



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:05 AM UTC

PDB ID : 6UEW / pdb_00006uew
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

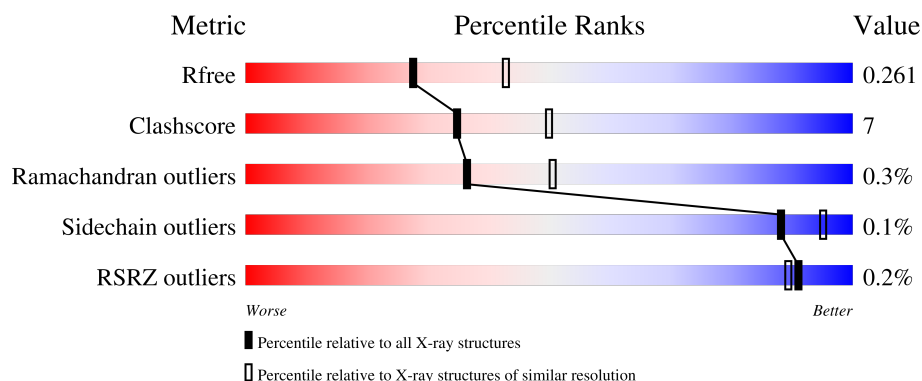
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	506	 74% 16% 10%
1	C	506	 74% 16% 10%
1	E	506	 72% 17% 11%
1	G	506	 74% 16% 10%
2	B	110	 77% 17% 5%

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Mol	Chain	Length	Quality of chain
2	D	110	82% 15%
2	F	110	82% 13% • 5%
2	H	110	% 77% 15% 8%

2 Entry composition

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 biphosphate 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 biphosphate 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			

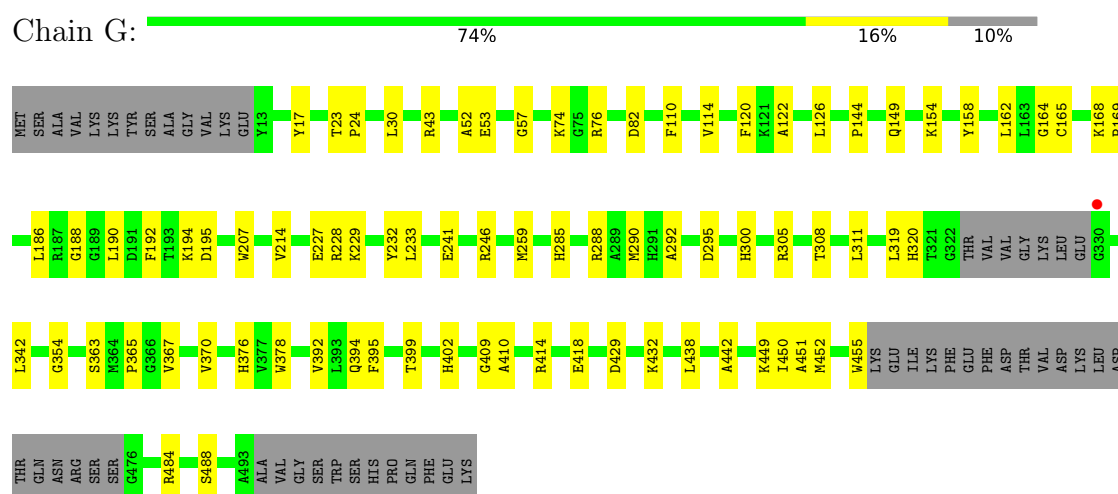
- Molecule 3 is water.

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		

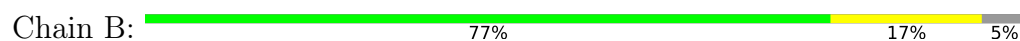
- Molecule 1: Ribulose biphosphate carboxylase large chain, CsoS2 N-peptide fusion



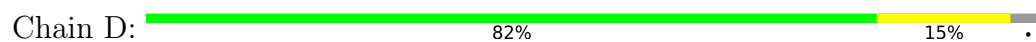
- Molecule 1: Ribulose biphosphate carboxylase large chain, CsoS2 N-peptide fusion



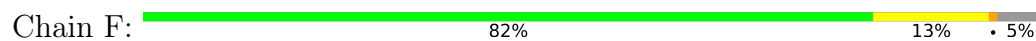
- Molecule 2: Ribulose biphosphate carboxylase small chain



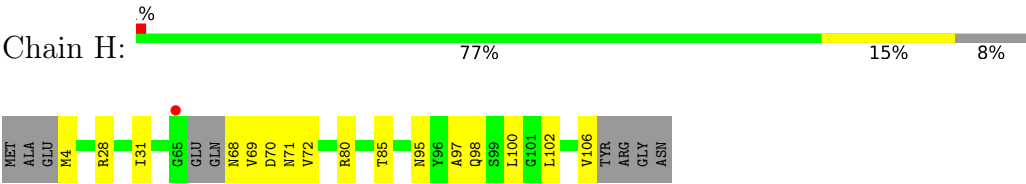
- Molecule 2: Ribulose biphosphate carboxylase small chain



- Molecule 2: Ribulose biphosphate carboxylase small chain



● Molecule 2: Ribulose biphosphate carboxylase small chain



4 Data and refinement statistics

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 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (104.08-2.40) 92.6 (104.08-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.188 , 0.259 0.192 , 0.261	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 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	0.35	0/3638	0.54	0/4929
1	C	0.37	0/3653	0.54	0/4948
1	E	0.37	0/3613	0.54	0/4896
1	G	0.37	0/3641	0.55	0/4933
2	B	0.33	0/890	0.48	0/1209
2	D	0.36	0/902	0.50	0/1224
2	F	0.35	0/898	0.53	0/1219
2	H	0.30	0/855	0.44	0/1160
All	All	0.36	0/18090	0.53	0/24518

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	3550	0	3442	59	0
1	C	3565	0	3460	53	1
1	E	3525	0	3418	64	0
1	G	3553	0	3443	62	0
2	B	864	0	830	11	0
2	D	876	0	842	11	0
2	F	872	0	839	11	0
2	H	831	0	802	14	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	7	1
3	H	17	0	0	1	0
All	All	18304	0	17076	260	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 (260) 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:HB2	1:G:452:MET:HE3	1.69	0.74
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
1:E:64:THR:HA	1:E:67:LEU:HD23	1.75	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:450:ILE:HD12	1:G:450:ILE:C	2.23	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:290:MET:HE2	1:E:110:PHE:HE2	1.63	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:C:404:TRP:HA	2:D:4:MET:HE3	1.82	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:E:155:MET:HE2	1:E:155:MET:HA	1.84	0.59
1:A:162:LEU:HB2	1:A:392:VAL:HG22	1.85	0.59
1:E:404:TRP:HA	2:F:4:MET:HE3	1.85	0.58
2:D:86:HIS:NE2	3:D:205:HOH:O	2.32	0.58
1:C:442:ALA:HB2	1:C:452:MET:HE2	1.85	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
1:G:438:LEU:C	1:G:452:MET:HE1	2.30	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:G:74:LYS:NZ	3:G:609:HOH:O	2.39	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
1:A:442:ALA:HB2	1:A:452:MET:HE1	1.89	0.54
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
2:D:58:MET:HE3	1:E:180:ARG:HD2	1.91	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:G:450:ILE:C	1:G:450:ILE:CD1	2.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:ARG:HG3	2:D:69:VAL:HG11	1.94	0.49
1:G:429:ASP:HB3	1:G:432:LYS:HZ3	1.76	0.49
1:A:320:HIS:HA	1:A:370:VAL:HB	1.94	0.49
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:A:263:ILE:HG22	1:A:290:MET:HE3	1.95	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:173:LEU:O	1:A:205:MET:HE2	2.13	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:85:GLY:O	1:E:86:ASP:C	2.56	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:38:GLN:CD	1:A:124:ARG:HG2	2.39	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:19:MET:HB2	1:E:19:MET:HE3	1.59	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
1:A:438:LEU:O	1:A:452:MET:HE1	2.17	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:G:186:LEU:O	1:G:229:LYS:NZ	2.36	0.44
1:A:240:PRO:HD3	1:E:268:THR:O	2.17	0.44
1:G:144:PRO:HG2	1:G:365:PRO:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:120:PHE:CE1	1:E:122:ALA:HB3	2.53	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
1:G:168:LYS:HA	1:G:169:PRO:C	2.43	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: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
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: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
2:H:4:MET:HB3	2:H:4:MET:HE2	1.59	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: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:G:429:ASP:OD1	1:G:429:ASP:C	2.64	0.40
1:G:438:LEU:O	1:G:452:MET:HE1	2.22	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

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	447/506 (88%)	431 (96%)	16 (4%)	0	100	100
1	C	449/506 (89%)	432 (96%)	15 (3%)	2 (0%)	30	43
1	E	444/506 (88%)	426 (96%)	16 (4%)	2 (0%)	24	37
1	G	448/506 (88%)	429 (96%)	18 (4%)	1 (0%)	43	58
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%)	12	20
2	H	97/110 (88%)	93 (96%)	4 (4%)	0	100	100
All	All	2194/2464 (89%)	2102 (96%)	86 (4%)	6 (0%)	36	50

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

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%)	361 (100%)	0	100	100
1	C	363/407 (89%)	363 (100%)	0	100	100
1	E	359/407 (88%)	359 (100%)	0	100	100
1	G	361/407 (89%)	360 (100%)	1 (0%)	86	93
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%)	91 (100%)	0	100	100
2	H	87/94 (93%)	87 (100%)	0	100	100
All	All	1803/2004 (90%)	1802 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	76	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	413	ASN
2	B	5	GLN
2	B	9	GLN
1	C	303	HIS
1	C	376	HIS
1	C	413	ASN
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 [i](#)

There are no oligosaccharides 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	453/506 (89%)	-0.38	1 (0%) 91 89	26, 38, 61, 72	0
1	C	455/506 (89%)	-0.42	1 (0%) 91 89	23, 36, 66, 79	0
1	E	450/506 (88%)	-0.34	1 (0%) 91 89	22, 38, 61, 87	0
1	G	454/506 (89%)	-0.29	1 (0%) 91 89	26, 39, 62, 74	0
2	B	104/110 (94%)	-0.32	0 100 100	32, 42, 58, 69	0
2	D	106/110 (96%)	-0.37	0 100 100	27, 38, 56, 64	0
2	F	105/110 (95%)	-0.12	0 100 100	28, 45, 61, 71	0
2	H	101/110 (91%)	0.15	1 (0%) 79 76	35, 54, 70, 82	0
All	All	2228/2464 (90%)	-0.32	5 (0%) 91 89	22, 39, 63, 87	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	378	TRP	3.0
2	H	65	GLY	2.9
1	A	476	GLY	2.6
1	C	59	TRP	2.3
1	G	330	GLY	2.3

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 oligosaccharides 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.