HIS:HA	1:A:370:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:ARG:HG3	1:E:127:ARG:HH11	1.77	0.49
2:H:31:ILE:HD11	2:H:72:VAL:CB	2.43	0.49
1:C:375:ILE:HG13	1:C:395:PHE:CE2	2.47	0.49
1:G:402:HIS:CD2	1:G:409:GLY:HA2	2.47	0.49
1:C:194:LYS:HG2	1:C:195:ASP:O	2.12	0.49
1:G:149:GLN:HB3	3:G:699:HOH:O	2.11	0.49
1:E:127:ARG:HH11	1:E:127:ARG:CG	2.25	0.48
1:A:450:ILE:O	1:A:454:THR:HG23	2.14	0.48
1:E:188:GLY:HA3	1:E:410:ALA:HB3	1.95	0.48
1:A:207:TRP:CE3	1:A:246:ARG:HG2	2.49	0.48
1:A:378:TRP:CZ2	1:A:452:MET:HG2	2.48	0.48
1:E:320:HIS:HA	1:E:370:VAL:HB	1.95	0.48
1:A:190:LEU:HG	1:A:410:ALA:HB1	1.94	0.48
2:B:56:TRP:CZ3	2:B:89:LYS:HB2	2.49	0.48
1:A:83:VAL:HG23	1:A:90:PHE:HA	1.95	0.48
1:G:305:ARG:NH2	1:G:354:GLY:HA3	2.28	0.48
1:A:12:GLU:HG3	1:A:45:GLU:OE1	2.14	0.47
1:C:194:LYS:HG3	1:C:232:TYR:HD2	1.78	0.47
1:E:259:MET:HA	1:E:285:HIS:O	2.14	0.47
1:G:214:VAL:HG11	1:G:233:LEU:HD21	1.96	0.47
1:G:429:ASP:HB3	1:G:432:LYS:HZ3	1.79	0.47
1:E:375:ILE:HG13	1:E:395:PHE:CE2	2.49	0.47
1:A:47:ALA:HB2	1:A:80:ILE:HD11	1.97	0.47
1:C:146:HIS:NE2	1:C:154:LYS:HE3	2.29	0.47
1:C:192:PHE:HA	1:C:230:GLY:O	2.14	0.47
2:F:90:LEU:O	2:F:103:ALA:HA	2.14	0.47
2:B:33:TYR:O	2:B:37:GLN:HG2	2.15	0.46
1:C:342:LEU:HG	1:C:367:VAL:HB	1.98	0.46
2:F:62:PRO:HB2	2:F:64:PHE:CZ	2.50	0.46
1:G:450:ILE:C	1:G:450:ILE:CD1	2.83	0.46
1:C:346:PHE:CD2	1:C:483:ARG:HD2	2.51	0.46
1:E:36:THR:O	1:E:124:ARG:N	2.46	0.46
1:A:438:LEU:O	1:A:452:MET:HE1	2.16	0.46
1:A:173:LEU:O	1:A:205:MET:HE2	2.15	0.46
1:G:165:CYS:HA	1:G:395:PHE:O	2.15	0.46
1:A:194:LYS:HG2	1:A:195:ASP:O	2.15	0.46
1:C:448:LEU:O	1:C:452:MET:HG3	2.15	0.46
1:E:18:TRP:CE2	1:E:44:GLU:HG2	2.50	0.46
1:E:193:THR:O	1:E:231:HIS:HA	2.16	0.46
1:C:232:TYR:HB3	1:C:259:MET:HB2	1.98	0.46
1:G:110:PHE:O	1:G:114:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:THR:O	1:C:491:GLY:HA3	2.15	0.45
1:C:197:GLU:OE2	3:C:602:HOH:O	2.21	0.45
1:A:205:MET:SD	1:A:210:ARG:HD3	2.56	0.45
1:C:190:LEU:HG	1:C:410:ALA:HB1	1.97	0.45
1:C:332:ARG:HG3	1:C:333:ALA:H	1.80	0.45
2:D:6:ASP:OD2	3:D:201:HOH:O	2.21	0.45
3:C:683:HOH:O	2:D:102:LEU:HD23	2.16	0.45
1:G:308:THR:HG23	1:G:342:LEU:HD13	1.99	0.45
1:A:402:HIS:CG	1:A:403:PRO:HD2	2.52	0.45
1:E:166:THR:HG23	1:E:194:LYS:HG2	1.98	0.45
1:C:47:ALA:HB2	1:C:80:ILE:HD11	1.99	0.45
1:A:491:GLY:HA3	1:C:23:THR:O	2.16	0.45
2:B:40:SER:HG	2:B:64:PHE:HD1	1.64	0.45
2:B:90:LEU:HD12	2:B:104:PHE:CE1	2.51	0.45
1:E:43:ARG:CZ	1:E:90:PHE:HB3	2.46	0.45
1:E:375:ILE:HG13	1:E:395:PHE:CD2	2.51	0.45
1:E:43:ARG:NH1	1:E:82:ASP:OD1	2.46	0.45
1:E:319:LEU:HB3	1:E:342:LEU:HD21	1.98	0.45
1:E:37:PRO:HD2	1:E:88:ALA:O	2.17	0.45
1:G:164:GLY:HA3	1:G:394:GLN:OE1	2.17	0.45
1:C:37:PRO:HD2	1:C:88:ALA:O	2.17	0.45
1:E:66:LEU:O	2:H:95:ASN:ND2	2.38	0.45
1:G:292:ALA:HA	1:G:295:ASP:OD1	2.17	0.45
1:C:163:LEU:HD23	1:C:393:LEU:HB2	1.99	0.44
1:A:146:HIS:CD2	1:A:154:LYS:HE3	2.53	0.44
2:D:62:PRO:HB2	2:D:64:PHE:CZ	2.53	0.44
1:E:164:GLY:HA2	1:E:192:PHE:O	2.17	0.44
1:E:99:ASP:OD2	1:G:363:SER:HB3	2.17	0.44
1:G:227:GLU:O	1:G:229:LYS:HG2	2.17	0.44
1:G:378:TRP:NE1	1:G:455:TRP:O	2.50	0.44
1:G:450:ILE:HD12	1:G:451:ALA:H	1.74	0.44
2:B:102:LEU:HD12	2:B:103:ALA:H	1.82	0.44
1:C:207:TRP:CD2	1:C:246:ARG:HG2	2.53	0.44
1:C:211:PHE:CD1	1:C:233:LEU:HD22	2.53	0.44
1:A:240:PRO:HD3	1:E:268:THR:O	2.17	0.44
1:C:178:TYR:HH	1:C:195:ASP:HA	1.82	0.44
1:G:144:PRO:HG2	1:G:365:PRO:O	2.18	0.44
1:A:197:GLU:HG2	1:A:198:ASN:N	2.33	0.43
1:A:336:LEU:HD23	1:A:336:LEU:H	1.82	0.43
1:E:85:GLY:O	1:E:86:ASP:C	2.56	0.43
1:E:120:PHE:CE1	1:E:122:ALA:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:442:ALA:HB2	1:G:452:MET:HE3	2.00	0.43
2:B:13:TYR:HB3	2:B:105:VAL:HG21	2.00	0.43
1:C:14:ARG:HB2	1:C:45:GLU:OE2	2.18	0.43
1:E:288:ARG:NH2	1:E:322:GLY:HA2	2.34	0.43
3:G:635:HOH:O	2:H:102:LEU:HD13	2.18	0.43
1:C:24:PRO:HB3	1:C:30:LEU:HD21	2.00	0.43
1:C:332:ARG:O	1:C:336:LEU:HD23	2.18	0.43
1:E:346:PHE:CD2	1:E:483:ARG:HD3	2.54	0.43
1:A:38:GLN:CD	1:A:124:ARG:HG2	2.39	0.43
1:A:158:TYR:CD1	2:B:100:LEU:HB2	2.54	0.43
1:G:232:TYR:CE2	1:G:285:HIS:CE1	3.06	0.43
2:H:28:ARG:HG3	2:H:69:VAL:HG11	2.00	0.43
2:H:31:ILE:CG2	2:H:69:VAL:HG13	2.48	0.43
1:A:62:VAL:HG22	1:A:63:TRP:N	2.34	0.43
1:A:110:PHE:O	1:A:114:VAL:HG22	2.18	0.43
1:A:174:SER:HB3	2:H:98:GLN:HB3	2.01	0.43
1:E:121:LYS:H	1:E:121:LYS:CE	2.31	0.43
1:C:491:GLY:O	1:C:493:ALA:N	2.51	0.43
1:E:127:ARG:NH1	1:E:129:GLU:OE2	2.52	0.43
1:G:207:TRP:CD2	1:G:246:ARG:HG2	2.54	0.43
1:A:169:PRO:HD2	1:A:173:LEU:HD11	2.01	0.42
1:E:190:LEU:HG	1:E:410:ALA:HB1	1.99	0.42
2:F:12:LYS:HG3	2:F:18:TYR:CE1	2.54	0.42
1:G:194:LYS:NZ	3:G:601:HOH:O	2.10	0.42
1:A:62:VAL:HG23	1:E:401:GLY:HA2	2.00	0.42
1:C:343:ARG:HG2	1:C:367:VAL:O	2.19	0.42
1:C:414:ARG:O	1:C:418:GLU:HG3	2.19	0.42
1:E:308:THR:HG23	1:E:342:LEU:HD13	2.02	0.42
1:A:47:ALA:CB	1:A:80:ILE:HD11	2.50	0.42
1:G:259:MET:HA	1:G:285:HIS:O	2.20	0.42
2:B:14:GLU:HA	2:B:14:GLU:OE1	2.19	0.42
1:G:442:ALA:HB2	1:G:452:MET:CE	2.50	0.42
2:D:46:VAL:HG13	2:D:47:GLU:O	2.19	0.42
2:F:12:LYS:HD3	2:F:12:LYS:HA	1.72	0.42
1:A:335:THR:HA	1:A:338:TRP:CE2	2.54	0.42
2:D:22:MET:HA	2:D:26:ARG:NH1	2.34	0.42
1:E:481:ARG:NH1	3:E:618:HOH:O	2.47	0.42
1:A:263:ILE:HG22	1:A:290:MET:HE3	2.02	0.41
1:E:149:GLN:HG2	2:F:97:ALA:O	2.20	0.41
1:E:24:PRO:HB3	1:E:30:LEU:HD21	2.02	0.41
1:G:53:GLU:HA	1:G:57:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:SER:O	1:A:98:ILE:HB	2.20	0.41
1:E:277:CYS:HB3	1:E:282:VAL:O	2.20	0.41
1:E:126:LEU:O	1:E:300:HIS:HA	2.21	0.41
1:E:491:GLY:HA3	1:G:23:THR:O	2.21	0.41
1:G:186:LEU:O	1:G:229:LYS:NZ	2.36	0.41
1:C:288:ARG:HG3	1:C:291:HIS:CD2	2.56	0.41
1:A:24:PRO:HB3	1:A:30:LEU:HD21	2.02	0.41
1:E:492:LYS:HE3	1:G:24:PRO:O	2.20	0.41
1:G:288:ARG:HG2	3:G:711:HOH:O	2.20	0.41
1:A:259:MET:HA	1:A:285:HIS:O	2.21	0.41
1:A:442:ALA:HB2	1:A:452:MET:HE3	2.03	0.41
1:E:17:TYR:HB2	1:E:48:ALA:HB1	2.03	0.41
1:E:289:ALA:O	1:E:290:MET:HG2	2.21	0.41
1:A:364:MET:HA	1:A:365:PRO:HD3	1.93	0.41
1:C:27:SER:O	1:C:98:ILE:HB	2.21	0.41
1:C:193:THR:O	1:C:231:HIS:HA	2.21	0.41
1:E:485:GLU:O	1:E:489:GLN:HG2	2.20	0.41
1:G:17:TYR:CD2	1:G:52:ALA:HB2	2.56	0.41
1:A:402:HIS:CD2	1:A:451:ALA:HB2	2.56	0.40
1:A:442:ALA:HB2	1:A:452:MET:CE	2.51	0.40
2:B:98:GLN:NE2	1:C:67:LEU:O	2.52	0.40
1:C:207:TRP:CE3	1:C:246:ARG:HG2	2.56	0.40
2:F:59:TRP:CD1	2:F:60:LYS:HG2	2.56	0.40
1:G:164:GLY:HA2	1:G:192:PHE:O	2.20	0.40
1:A:403:PRO:O	1:A:404:TRP:HD1	2.05	0.40
2:B:45:HIS:HA	2:B:87:GLN:O	2.21	0.40
1:G:154:LYS:NZ	3:G:630:HOH:O	2.54	0.40
1:E:346:PHE:CG	1:E:483:ARG:HD3	2.56	0.40
1:A:214:VAL:HG11	1:A:231:HIS:CD2	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:608:HOH:O	3:G:633:HOH:O[2_555]	2.17	0.03
1:C:15:GLN:NE2	2:H:71:ASN:OD1[4_454]	2.18	0.02

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	447/506 (88%)	431 (96%)	16 (4%)	0	100	100
1	C	449/506 (89%)	432 (96%)	15 (3%)	2 (0%)	34	48
1	E	444/506 (88%)	426 (96%)	16 (4%)	2 (0%)	29	41
1	G	448/506 (88%)	429 (96%)	18 (4%)	1 (0%)	47	62
2	B	102/110 (93%)	96 (94%)	6 (6%)	0	100	100
2	D	104/110 (94%)	100 (96%)	4 (4%)	0	100	100
2	F	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	15	23
2	H	97/110 (88%)	93 (96%)	4 (4%)	0	100	100
All	All	2194/2464 (89%)	2102 (96%)	86 (4%)	6 (0%)	41	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	86	ASP
2	F	23	ASN
1	C	492	LYS
1	E	396	GLY
1	G	290	MET
1	C	396	GLY

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	361/407 (89%)	359 (99%)	2 (1%)	86 94
1	C	363/407 (89%)	358 (99%)	5 (1%)	67 82
1	E	359/407 (88%)	354 (99%)	5 (1%)	67 82
1	G	361/407 (89%)	358 (99%)	3 (1%)	81 91
2	B	90/94 (96%)	90 (100%)	0	100 100
2	D	91/94 (97%)	91 (100%)	0	100 100
2	F	91/94 (97%)	90 (99%)	1 (1%)	73 87
2	H	87/94 (93%)	87 (100%)	0	100 100
All	All	1803/2004 (90%)	1787 (99%)	16 (1%)	78 90

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ARG
1	A	127	ARG
1	C	205	MET
1	C	232	TYR
1	C	275	LYS
1	C	290	MET
1	C	332	ARG
1	E	76	ARG
1	E	121	LYS
1	E	127	ARG
1	E	232	TYR
1	E	428	ARG
2	F	102	LEU
1	G	165	CYS
1	G	290	MET
1	G	353	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	413	ASN
2	B	5	GLN
1	C	303	HIS
2	H	5	GLN

5.3.3 RNA

There are no RNA molecules 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 monosaccharides 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, 95^{th} 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	453/506 (89%)	-0.58	1 (0%) 95 94	26, 38, 61, 72	0
1	C	455/506 (89%)	-0.54	3 (0%) 87 86	23, 36, 66, 79	0
1	E	450/506 (88%)	-0.54	1 (0%) 95 94	22, 38, 61, 87	0
1	G	454/506 (89%)	-0.55	1 (0%) 95 94	26, 39, 62, 74	0
2	B	104/110 (94%)	-0.58	0 100 100	32, 42, 58, 69	0
2	D	106/110 (96%)	-0.61	0 100 100	27, 38, 56, 64	0
2	F	105/110 (95%)	-0.33	1 (0%) 82 80	28, 45, 61, 71	0
2	H	101/110 (91%)	-0.28	0 100 100	35, 54, 70, 82	0
All	All	2228/2464 (90%)	-0.53	7 (0%) 94 93	22, 39, 63, 87	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	59	TRP	5.5
1	E	39	PRO	4.2
1	G	39	PRO	2.5
1	C	40	GLY	2.3
2	F	23	ASN	2.3
1	C	60	THR	2.2
1	A	59	TRP	2.1

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 monosaccharides 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.