



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:27 PM UTC

PDB ID : 2GPW / pdb_00002gpw
Title : Crystal Structure of the Biotin Carboxylase Subunit, F363A Mutant, of Acetyl-CoA Carboxylase from Escherichia coli.
Authors : Shen, Y.; Chou, C.Y.; Chang, G.G.; Tong, L.
Deposited on : 2006-04-18
Resolution : 2.20 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

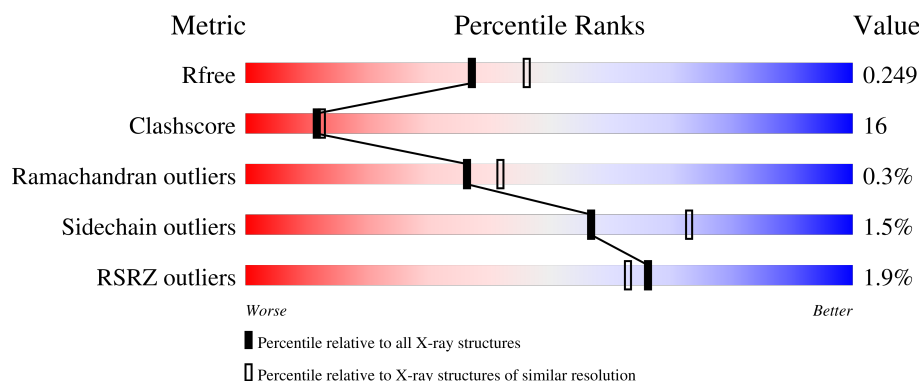
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	469	2% 71% 22% • 5%
1	B	469	2% 71% 22% • 6%
1	C	469	0% 71% 22% • 5%
1	D	469	2% 66% 27% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14802 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 Biotin carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3434	2162	615	635	22			
1	B	442	Total	C	N	O	S	0	0	0
			3410	2146	611	631	22			
1	C	446	Total	C	N	O	S	0	0	0
			3440	2165	616	637	22			
1	D	447	Total	C	N	O	S	0	0	0
			3447	2170	617	638	22			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	cloning artifact	UNP P24182
A	-18	GLY	-	cloning artifact	UNP P24182
A	-17	SER	-	cloning artifact	UNP P24182
A	-16	SER	-	cloning artifact	UNP P24182
A	-15	HIS	-	expression tag	UNP P24182
A	-14	HIS	-	expression tag	UNP P24182
A	-13	HIS	-	expression tag	UNP P24182
A	-12	HIS	-	expression tag	UNP P24182
A	-11	HIS	-	expression tag	UNP P24182
A	-10	HIS	-	expression tag	UNP P24182
A	-9	SER	-	cloning artifact	UNP P24182
A	-8	SER	-	cloning artifact	UNP P24182
A	-7	GLY	-	cloning artifact	UNP P24182
A	-6	LEU	-	cloning artifact	UNP P24182
A	-5	VAL	-	cloning artifact	UNP P24182
A	-4	PRO	-	cloning artifact	UNP P24182
A	-3	ARG	-	cloning artifact	UNP P24182
A	-2	GLY	-	cloning artifact	UNP P24182
A	-1	SER	-	cloning artifact	UNP P24182
A	0	HIS	-	cloning artifact	UNP P24182
A	363	ALA	PHE	engineered mutation	UNP P24182

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	cloning artifact	UNP P24182
B	-18	GLY	-	cloning artifact	UNP P24182
B	-17	SER	-	cloning artifact	UNP P24182
B	-16	SER	-	cloning artifact	UNP P24182
B	-15	HIS	-	expression tag	UNP P24182
B	-14	HIS	-	expression tag	UNP P24182
B	-13	HIS	-	expression tag	UNP P24182
B	-12	HIS	-	expression tag	UNP P24182
B	-11	HIS	-	expression tag	UNP P24182
B	-10	HIS	-	expression tag	UNP P24182
B	-9	SER	-	cloning artifact	UNP P24182
B	-8	SER	-	cloning artifact	UNP P24182
B	-7	GLY	-	cloning artifact	UNP P24182
B	-6	LEU	-	cloning artifact	UNP P24182
B	-5	VAL	-	cloning artifact	UNP P24182
B	-4	PRO	-	cloning artifact	UNP P24182
B	-3	ARG	-	cloning artifact	UNP P24182
B	-2	GLY	-	cloning artifact	UNP P24182
B	-1	SER	-	cloning artifact	UNP P24182
B	0	HIS	-	cloning artifact	UNP P24182
B	363	ALA	PHE	engineered mutation	UNP P24182
C	-19	MET	-	cloning artifact	UNP P24182
C	-18	GLY	-	cloning artifact	UNP P24182
C	-17	SER	-	cloning artifact	UNP P24182
C	-16	SER	-	cloning artifact	UNP P24182
C	-15	HIS	-	expression tag	UNP P24182
C	-14	HIS	-	expression tag	UNP P24182
C	-13	HIS	-	expression tag	UNP P24182
C	-12	HIS	-	expression tag	UNP P24182
C	-11	HIS	-	expression tag	UNP P24182
C	-10	HIS	-	expression tag	UNP P24182
C	-9	SER	-	cloning artifact	UNP P24182
C	-8	SER	-	cloning artifact	UNP P24182
C	-7	GLY	-	cloning artifact	UNP P24182
C	-6	LEU	-	cloning artifact	UNP P24182
C	-5	VAL	-	cloning artifact	UNP P24182
C	-4	PRO	-	cloning artifact	UNP P24182
C	-3	ARG	-	cloning artifact	UNP P24182
C	-2	GLY	-	cloning artifact	UNP P24182
C	-1	SER	-	cloning artifact	UNP P24182
C	0	HIS	-	cloning artifact	UNP P24182
C	363	ALA	PHE	engineered mutation	UNP P24182

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	cloning artifact	UNP P24182
D	-18	GLY	-	cloning artifact	UNP P24182
D	-17	SER	-	cloning artifact	UNP P24182
D	-16	SER	-	cloning artifact	UNP P24182
D	-15	HIS	-	expression tag	UNP P24182
D	-14	HIS	-	expression tag	UNP P24182
D	-13	HIS	-	expression tag	UNP P24182
D	-12	HIS	-	expression tag	UNP P24182
D	-11	HIS	-	expression tag	UNP P24182
D	-10	HIS	-	expression tag	UNP P24182
D	-9	SER	-	cloning artifact	UNP P24182
D	-8	SER	-	cloning artifact	UNP P24182
D	-7	GLY	-	cloning artifact	UNP P24182
D	-6	LEU	-	cloning artifact	UNP P24182
D	-5	VAL	-	cloning artifact	UNP P24182
D	-4	PRO	-	cloning artifact	UNP P24182
D	-3	ARG	-	cloning artifact	UNP P24182
D	-2	GLY	-	cloning artifact	UNP P24182
D	-1	SER	-	cloning artifact	UNP P24182
D	0	HIS	-	cloning artifact	UNP P24182
D	363	ALA	PHE	engineered mutation	UNP P24182

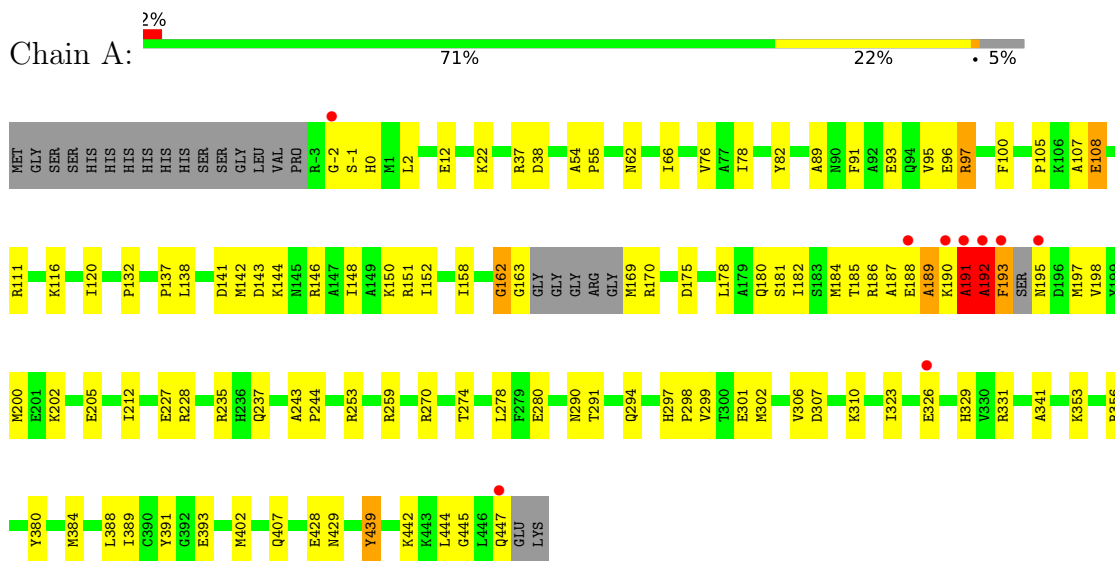
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	272	Total	O	0	0
			272	272		
2	B	247	Total	O	0	0
			247	247		
2	C	291	Total	O	0	0
			291	291		
2	D	261	Total	O	0	0
			261	261		

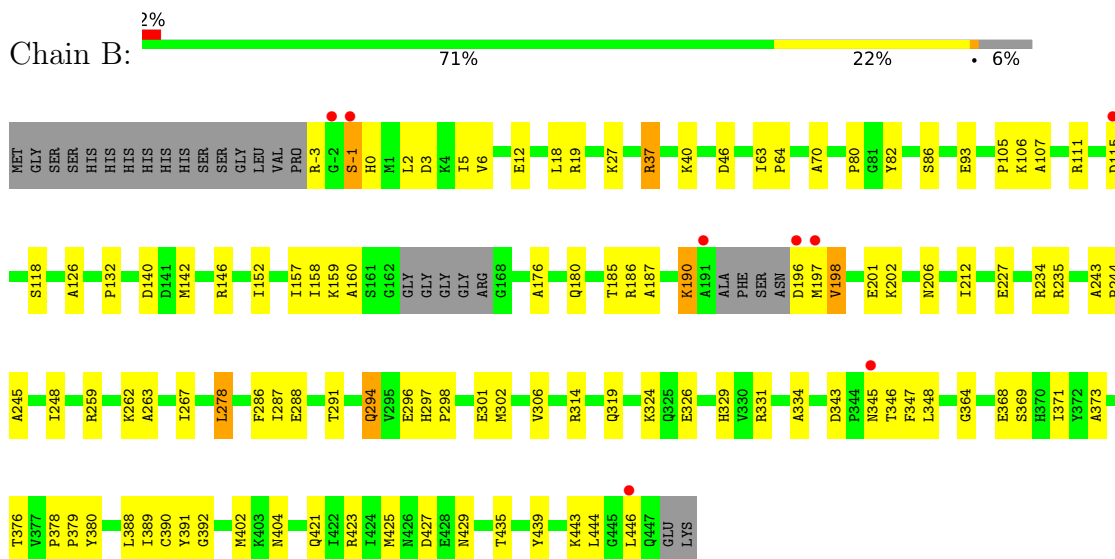
3 Residue-property plots

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.

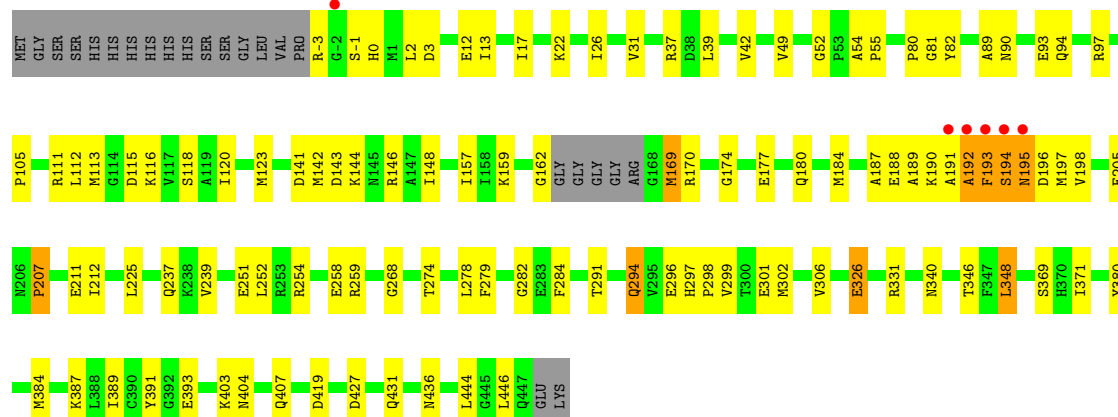
• Molecule 1: Biotin carboxylase



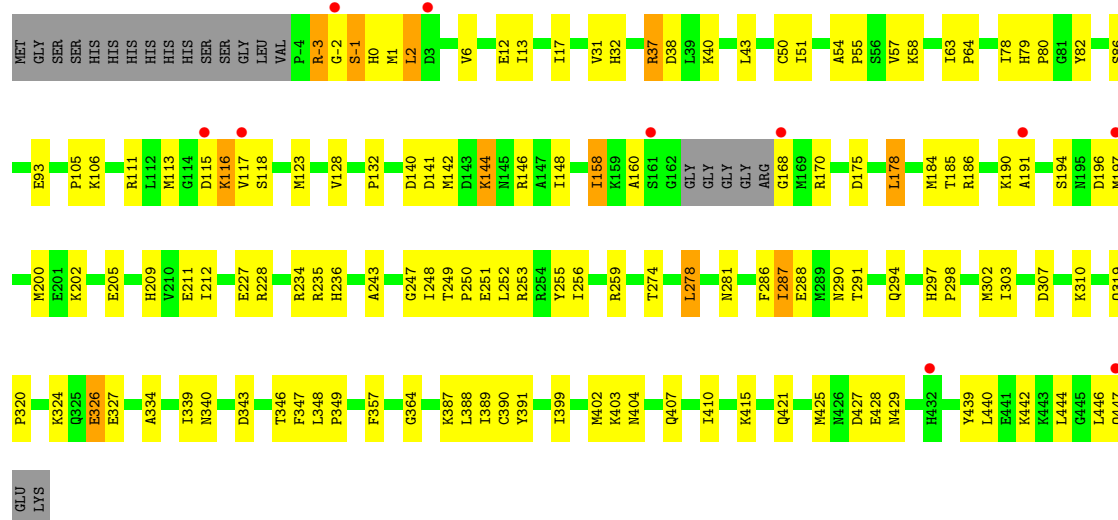
• Molecule 1: Biotin carboxylase



• Molecule 1: Biotin carboxylase



• Molecule 1: Biotin carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.35Å 81.50Å 176.65Å 90.00° 97.69° 90.00°	Depositor
Resolution (Å)	29.75 – 2.20 29.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.8 (29.75-2.20) 87.8 (29.75-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.192 , 0.250 0.192 , 0.249	Depositor DCC
R_{free} test set	6090 reflections (7.55%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14802	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.54% 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	0.50	2/3495 (0.1%)	0.92	9/4715 (0.2%)
1	B	0.42	1/3470 (0.0%)	0.90	4/4681 (0.1%)
1	C	0.44	2/3502 (0.1%)	0.95	12/4726 (0.3%)
1	D	0.40	0/3510	0.91	9/4737 (0.2%)
All	All	0.44	5/13977 (0.0%)	0.92	34/18859 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	ALA	C-O	-6.64	1.15	1.24
1	C	192	ALA	CA-C	-5.69	1.45	1.52
1	C	192	ALA	N-CA	-5.69	1.38	1.46
1	A	192	ALA	C-N	-5.58	1.25	1.33
1	B	198	VAL	C-N	-5.10	1.26	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	-1	SER	N-CA-C	-14.10	96.98	114.75
1	D	-1	SER	N-CA-C	-13.19	97.81	114.56
1	A	-1	SER	N-CA-C	-12.36	98.86	114.56
1	B	-1	SER	N-CA-C	-10.93	98.03	114.64
1	C	191	ALA	CA-C-N	-10.31	104.09	121.92
1	C	191	ALA	C-N-CA	-10.31	104.09	121.92
1	C	192	ALA	N-CA-C	8.76	124.28	113.50
1	A	205	GLU	N-CA-C	8.34	120.00	111.07
1	C	380	TYR	N-CA-C	7.82	122.40	113.01
1	B	278	LEU	N-CA-C	-7.66	97.26	109.59
1	A	439	TYR	N-CA-C	7.29	119.85	111.11
1	D	287	ILE	CB-CA-C	-7.13	105.65	111.71
1	C	205	GLU	N-CA-C	7.06	119.05	111.36
1	C	194	SER	O-C-N	6.98	130.76	121.97
1	D	439	TYR	N-CA-C	6.97	119.53	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	144	LYS	N-CA-C	-6.87	104.04	113.18
1	D	205	GLU	N-CA-C	6.59	118.25	111.14
1	C	195	ASN	CA-CB-CG	-6.45	106.16	112.60
1	A	380	TYR	N-CA-C	6.42	120.38	112.54
1	B	439	TYR	N-CA-C	6.27	118.67	111.02
1	D	278	LEU	N-CA-C	-6.12	99.21	109.07
1	A	191	ALA	O-C-N	6.09	130.70	122.59
1	A	278	LEU	N-CA-C	-6.00	99.45	109.24
1	B	190	LYS	CA-C-O	5.91	126.64	119.49
1	C	52	GLY	CA-C-N	5.83	125.81	120.21
1	C	52	GLY	C-N-CA	5.83	125.81	120.21
1	D	2	LEU	CA-C-N	5.83	128.40	120.54
1	D	2	LEU	C-N-CA	5.83	128.40	120.54
1	C	193	PHE	N-CA-C	-5.80	106.05	114.12
1	C	278	LEU	N-CA-C	-5.56	100.12	109.07
1	A	189	ALA	O-C-N	5.27	128.16	122.15
1	A	193	PHE	CA-CB-CG	-5.15	108.65	113.80
1	A	341	ALA	N-CA-C	-5.02	97.84	107.57
1	D	178	LEU	N-CA-C	5.00	116.42	111.07

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	3434	0	3459	116	1
1	B	3410	0	3439	97	0
1	C	3440	0	3465	95	1
1	D	3447	0	3472	135	1
2	A	272	0	0	30	0
2	B	247	0	0	15	0
2	C	291	0	0	22	0
2	D	261	0	0	29	0
All	All	14802	0	13835	437	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 16.

All (437) 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:162:GLY:O	1:C:193:PHE:CE2	1.83	1.30
1:A:162:GLY:O	1:A:193:PHE:CD2	2.01	1.13
1:B:302:MET:HE3	1:B:391:TYR:HB2	1.43	0.98
1:A:163:GLY:HA2	1:A:193:PHE:CE2	1.97	0.97
1:C:162:GLY:O	1:C:193:PHE:CZ	2.18	0.95
1:C:162:GLY:O	1:C:193:PHE:CD2	2.21	0.93
1:C:193:PHE:O	1:C:194:SER:HB2	1.70	0.91
1:D:186:ARG:HG2	1:D:196:ASP:HB2	1.51	0.90
1:A:162:GLY:O	1:A:193:PHE:CE2	2.24	0.89
1:B:196:ASP:O	1:B:196:ASP:OD2	1.92	0.87
1:D:146:ARG:HD2	1:D:175:ASP:OD1	1.74	0.87
1:C:97:ARG:HG2	1:C:97:ARG:HH11	1.39	0.85
1:D:128:VAL:HG12	2:D:513:HOH:O	1.76	0.84
1:B:343:ASP:OD2	1:B:345:ASN:HB2	1.78	0.83
1:A:302:MET:HE2	1:A:389:ILE:HG22	1.61	0.82
1:C:162:GLY:C	1:C:193:PHE:CD2	2.58	0.82
1:A:290:ASN:HD22	1:A:294:GLN:HE22	1.25	0.81
1:D:334:ALA:HB2	2:D:623:HOH:O	1.81	0.80
1:A:141:ASP:OD1	1:A:144:LYS:HE3	1.82	0.80
1:C:162:GLY:C	1:C:193:PHE:CE2	2.61	0.79
1:C:302:MET:HE2	1:C:389:ILE:HG22	1.64	0.79
1:A:290:ASN:HD22	1:A:294:GLN:NE2	1.80	0.79
1:B:37:ARG:HH11	1:B:37:ARG:HB3	1.47	0.79
1:B:187:ALA:HA	1:B:190:LYS:HD2	1.64	0.79
1:D:0:HIS:HD2	1:D:2:LEU:H	1.28	0.79
1:C:302:MET:HE3	1:C:391:TYR:HB2	1.63	0.79
1:D:197:MET:HB3	2:D:641:HOH:O	1.84	0.78
1:A:163:GLY:HA2	1:A:193:PHE:HE2	1.44	0.78
1:A:302:MET:HE3	1:A:391:TYR:HB2	1.66	0.77
1:C:144:LYS:HG3	2:C:496:HOH:O	1.85	0.77
1:B:12:GLU:HB2	2:B:655:HOH:O	1.82	0.77
1:B:142:MET:O	1:B:146:ARG:HG3	1.83	0.77
1:A:243:ALA:HB3	1:A:299:VAL:HG12	1.66	0.76
1:B:196:ASP:O	1:B:196:ASP:CG	2.29	0.75
1:D:248:ILE:HB	1:D:253:ARG:HE	1.50	0.75
1:A:163:GLY:CA	1:A:193:PHE:CE2	2.69	0.75
1:A:138:LEU:HD11	1:A:200:MET:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-1:SER:HA	2:D:455:HOH:O	1.87	0.74
1:B:-1:SER:HA	2:B:461:HOH:O	1.86	0.74
1:A:97:ARG:HG2	1:A:97:ARG:HH11	1.51	0.73
1:D:303:ILE:HG23	2:D:623:HOH:O	1.89	0.73
1:B:348:LEU:HD21	1:D:43:LEU:HD23	1.72	0.70
1:D:158:ILE:HG22	1:D:185:THR:HG21	1.72	0.70
1:D:290:ASN:HD22	1:D:294:GLN:NE2	1.89	0.70
1:A:290:ASN:ND2	1:A:294:GLN:HE22	1.89	0.69
1:C:326:GLU:HB3	2:C:607:HOH:O	1.92	0.69
1:C:12:GLU:HG2	1:C:384:MET:HE3	1.74	0.69
1:A:195:ASN:HD21	1:A:197:MET:HB2	1.57	0.69
1:A:189:ALA:O	1:A:190:LYS:C	2.36	0.68
1:B:297:HIS:ND1	1:B:298:PRO:HD3	2.09	0.68
1:B:368:GLU:HB3	2:B:655:HOH:O	1.94	0.68
1:A:175:ASP:HB3	2:A:612:HOH:O	1.93	0.68
1:D:287:ILE:HG12	2:D:683:HOH:O	1.94	0.68
1:C:190:LYS:HG2	1:C:196:ASP:HB3	1.74	0.67
1:A:191:ALA:O	1:A:192:ALA:C	2.37	0.67
1:D:191:ALA:HB3	2:D:700:HOH:O	1.93	0.67
1:D:146:ARG:HG2	1:D:178:LEU:HD23	1.75	0.66
1:D:132:PRO:HG2	1:D:202:LYS:HB2	1.77	0.66
1:A:302:MET:HE2	1:A:389:ILE:CG2	2.24	0.66
1:D:212:ILE:HD13	1:D:227:GLU:HB3	1.77	0.65
1:D:-3:ARG:HH11	1:D:-3:ARG:HB3	1.61	0.65
1:A:180:GLN:HG3	2:A:495:HOH:O	1.97	0.65
1:C:301:GLU:HG2	1:C:306:VAL:O	1.98	0.64
1:A:442:LYS:HB2	2:A:719:HOH:O	1.97	0.64
1:A:445:GLY:HA2	1:A:447:GLN:HE21	1.63	0.64
1:A:142:MET:O	1:A:146:ARG:HG3	1.96	0.64
1:C:97:ARG:HG2	1:C:97:ARG:NH1	2.12	0.64
1:D:248:ILE:HB	1:D:253:ARG:NE	2.12	0.64
1:B:37:ARG:HB3	1:B:37:ARG:NH1	2.13	0.63
1:D:302:MET:HE2	1:D:389:ILE:HG22	1.80	0.63
1:A:270:ARG:HD2	2:A:555:HOH:O	1.99	0.63
1:D:444:LEU:HB3	1:D:446:LEU:HD13	1.81	0.63
1:B:160:ALA:HA	1:B:198:VAL:HG12	1.81	0.63
1:A:302:MET:CE	1:A:389:ILE:HG22	2.27	0.62
1:B:37:ARG:HH11	1:B:37:ARG:CB	2.13	0.62
1:D:302:MET:CE	1:D:389:ILE:HG22	2.30	0.62
1:D:442:LYS:HD2	1:D:447:GLN:CD	2.25	0.62
1:A:182:ILE:HG13	2:A:560:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:O	1:A:169:MET:HA	1.99	0.62
1:B:346:THR:OG1	1:B:348:LEU:HB2	2.00	0.62
1:B:346:THR:HB	1:B:348:LEU:HD13	1.81	0.62
1:D:209:HIS:HA	2:D:587:HOH:O	1.99	0.62
1:A:323:ILE:HG12	2:A:565:HOH:O	1.98	0.61
1:D:116:LYS:N	1:D:116:LYS:HD2	2.15	0.61
1:A:150:LYS:HE3	2:A:622:HOH:O	1.99	0.61
1:C:297:HIS:ND1	1:C:298:PRO:HD3	2.14	0.61
1:A:182:ILE:O	1:A:186:ARG:HG2	1.99	0.61
1:C:340:ASN:HD22	1:C:384:MET:HA	1.65	0.61
1:C:115:ASP:HB3	1:C:118:SER:HB3	1.82	0.61
1:A:144:LYS:O	1:A:148:ILE:HG13	2.00	0.61
1:D:141:ASP:OD2	1:D:144:LYS:HB2	2.01	0.61
1:A:190:LYS:HA	1:A:195:ASN:O	2.00	0.61
1:B:302:MET:CE	1:B:389:ILE:HG22	2.31	0.61
1:D:113:MET:HE1	1:D:123:MET:HE3	1.83	0.60
1:A:243:ALA:CB	1:A:299:VAL:HG12	2.31	0.60
1:B:206:ASN:HB3	2:B:586:HOH:O	1.99	0.60
1:C:258:GLU:HB2	2:C:629:HOH:O	2.00	0.60
1:A:105:PRO:HG3	1:A:291:THR:HB	1.82	0.60
1:D:160:ALA:HB2	1:D:168:GLY:HA3	1.83	0.60
1:D:0:HIS:CD2	1:D:2:LEU:H	2.16	0.60
1:D:391:TYR:HD2	2:D:623:HOH:O	1.83	0.60
1:A:323:ILE:HD13	2:A:656:HOH:O	2.00	0.60
1:B:105:PRO:HG3	1:B:291:THR:HB	1.84	0.60
1:B:314:ARG:HD3	1:B:319:GLN:HE22	1.66	0.60
1:A:158:ILE:HG22	1:A:185:THR:HG21	1.82	0.60
1:D:307:ASP:OD1	1:D:310:LYS:HE2	2.02	0.60
1:B:286:PHE:CZ	1:B:288:GLU:HA	2.37	0.59
1:D:302:MET:HB2	2:D:623:HOH:O	2.01	0.59
1:A:326:GLU:HB3	2:A:631:HOH:O	2.01	0.59
1:D:37:ARG:CB	1:D:37:ARG:HH11	2.16	0.59
1:A:329:HIS:HB2	1:A:331:ARG:NH1	2.18	0.59
1:A:407:GLN:HG2	2:A:613:HOH:O	2.02	0.59
1:D:252:LEU:HD12	2:D:656:HOH:O	2.02	0.59
1:D:326:GLU:H	1:D:326:GLU:CD	2.09	0.59
1:B:157:ILE:HG23	1:B:159:LYS:HZ2	1.66	0.59
1:C:268:GLY:HA3	2:C:668:HOH:O	2.03	0.58
1:A:189:ALA:HA	1:A:192:ALA:HB3	1.85	0.58
1:B:301:GLU:HG2	1:B:306:VAL:O	2.02	0.58
1:C:90:ASN:O	1:C:94:GLN:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ALA:O	1:A:190:LYS:HB2	2.04	0.58
1:D:140:ASP:HB3	2:D:562:HOH:O	2.04	0.58
1:B:93:GLU:CD	1:B:111:ARG:HH21	2.11	0.58
1:D:235:ARG:HH12	1:D:446:LEU:HD23	1.69	0.58
1:D:388:LEU:O	1:D:402:MET:HE1	2.03	0.57
1:B:343:ASP:C	1:B:345:ASN:H	2.12	0.57
1:A:191:ALA:O	1:A:193:PHE:N	2.37	0.57
1:C:302:MET:CE	1:C:389:ILE:HG22	2.32	0.57
1:A:307:ASP:OD1	1:A:310:LYS:HG3	2.05	0.56
1:B:196:ASP:OD2	1:B:197:MET:HE2	2.04	0.56
1:B:444:LEU:C	1:B:446:LEU:H	2.12	0.56
1:C:180:GLN:HB3	2:C:609:HOH:O	2.05	0.56
1:C:407:GLN:HG3	2:C:559:HOH:O	2.06	0.56
1:D:339:ILE:C	1:D:340:ASN:HD22	2.13	0.56
1:A:188:GLU:O	1:A:192:ALA:N	2.38	0.56
1:A:307:ASP:CG	1:A:310:LYS:HG3	2.30	0.56
1:B:-3:ARG:HG2	1:B:3:ASP:OD1	2.06	0.56
1:C:82:TYR:OH	1:C:384:MET:HE1	2.05	0.56
1:D:158:ILE:CG2	1:D:185:THR:HG21	2.35	0.56
1:D:278:LEU:HD23	2:D:587:HOH:O	2.05	0.56
1:B:132:PRO:HG2	1:B:202:LYS:HB2	1.88	0.56
1:C:340:ASN:ND2	1:C:384:MET:HA	2.20	0.56
1:B:297:HIS:CG	1:B:298:PRO:HD3	2.41	0.56
1:D:302:MET:HE2	1:D:389:ILE:CG2	2.36	0.56
1:A:37:ARG:HG3	2:A:677:HOH:O	2.06	0.55
1:B:-3:ARG:HA	2:B:680:HOH:O	2.05	0.55
1:C:54:ALA:HB3	1:C:55:PRO:HD3	1.88	0.55
1:B:427:ASP:HB2	1:B:443:LYS:NZ	2.21	0.55
1:D:190:LYS:O	1:D:194:SER:HA	2.06	0.55
1:A:170:ARG:NH1	2:A:611:HOH:O	2.38	0.55
1:C:22:LYS:NZ	1:D:404:ASN:ND2	2.54	0.55
1:A:37:ARG:HG2	2:A:610:HOH:O	2.06	0.55
1:A:116:LYS:O	1:A:120:ILE:HG12	2.07	0.55
1:A:356:ARG:HD2	2:A:693:HOH:O	2.07	0.54
1:B:187:ALA:HA	1:B:190:LYS:CD	2.36	0.54
1:C:141:ASP:HB3	2:C:673:HOH:O	2.06	0.54
1:A:62:ASN:O	1:A:66:ILE:HG13	2.07	0.54
1:A:97:ARG:NH1	2:A:624:HOH:O	2.40	0.54
1:A:82:TYR:OH	1:A:384:MET:HE1	2.08	0.54
1:B:196:ASP:OD2	1:B:196:ASP:C	2.48	0.54
1:B:263:ALA:O	1:B:267:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ARG:HH11	1:C:97:ARG:CG	2.16	0.54
1:C:0:HIS:CD2	1:C:2:LEU:H	2.25	0.54
1:D:54:ALA:HB3	1:D:55:PRO:HD3	1.90	0.54
1:D:158:ILE:HD12	1:D:158:ILE:N	2.23	0.54
1:A:22:LYS:HE2	1:B:404:ASN:ND2	2.22	0.54
1:D:0:HIS:HD2	1:D:2:LEU:N	2.02	0.54
1:A:158:ILE:CG2	1:A:198:VAL:HG11	2.38	0.54
1:D:290:ASN:ND2	1:D:294:GLN:HE22	2.06	0.53
1:A:187:ALA:HA	1:A:190:LYS:HG3	1.90	0.53
1:B:157:ILE:CG2	1:B:159:LYS:HZ2	2.21	0.53
1:B:423:ARG:HD3	2:B:666:HOH:O	2.08	0.53
1:A:163:GLY:CA	1:A:193:PHE:CZ	2.91	0.53
1:D:37:ARG:HB3	1:D:37:ARG:NH1	2.23	0.53
1:D:247:GLY:O	1:D:248:ILE:HD13	2.09	0.53
1:A:97:ARG:HG2	1:A:97:ARG:NH1	2.21	0.53
1:A:132:PRO:HB2	1:A:152:ILE:HG23	1.90	0.53
1:A:329:HIS:HB2	1:A:331:ARG:HH12	1.74	0.53
1:C:193:PHE:O	1:C:194:SER:CB	2.44	0.53
1:D:105:PRO:HD3	2:D:607:HOH:O	2.08	0.53
1:B:0:HIS:CD2	1:B:2:LEU:HB2	2.43	0.53
1:C:22:LYS:HZ2	1:D:404:ASN:ND2	2.07	0.53
1:C:197:MET:HE2	1:C:197:MET:HA	1.91	0.52
1:C:211:GLU:C	1:C:212:ILE:HD12	2.33	0.52
1:D:290:ASN:ND2	1:D:294:GLN:NE2	2.57	0.52
1:D:111:ARG:HH11	1:D:111:ARG:HG2	1.74	0.52
1:A:38:ASP:HB2	2:A:678:HOH:O	2.09	0.52
1:B:288:GLU:HB2	2:B:656:HOH:O	2.09	0.52
1:B:278:LEU:HG	1:B:287:ILE:HD11	1.90	0.52
1:C:105:PRO:HG3	1:C:291:THR:HB	1.92	0.52
1:D:274:THR:OG1	1:D:294:GLN:HG3	2.10	0.52
1:A:91:PHE:O	1:A:95:VAL:HG23	2.10	0.52
1:A:297:HIS:CG	1:A:298:PRO:HD3	2.45	0.52
1:A:280:GLU:HA	2:A:669:HOH:O	2.10	0.52
1:A:428:GLU:HB3	2:A:526:HOH:O	2.09	0.52
1:B:376:THR:O	1:B:378:PRO:HD3	2.09	0.52
1:C:0:HIS:CD2	1:C:26:ILE:HD11	2.45	0.52
1:C:302:MET:HE2	1:C:389:ILE:CG2	2.36	0.52
1:D:148:ILE:HG22	1:D:200:MET:HE3	1.91	0.52
1:D:-1:SER:N	2:D:457:HOH:O	2.42	0.51
1:B:212:ILE:HD13	1:B:227:GLU:HB3	1.91	0.51
1:D:38:ASP:HB2	2:D:652:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLY:HA3	1:A:193:PHE:CZ	2.45	0.51
1:D:12:GLU:CD	1:D:387:LYS:HE2	2.35	0.51
1:D:190:LYS:HG2	1:D:196:ASP:HB3	1.91	0.51
1:C:297:HIS:CG	1:C:298:PRO:HD3	2.45	0.51
1:D:115:ASP:HB3	1:D:118:SER:OG	2.11	0.51
1:A:188:GLU:O	1:A:192:ALA:CB	2.59	0.51
1:C:427:ASP:O	1:C:431:GLN:HG3	2.10	0.51
1:B:302:MET:HE2	1:B:389:ILE:HG22	1.93	0.51
1:D:297:HIS:CG	1:D:298:PRO:HD3	2.46	0.50
1:D:442:LYS:HD2	1:D:447:GLN:OE1	2.12	0.50
1:C:212:ILE:HD12	1:C:212:ILE:N	2.26	0.50
1:D:248:ILE:HG22	1:D:253:ARG:HG3	1.93	0.50
1:A:151:ARG:HD3	2:A:489:HOH:O	2.11	0.50
1:A:190:LYS:O	1:A:191:ALA:O	2.30	0.50
1:C:0:HIS:CD2	1:C:2:LEU:HB2	2.47	0.50
1:D:346:THR:HB	1:D:348:LEU:HD13	1.93	0.50
1:B:159:LYS:NZ	1:B:201:GLU:HB3	2.27	0.50
1:B:314:ARG:HD3	1:B:319:GLN:NE2	2.27	0.50
1:D:234:ARG:HG2	1:D:235:ARG:HD3	1.94	0.50
1:B:93:GLU:HG3	1:B:107:ALA:CB	2.42	0.50
1:B:37:ARG:NE	2:B:677:HOH:O	2.45	0.49
1:B:-1:SER:N	2:B:462:HOH:O	2.46	0.49
1:B:369:SER:OG	1:B:371:ILE:HG12	2.12	0.49
1:D:234:ARG:NH2	1:D:347:PHE:HB3	2.26	0.49
1:D:324:LYS:HE3	1:D:327:GLU:CD	2.38	0.49
1:D:63:ILE:HB	1:D:64:PRO:HD3	1.93	0.49
1:A:297:HIS:ND1	1:A:298:PRO:HD3	2.26	0.49
1:B:152:ILE:HG23	1:B:202:LYS:HB2	1.95	0.49
1:D:297:HIS:ND1	1:D:298:PRO:HD3	2.27	0.49
1:D:319:GLN:HG2	2:D:669:HOH:O	2.11	0.49
1:D:146:ARG:HA	1:D:178:LEU:CD2	2.42	0.49
1:B:444:LEU:C	1:B:446:LEU:N	2.70	0.49
1:C:-3:ARG:HD3	1:C:3:ASP:OD2	2.13	0.49
1:D:190:LYS:CG	1:D:196:ASP:HB3	2.42	0.49
2:C:692:HOH:O	1:D:40:LYS:HG2	2.12	0.49
1:B:259:ARG:HG3	1:B:259:ARG:HH11	1.78	0.49
1:A:107:ALA:O	1:A:111:ARG:HG3	2.13	0.48
1:C:195:ASN:OD1	1:C:197:MET:N	2.46	0.48
1:D:407:GLN:HB3	2:D:679:HOH:O	2.13	0.48
1:C:393:GLU:OE2	1:C:393:GLU:N	2.41	0.48
1:D:37:ARG:HH11	1:D:37:ARG:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:LYS:HG2	1:D:425:MET:HB3	1.94	0.48
1:A:274:THR:OG1	1:A:294:GLN:HG3	2.14	0.48
1:B:234:ARG:NH2	1:B:347:PHE:HB3	2.28	0.48
1:B:63:ILE:HB	1:B:64:PRO:HD3	1.95	0.48
1:C:22:LYS:HE3	2:D:695:HOH:O	2.13	0.48
1:C:419:ASP:HB2	2:C:575:HOH:O	2.13	0.48
1:D:160:ALA:CB	1:D:168:GLY:HA3	2.43	0.48
1:D:13:ILE:HB	1:D:82:TYR:CE2	2.48	0.48
1:D:185:THR:HA	2:D:628:HOH:O	2.14	0.48
1:A:259:ARG:HD2	2:A:717:HOH:O	2.14	0.47
1:C:239:VAL:HG22	2:C:625:HOH:O	2.15	0.47
1:A:2:LEU:HA	1:A:76:VAL:HG21	1.96	0.47
1:A:12:GLU:HG2	1:A:384:MET:HE3	1.96	0.47
1:A:195:ASN:ND2	1:A:197:MET:H	2.12	0.47
1:D:251:GLU:OE1	1:D:251:GLU:N	2.40	0.47
1:A:152:ILE:CG2	1:A:202:LYS:HB2	2.44	0.47
1:B:126:ALA:O	1:B:262:LYS:HD2	2.14	0.47
1:B:435:THR:HA	2:B:688:HOH:O	2.14	0.47
1:C:22:LYS:NZ	1:C:22:LYS:HB3	2.28	0.47
1:A:439:TYR:O	1:A:442:LYS:HB3	2.13	0.47
1:D:105:PRO:HG3	1:D:291:THR:HB	1.95	0.47
1:A:189:ALA:O	1:A:190:LYS:O	2.32	0.47
1:A:228:ARG:NH2	1:A:294:GLN:HG3	2.28	0.47
1:B:159:LYS:O	1:B:198:VAL:HA	2.14	0.47
1:C:297:HIS:N	1:C:298:PRO:CD	2.77	0.47
1:D:250:PRO:HD2	1:D:251:GLU:OE1	2.14	0.47
1:D:255:TYR:O	1:D:259:ARG:HG2	2.15	0.47
1:C:141:ASP:OD2	1:C:144:LYS:HB2	2.14	0.47
1:D:228:ARG:HG2	1:D:243:ALA:HB2	1.97	0.47
1:D:235:ARG:NH1	1:D:446:LEU:HD23	2.28	0.47
1:D:444:LEU:CB	1:D:446:LEU:HD13	2.43	0.47
1:A:329:HIS:HD2	2:A:704:HOH:O	1.98	0.47
1:C:225:LEU:N	1:C:225:LEU:HD12	2.30	0.47
1:D:141:ASP:HB3	2:D:701:HOH:O	2.14	0.47
1:B:297:HIS:CE1	1:B:298:PRO:HD3	2.49	0.47
1:C:393:GLU:H	1:C:393:GLU:CD	2.21	0.47
1:C:89:ALA:O	1:C:93:GLU:HG3	2.15	0.47
1:C:93:GLU:CD	1:C:111:ARG:HH21	2.23	0.47
1:D:209:HIS:HE1	1:D:211:GLU:OE2	1.97	0.47
1:D:348:LEU:HD12	2:D:543:HOH:O	2.15	0.47
1:C:13:ILE:HG22	2:C:623:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:LYS:HD2	1:D:116:LYS:H	1.79	0.46
1:D:428:GLU:HG2	2:D:646:HOH:O	2.15	0.46
1:B:105:PRO:HD3	2:B:616:HOH:O	2.16	0.46
1:C:187:ALA:O	1:C:190:LYS:HB2	2.15	0.46
1:D:106:LYS:HG3	2:D:452:HOH:O	2.16	0.46
1:C:97:ARG:NH1	2:C:454:HOH:O	2.32	0.46
1:A:54:ALA:HB3	1:A:55:PRO:HD3	1.98	0.46
1:B:364:GLY:O	1:B:390:CYS:HA	2.15	0.46
1:A:190:LYS:O	1:A:191:ALA:C	2.58	0.46
1:B:297:HIS:N	1:B:298:PRO:CD	2.79	0.46
1:B:346:THR:HA	1:D:37:ARG:HH11	1.81	0.46
1:D:80:PRO:HB2	1:D:86:SER:HA	1.98	0.46
1:A:301:GLU:HG2	1:A:306:VAL:O	2.15	0.46
1:D:158:ILE:N	1:D:158:ILE:CD1	2.79	0.46
1:B:343:ASP:C	1:B:345:ASN:N	2.74	0.46
1:A:146:ARG:HD3	2:A:627:HOH:O	2.15	0.45
1:A:96:GLU:HA	1:A:100:PHE:O	2.16	0.45
1:A:105:PRO:HD3	2:A:640:HOH:O	2.16	0.45
1:B:80:PRO:HB2	1:B:86:SER:HA	1.97	0.45
1:D:440:LEU:O	1:D:444:LEU:HG	2.17	0.45
1:A:393:GLU:H	1:A:393:GLU:CD	2.24	0.45
1:D:340:ASN:HD22	1:D:340:ASN:N	2.13	0.45
1:A:89:ALA:O	1:A:93:GLU:HG3	2.15	0.45
1:C:302:MET:CE	1:C:391:TYR:HB2	2.40	0.45
1:A:388:LEU:O	1:A:402:MET:HE1	2.16	0.45
1:A:181:SER:HB2	2:A:560:HOH:O	2.17	0.45
1:A:137:PRO:HG3	2:A:482:HOH:O	2.17	0.45
1:B:421:GLN:O	1:B:425:MET:HG2	2.17	0.45
1:C:403:LYS:HD3	2:C:614:HOH:O	2.17	0.45
1:D:343:ASP:OD2	1:D:415:LYS:HD3	2.17	0.45
1:B:423:ARG:NH2	1:B:443:LYS:HE2	2.32	0.45
1:D:116:LYS:H	1:D:116:LYS:CD	2.26	0.44
1:A:0:HIS:CD2	1:A:2:LEU:H	2.35	0.44
1:B:388:LEU:O	1:B:402:MET:HE1	2.17	0.44
1:B:391:TYR:CD1	1:B:392:GLY:N	2.85	0.44
1:B:427:ASP:OD2	1:B:429:ASN:N	2.50	0.44
1:B:186:ARG:C	1:B:190:LYS:HE3	2.43	0.44
1:C:189:ALA:O	1:C:192:ALA:N	2.51	0.44
1:D:31:VAL:HB	1:D:51:ILE:HG21	1.99	0.44
1:D:297:HIS:N	1:D:298:PRO:CD	2.80	0.44
1:A:244:PRO:HB2	1:A:253:ARG:HH21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ALA:HB3	2:B:644:HOH:O	2.15	0.44
1:D:251:GLU:H	1:D:251:GLU:CD	2.24	0.44
1:A:142:MET:HB3	2:A:627:HOH:O	2.16	0.44
1:B:106:LYS:NZ	2:B:548:HOH:O	2.46	0.44
1:C:113:MET:HE1	1:C:123:MET:HE3	1.99	0.44
1:C:12:GLU:CD	1:C:387:LYS:HE2	2.43	0.44
1:D:442:LYS:HD2	1:D:447:GLN:NE2	2.32	0.44
1:A:143:ASP:OD1	1:A:146:ARG:NH2	2.51	0.44
1:C:184:MET:O	1:C:188:GLU:HG2	2.18	0.44
1:C:39:LEU:HB2	1:C:42:VAL:HG23	2.00	0.44
1:C:252:LEU:HG	1:C:284:PHE:HE1	1.83	0.44
1:B:115:ASP:HB3	1:B:118:SER:OG	2.18	0.44
1:B:187:ALA:HA	1:B:190:LYS:CE	2.48	0.44
1:B:296:GLU:C	1:B:298:PRO:HD2	2.43	0.44
1:A:108:GLU:CD	1:A:108:GLU:H	2.26	0.43
1:A:235:ARG:HG2	2:A:633:HOH:O	2.17	0.43
1:D:234:ARG:O	1:D:235:ARG:HB2	2.17	0.43
1:D:421:GLN:OE1	1:D:421:GLN:HA	2.18	0.43
1:C:97:ARG:NH1	1:C:97:ARG:CG	2.75	0.43
1:D:326:GLU:OE1	1:D:326:GLU:N	2.33	0.43
1:A:297:HIS:N	1:A:298:PRO:CD	2.81	0.43
1:D:249:THR:HG23	2:D:656:HOH:O	2.17	0.43
1:A:184:MET:O	1:A:188:GLU:HG3	2.19	0.43
1:D:144:LYS:O	1:D:148:ILE:HG13	2.18	0.43
1:C:112:LEU:HD12	1:C:118:SER:OG	2.17	0.43
1:C:116:LYS:O	1:C:120:ILE:HG12	2.18	0.43
1:D:6:VAL:HB	1:D:78:ILE:HG12	2.00	0.43
1:A:393:GLU:OE2	1:A:393:GLU:N	2.46	0.43
1:C:369:SER:OG	1:C:371:ILE:HG12	2.19	0.43
1:C:444:LEU:CB	1:C:446:LEU:HD13	2.48	0.43
1:C:31:VAL:HA	1:C:49:VAL:O	2.18	0.43
1:A:138:LEU:O	1:A:186:ARG:NH2	2.50	0.43
1:A:302:MET:CE	1:A:391:TYR:HB2	2.43	0.43
1:B:329:HIS:HB2	1:B:331:ARG:HH12	1.83	0.43
1:C:331:ARG:HD2	2:C:480:HOH:O	2.19	0.43
1:D:186:ARG:HG3	2:D:675:HOH:O	2.18	0.43
1:D:228:ARG:NH2	1:D:294:GLN:HG3	2.34	0.43
1:B:259:ARG:HG3	1:B:259:ARG:NH1	2.34	0.43
1:B:329:HIS:HB2	1:B:331:ARG:NH1	2.34	0.43
1:C:170:ARG:HD3	2:C:611:HOH:O	2.19	0.43
1:D:55:PRO:HA	2:D:586:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:ASP:OD2	1:D:429:ASN:HB2	2.19	0.43
1:A:97:ARG:NH1	1:A:97:ARG:CG	2.81	0.42
1:C:148:ILE:HG13	2:C:496:HOH:O	2.18	0.42
1:C:159:LYS:O	1:C:198:VAL:HA	2.19	0.42
1:C:80:PRO:O	1:C:81:GLY:C	2.62	0.42
1:D:281:ASN:HB2	2:D:484:HOH:O	2.19	0.42
1:C:13:ILE:O	1:C:17:ILE:HG13	2.19	0.42
1:C:142:MET:O	1:C:146:ARG:HG3	2.20	0.42
1:D:286:PHE:CZ	1:D:288:GLU:HA	2.54	0.42
1:A:227:GLU:N	1:A:227:GLU:OE1	2.52	0.42
1:A:243:ALA:HA	1:A:244:PRO:C	2.44	0.42
1:C:174:GLY:HA3	2:C:511:HOH:O	2.19	0.42
1:C:157:ILE:HD11	1:C:169:MET:HB2	2.01	0.42
1:B:18:LEU:C	1:B:18:LEU:HD23	2.45	0.42
1:C:207:PRO:O	1:C:436:ASN:HB2	2.20	0.42
1:D:142:MET:C	1:D:144:LYS:H	2.26	0.42
1:D:186:ARG:CG	1:D:196:ASP:HB2	2.36	0.42
1:A:407:GLN:HG3	2:A:599:HOH:O	2.18	0.42
1:D:17:ILE:HD13	1:D:79:HIS:CG	2.54	0.42
1:B:140:ASP:HB3	2:B:692:HOH:O	2.20	0.42
1:B:245:ALA:HB3	1:B:248:ILE:HG13	2.01	0.42
1:C:143:ASP:CG	1:C:146:ARG:HH21	2.27	0.42
1:C:279:PHE:CZ	1:C:282:GLY:HA2	2.55	0.42
1:C:251:GLU:CD	1:C:251:GLU:H	2.28	0.42
1:C:404:ASN:ND2	2:C:622:HOH:O	2.53	0.42
1:D:111:ARG:HG2	1:D:111:ARG:NH1	2.35	0.42
1:C:195:ASN:OD1	1:C:197:MET:HG2	2.20	0.42
1:D:278:LEU:HD23	1:D:278:LEU:HA	1.92	0.41
1:A:2:LEU:HA	1:A:76:VAL:CG2	2.50	0.41
1:A:178:LEU:HD12	2:A:560:HOH:O	2.19	0.41
1:C:296:GLU:O	1:C:299:VAL:HG22	2.20	0.41
1:B:287:ILE:O	1:B:288:GLU:HB3	2.20	0.41
1:B:346:THR:HA	1:D:37:ARG:HB2	2.02	0.41
1:D:57:VAL:HG23	1:D:58:LYS:HG3	2.01	0.41
1:A:78:ILE:HD12	1:A:95:VAL:HG13	2.02	0.41
1:A:162:GLY:O	1:A:193:PHE:HD2	1.83	0.41
1:B:6:VAL:HG21	1:B:70:ALA:HB2	2.03	0.41
1:B:27:LYS:HA	1:B:46:ASP:OD1	2.20	0.41
1:D:399:ILE:O	1:D:403:LYS:HG3	2.21	0.41
1:A:274:THR:OG1	1:A:294:GLN:CG	2.68	0.41
1:B:243:ALA:HA	1:B:244:PRO:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:LYS:HB3	1:B:326:GLU:OE1	2.20	0.41
1:D:32:HIS:O	1:D:50:CYS:HA	2.20	0.41
1:C:403:LYS:HE3	2:C:734:HOH:O	2.21	0.41
1:B:158:ILE:HG22	1:B:185:THR:HG21	2.03	0.41
1:D:256:ILE:HD12	1:D:256:ILE:HA	1.94	0.41
1:A:237:GLN:NE2	2:A:695:HOH:O	2.53	0.41
1:B:379:PRO:HD2	1:B:380:TYR:CE1	2.55	0.41
1:C:259:ARG:NH1	2:C:629:HOH:O	2.53	0.41
1:C:37:ARG:CZ	2:C:730:HOH:O	2.69	0.41
1:C:254:ARG:HD2	2:C:602:HOH:O	2.20	0.41
1:C:346:THR:C	1:C:348:LEU:H	2.29	0.41
1:D:93:GLU:CD	1:D:111:ARG:HH21	2.29	0.41
1:D:302:MET:HE1	1:D:389:ILE:HG22	2.02	0.41
1:D:348:LEU:O	1:D:349:PRO:C	2.63	0.41
1:B:427:ASP:HB2	1:B:443:LYS:HZ2	1.83	0.41
1:B:12:GLU:OE2	1:B:82:TYR:OH	2.36	0.40
1:C:274:THR:OG1	1:C:294:GLN:HG3	2.21	0.40
1:D:170:ARG:NH2	1:D:184:MET:HE1	2.36	0.40
1:D:235:ARG:O	1:D:236:HIS:HB2	2.21	0.40
1:D:364:GLY:O	1:D:390:CYS:HA	2.21	0.40
1:A:212:ILE:N	1:A:212:ILE:HD12	2.37	0.40
1:B:421:GLN:HA	1:B:421:GLN:OE1	2.22	0.40
1:B:294:GLN:HE21	1:B:294:GLN:HA	1.85	0.40
1:D:319:GLN:HA	1:D:320:PRO:HD3	1.97	0.40
1:A:195:ASN:HD21	1:A:197:MET:CB	2.31	0.40
1:A:429:ASN:ND2	1:A:439:TYR:OH	2.48	0.40
1:B:302:MET:HE2	1:B:334:ALA:HB1	2.04	0.40
1:D:37:ARG:NE	2:D:598:HOH:O	2.55	0.40
1:D:357:PHE:HA	1:D:410:ILE:O	2.22	0.40
1:B:19:ARG:HD2	2:B:559:HOH:O	2.22	0.40
1:C:346:THR:C	1:C:348:LEU:N	2.78	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)
1:A:353:LYS:NZ	1:C:192:ALA:O[1_545]	2.14	0.06
1:D:1:MET:O	1:D:170:ARG:NH2[1_455]	2.19	0.01

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	439/469 (94%)	418 (95%)	17 (4%)	4 (1%)	14	14
1	B	436/469 (93%)	412 (94%)	23 (5%)	1 (0%)	43	51
1	C	442/469 (94%)	423 (96%)	19 (4%)	0	100	100
1	D	443/469 (94%)	421 (95%)	21 (5%)	1 (0%)	43	51
All	All	1760/1876 (94%)	1674 (95%)	80 (4%)	6 (0%)	36	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	ALA
1	A	192	ALA
1	A	-2	GLY
1	A	162	GLY
1	B	176	ALA
1	D	-2	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	359/377 (95%)	356 (99%)	3 (1%)	73	85
1	B	357/377 (95%)	351 (98%)	6 (2%)	53	69
1	C	360/377 (96%)	353 (98%)	7 (2%)	50	66
1	D	361/377 (96%)	355 (98%)	6 (2%)	53	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1437/1508 (95%)	1415 (98%)	22 (2%)	57 73

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	A	108	GLU
1	A	444	LEU
1	B	5	ILE
1	B	37	ARG
1	B	40	LYS
1	B	180	GLN
1	B	235	ARG
1	B	294	GLN
1	C	169	MET
1	C	177	GLU
1	C	207	PRO
1	C	237	GLN
1	C	294	GLN
1	C	326	GLU
1	C	348	LEU
1	D	-3	ARG
1	D	37	ARG
1	D	116	LYS
1	D	117	VAL
1	D	158	ILE
1	D	326	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	94	GLN
1	A	145	ASN
1	A	195	ASN
1	A	281	ASN
1	A	294	GLN
1	A	319	GLN
1	A	340	ASN
1	A	407	GLN
1	A	429	ASN

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Mol	Chain	Res	Type
1	A	431	GLN
1	A	432	HIS
1	A	447	GLN
1	B	145	ASN
1	B	180	GLN
1	B	206	ASN
1	B	209	HIS
1	B	237	GLN
1	B	290	ASN
1	B	294	GLN
1	B	319	GLN
1	B	404	ASN
1	B	429	ASN
1	B	438	HIS
1	B	447	GLN
1	C	0	HIS
1	C	90	ASN
1	C	94	GLN
1	C	206	ASN
1	C	233	GLN
1	C	237	GLN
1	C	281	ASN
1	C	290	ASN
1	C	294	GLN
1	C	340	ASN
1	C	345	ASN
1	C	404	ASN
1	C	429	ASN
1	C	438	HIS
1	D	0	HIS
1	D	180	GLN
1	D	209	HIS
1	D	294	GLN
1	D	319	GLN
1	D	340	ASN
1	D	404	ASN
1	D	447	GLN

5.3.3 RNA ⓘ

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 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

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	445/469 (94%)	-0.19	9 (2%) 65 62	10, 20, 40, 55	2 (0%)
1	B	442/469 (94%)	-0.11	8 (1%) 67 64	12, 22, 40, 58	2 (0%)
1	C	446/469 (95%)	-0.28	6 (1%) 75 73	10, 19, 38, 52	2 (0%)
1	D	447/469 (95%)	-0.17	10 (2%) 62 59	9, 20, 39, 52	2 (0%)
All	All	1780/1876 (94%)	-0.19	33 (1%) 66 63	9, 21, 39, 58	8 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	PHE	5.9
1	C	192	ALA	5.5
1	C	193	PHE	5.0
1	A	192	ALA	4.7
1	A	191	ALA	4.2
1	B	197	MET	3.8
1	B	-2	GLY	3.6
1	B	191	ALA	3.4
1	A	190	LYS	3.4
1	B	196	ASP	3.3
1	D	161	SER	3.2
1	D	191	ALA	3.1
1	C	-2	GLY	3.0
1	C	191	ALA	2.9
1	D	-2	GLY	2.9
1	D	168	GLY	2.8
1	C	195	ASN	2.7
1	C	194	SER	2.6
1	D	197	MET	2.5
1	D	3	ASP	2.5
1	D	432	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	446	LEU	2.4
1	D	447	GLN	2.3
1	D	117	VAL	2.3
1	A	447	GLN	2.3
1	A	195	ASN	2.2
1	A	-2	GLY	2.2
1	A	188	GLU	2.2
1	B	-1	SER	2.2
1	B	115	ASP	2.1
1	B	345	ASN	2.1
1	D	115	ASP	2.1
1	A	326	GLU	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 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.