



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:05 PM UTC

PDB ID : 3X0X / pdb_00003x0x
Title : Crystal structure of apo-DszC from Rhodococcus erythropolis D-1
Authors : Guan, L.J.; Lee, W.C.; Wang, S.P.; Ohtsuka, J.; Tanokura, M.
Deposited on : 2014-10-23
Resolution : 2.11 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

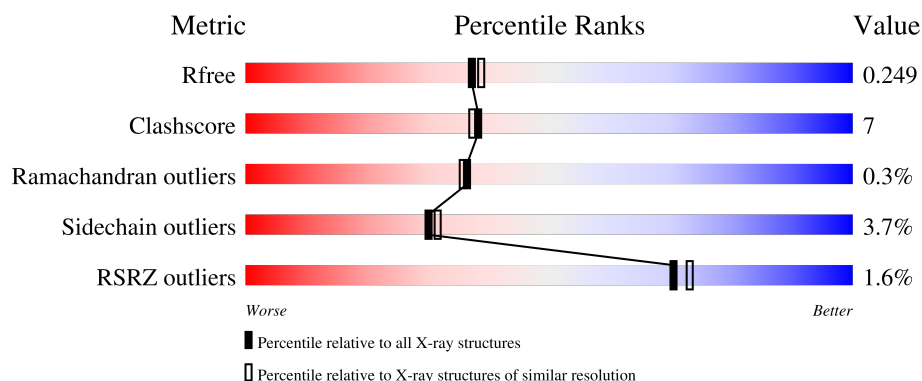
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	417	
1	B	417	
1	C	417	
1	D	417	
1	E	417	

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Mol	Chain	Length	Quality of chain
1	F	417	% 76% 17%
1	G	417	% 81% 14%
1	H	417	8% 69% 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25802 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 DszC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3054	1918	545	587	4			
1	B	400	Total	C	N	O	S	0	0	0
			3054	1918	545	587	4			
1	D	400	Total	C	N	O	S	0	0	0
			3054	1918	545	587	4			
1	C	400	Total	C	N	O	S	0	0	0
			3054	1918	545	587	4			
1	E	400	Total	C	N	O	S	0	0	0
			3054	1918	545	587	4			
1	F	400	Total	C	N	O	S	0	0	0
			3054	1918	545	587	4			
1	G	400	Total	C	N	O	S	0	0	0
			3054	1918	545	587	4			
1	H	400	Total	C	N	O	S	0	0	0
			3054	1918	545	587	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	189	Total	O	0	0
			189	189		
2	B	223	Total	O	0	0
			223	223		
2	D	196	Total	O	0	0
			196	196		
2	C	196	Total	O	0	0
			196	196		
2	E	191	Total	O	0	0
			191	191		
2	F	153	Total	O	0	0
			153	153		

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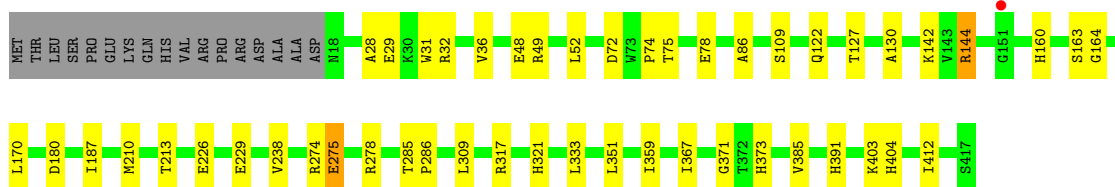
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	146	Total 146	O 146	0	0
2	H	76	Total 76	O 76	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DszC

Chain A: 



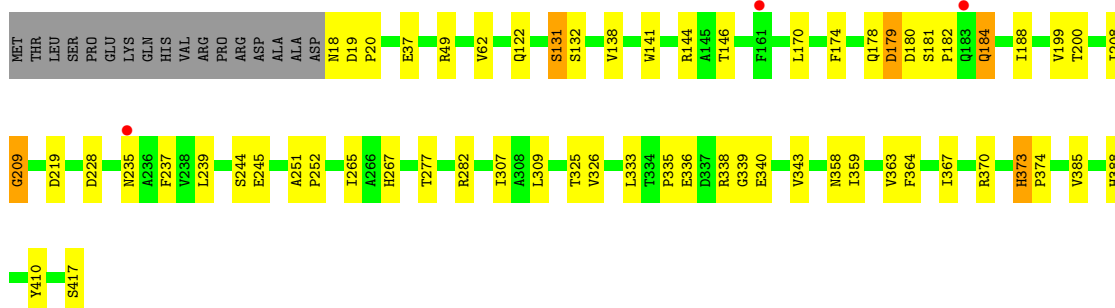
• Molecule 1: DszC

Chain B: 



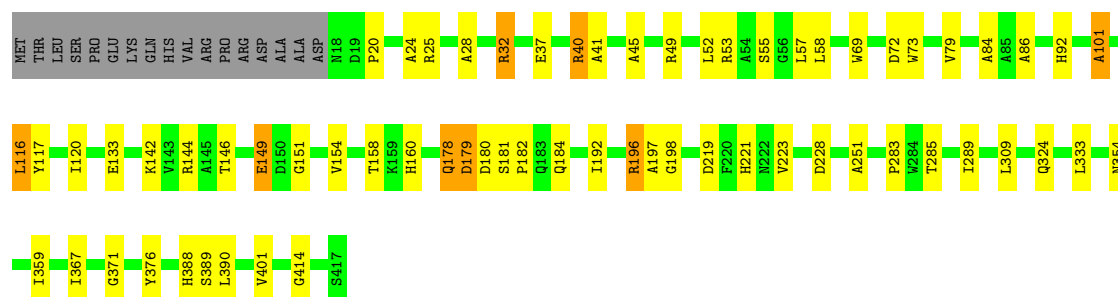
• Molecule 1: DszC

Chain D: 



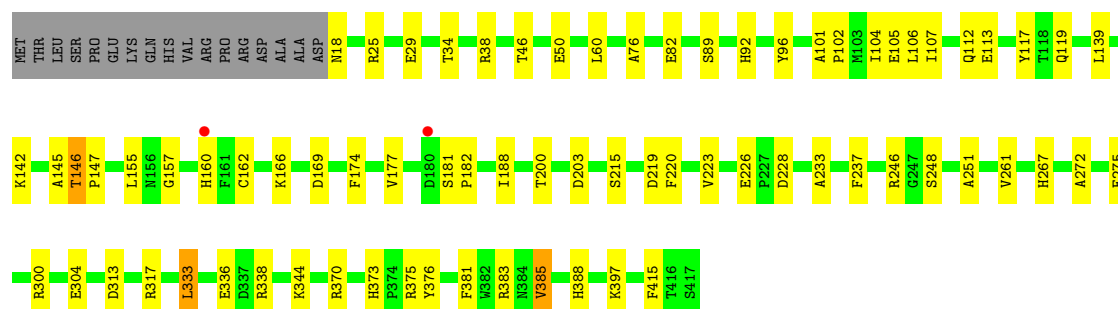
• Molecule 1: DszC

Chain C:  80% 14% . .



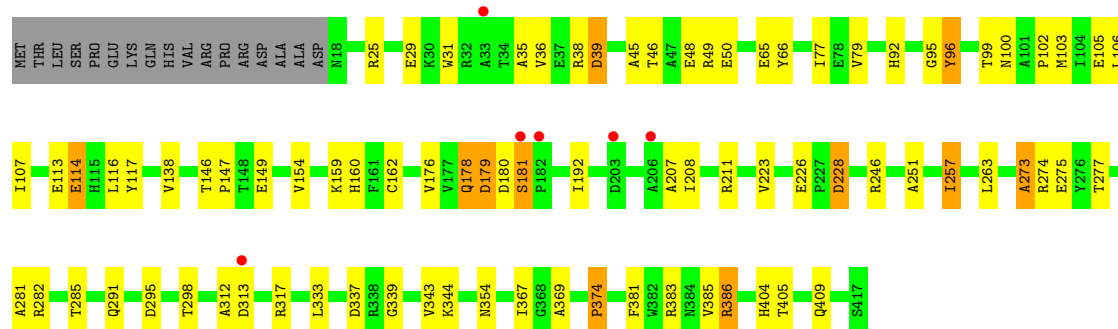
• Molecule 1: DszC

Chain E:  78% 17% . .



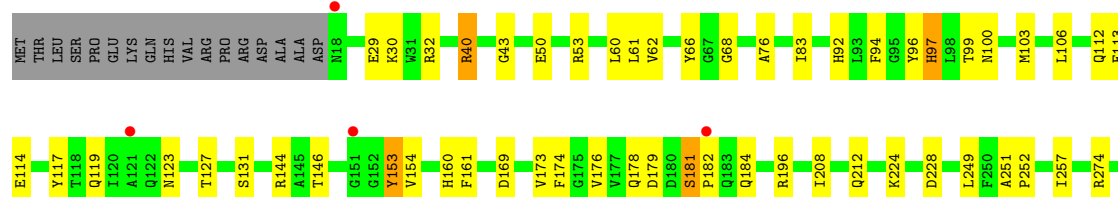
• Molecule 1: DszC

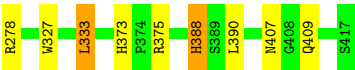
Chain F:  76% 17% . .



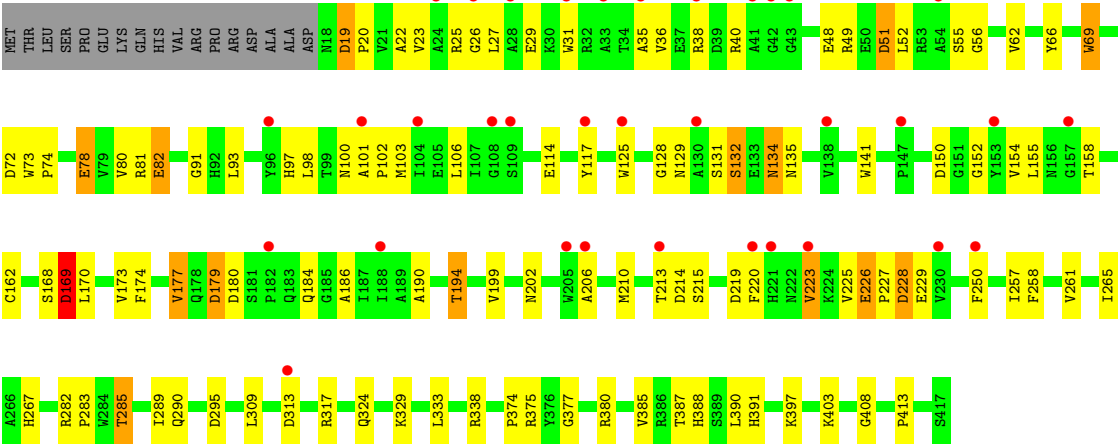
• Molecule 1: DszC

Chain G:  81% 14% . .





● Molecule 1: DszC



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.13Å 123.25Å 184.27Å 90.00° 101.21° 90.00°	Depositor
Resolution (Å)	43.91 – 2.11 43.91 – 2.11	Depositor EDS
% Data completeness (in resolution range)	98.2 (43.91-2.11) 98.2 (43.91-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.186 , 0.253 0.184 , 0.249	Depositor DCC
R_{free} test set	8996 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25802	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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

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	1.19	6/3129 (0.2%)	1.12	3/4265 (0.1%)
1	B	1.23	5/3129 (0.2%)	1.19	6/4265 (0.1%)
1	C	1.28	7/3129 (0.2%)	1.21	13/4265 (0.3%)
1	D	1.25	8/3129 (0.3%)	1.17	7/4265 (0.2%)
1	E	1.22	7/3129 (0.2%)	1.19	8/4265 (0.2%)
1	F	1.16	4/3129 (0.1%)	1.17	15/4265 (0.4%)
1	G	1.14	3/3129 (0.1%)	1.15	4/4265 (0.1%)
1	H	1.00	2/3129 (0.1%)	1.08	10/4265 (0.2%)
All	All	1.19	42/25032 (0.2%)	1.16	66/34120 (0.2%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	267	HIS	CG-CD2	7.36	1.44	1.35
1	C	84	ALA	CA-C	-7.10	1.43	1.52
1	D	131	SER	CA-C	6.64	1.56	1.52
1	D	373	HIS	CG-CD2	6.52	1.43	1.35
1	D	209	GLY	N-CA	6.32	1.51	1.45
1	C	388	HIS	CG-CD2	6.30	1.42	1.35
1	A	373	HIS	CG-CD2	6.25	1.42	1.35
1	C	388	HIS	ND1-CE1	6.01	1.38	1.32
1	D	170	LEU	CA-C	5.87	1.59	1.52
1	B	92	HIS	CG-CD2	5.85	1.42	1.35
1	D	326	VAL	CA-C	5.78	1.60	1.52
1	E	261	VAL	CA-C	5.54	1.59	1.52
1	D	388	HIS	CG-CD2	5.53	1.42	1.35
1	C	414	GLY	N-CA	5.46	1.51	1.44
1	H	295	ASP	CA-C	5.42	1.59	1.53
1	B	404	HIS	ND1-CE1	5.34	1.37	1.32
1	F	404	HIS	ND1-CE1	5.34	1.37	1.32
1	C	73	TRP	CA-C	-5.33	1.46	1.52
1	F	405	THR	C-O	-5.33	1.18	1.24
1	A	321	HIS	CE1-NE2	5.32	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	285	THR	C-O	-5.31	1.17	1.24
1	D	49	ARG	CA-C	5.28	1.59	1.52
1	E	373	HIS	CG-CD2	5.28	1.41	1.35
1	A	373	HIS	ND1-CE1	5.27	1.37	1.32
1	E	383	ARG	N-CA	5.26	1.52	1.46
1	G	388	HIS	CE1-NE2	5.20	1.37	1.32
1	C	389	SER	N-CA	5.19	1.52	1.46
1	E	160	HIS	CG-CD2	5.18	1.41	1.35
1	A	391	HIS	CG-CD2	5.18	1.41	1.35
1	E	92	HIS	CG-CD2	5.15	1.41	1.35
1	A	160	HIS	CG-CD2	5.14	1.41	1.35
1	F	386	ARG	N-CA	-5.14	1.39	1.46
1	C	101	ALA	N-CA	5.14	1.51	1.46
1	G	97	HIS	CG-CD2	5.13	1.41	1.35
1	B	388	HIS	CG-CD2	5.11	1.41	1.35
1	B	391	HIS	CG-CD2	5.09	1.41	1.35
1	B	404	HIS	CG-CD2	5.05	1.41	1.35
1	G	388	HIS	CG-CD2	5.04	1.41	1.35
1	D	267	HIS	CG-CD2	5.04	1.41	1.35
1	E	388	HIS	CG-CD2	5.03	1.41	1.35
1	A	404	HIS	CG-CD2	5.02	1.41	1.35
1	F	160	HIS	CG-CD2	5.02	1.41	1.35

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	385	VAL	CB-CA-C	-9.12	99.63	112.22
1	B	282	ARG	CA-C-N	8.16	128.18	119.78
1	B	282	ARG	C-N-CA	8.16	128.18	119.78
1	E	251	ALA	CA-C-N	-7.79	110.93	119.19
1	E	251	ALA	C-N-CA	-7.79	110.93	119.19
1	C	401	VAL	N-CA-C	-7.43	103.22	110.72
1	C	285	THR	CA-C-N	-7.18	112.78	119.82
1	C	285	THR	C-N-CA	-7.18	112.78	119.82
1	F	79	VAL	N-CA-C	-7.13	103.52	110.72
1	D	146	THR	CA-C-N	-6.74	113.00	120.14
1	D	146	THR	C-N-CA	-6.74	113.00	120.14
1	G	160	HIS	N-CA-C	6.53	118.06	111.07
1	E	146	THR	CB-CA-C	6.45	118.13	109.42
1	C	57	LEU	N-CA-C	6.31	119.82	111.75
1	H	128	GLY	N-CA-C	-6.18	100.82	111.57
1	F	50	GLU	N-CA-C	6.12	118.03	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	100	ASN	N-CA-C	5.94	117.44	110.97
1	A	130	ALA	N-CA-C	-5.91	98.20	110.80
1	H	285	THR	CA-C-N	-5.89	114.05	119.82
1	H	285	THR	C-N-CA	-5.89	114.05	119.82
1	F	192	ILE	N-CA-C	5.88	114.37	107.84
1	B	251	ALA	CA-C-N	-5.84	113.00	119.19
1	B	251	ALA	C-N-CA	-5.84	113.00	119.19
1	H	19	ASP	CA-C-N	5.84	125.46	119.56
1	H	19	ASP	C-N-CA	5.84	125.46	119.56
1	F	251	ALA	CA-C-N	-5.82	112.88	119.28
1	F	251	ALA	C-N-CA	-5.82	112.88	119.28
1	D	62	VAL	CA-C-N	-5.81	113.79	119.78
1	D	62	VAL	C-N-CA	-5.81	113.79	119.78
1	C	73	TRP	CA-C-N	-5.80	113.04	119.19
1	C	73	TRP	C-N-CA	-5.80	113.04	119.19
1	G	153	TYR	CA-C-N	-5.72	116.10	123.19
1	G	153	TYR	C-N-CA	-5.72	116.10	123.19
1	E	272	ALA	N-CA-C	-5.69	105.00	111.14
1	C	251	ALA	CA-C-N	-5.62	113.23	119.19
1	C	251	ALA	C-N-CA	-5.62	113.23	119.19
1	F	369	ALA	N-CA-C	5.60	117.38	111.28
1	C	86	ALA	N-CA-C	-5.57	105.61	112.90
1	C	160	HIS	N-CA-C	5.56	117.42	111.36
1	B	83	ILE	N-CA-C	-5.56	104.94	111.00
1	F	337	ASP	N-CA-C	-5.55	105.22	111.28
1	F	180	ASP	N-CA-C	-5.53	106.89	113.97
1	F	273	ALA	N-CA-C	-5.53	105.15	111.07
1	G	112	GLN	N-CA-C	-5.49	105.30	111.28
1	F	178	GLN	N-CA-C	-5.46	99.63	108.52
1	D	326	VAL	N-CA-C	5.43	116.16	110.62
1	D	199	VAL	CB-CA-C	-5.42	104.36	111.25
1	H	91	GLY	N-CA-C	-5.38	105.98	112.49
1	A	164	GLY	N-CA-C	-5.31	106.90	115.08
1	E	397	LYS	N-CA-C	-5.31	105.58	111.36
1	H	317	ARG	N-CA-C	5.30	117.06	111.28
1	E	89	SER	N-CA-C	5.30	116.74	110.97
1	A	385	VAL	CB-CA-C	-5.28	104.93	112.22
1	D	325	THR	N-CA-C	-5.24	105.48	111.14
1	F	25	ARG	CA-C-N	5.23	125.90	119.99
1	F	25	ARG	C-N-CA	5.23	125.90	119.99
1	C	41	ALA	N-CA-C	5.21	117.05	111.36
1	C	116	LEU	N-CA-C	5.20	116.94	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	ASN	N-CA-C	5.18	117.67	111.71
1	E	169	ASP	N-CA-C	-5.17	107.04	113.55
1	H	169	ASP	N-CA-C	-5.16	107.11	113.41
1	C	133	GLU	N-CA-C	-5.11	98.94	107.99
1	F	107	ILE	CB-CA-C	-5.10	105.83	110.63
1	F	106	LEU	N-CA-C	5.01	116.44	111.07
1	H	19	ASP	N-CA-C	5.01	117.00	110.08
1	H	261	VAL	N-CA-C	-5.01	105.71	110.42

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	3054	0	2932	25	0
1	B	3054	0	2932	36	0
1	C	3054	0	2932	34	0
1	D	3054	0	2932	37	0
1	E	3054	0	2932	38	0
1	F	3054	0	2932	50	0
1	G	3054	0	2932	38	0
1	H	3054	0	2932	84	0
2	A	189	0	0	9	0
2	B	223	0	0	8	0
2	C	196	0	0	4	0
2	D	196	0	0	7	0
2	E	191	0	0	7	0
2	F	153	0	0	3	0
2	G	146	0	0	1	0
2	H	76	0	0	9	0
All	All	25802	0	23456	332	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (332) 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:H:31:TRP:O	1:H:38:ARG:NH2	1.87	1.08
1:D:282:ARG:HD2	1:D:370:ARG:NH1	1.73	1.02
1:G:97:HIS:ND1	1:G:127:THR:HG22	1.75	1.01
1:E:370:ARG:HD3	1:G:161:PHE:CZ	2.06	0.91
1:B:181:SER:HB2	1:B:182:PRO:HD2	1.52	0.89
1:H:101:ALA:HB3	1:H:102:PRO:HD3	1.55	0.89
1:D:282:ARG:CD	1:D:370:ARG:NH1	2.43	0.81
1:D:282:ARG:HD2	1:D:370:ARG:HH12	1.47	0.80
1:H:377:GLY:O	1:H:380:ARG:NH1	2.14	0.80
1:D:282:ARG:CD	1:D:370:ARG:HH12	1.96	0.79
1:F:31:TRP:HB3	1:F:38:ARG:HH22	1.49	0.77
1:H:199:VAL:HG23	1:H:223:VAL:HG11	1.67	0.77
1:E:155:LEU:HB2	1:E:223:VAL:HB	1.66	0.76
1:H:62:VAL:HG13	1:H:117:TYR:HD2	1.51	0.75
1:F:31:TRP:HB3	1:F:38:ARG:NH2	2.01	0.74
1:E:370:ARG:HD3	1:G:161:PHE:HZ	1.55	0.72
1:D:282:ARG:HD2	1:D:370:ARG:HH11	1.54	0.71
1:G:181:SER:HB2	1:G:182:PRO:CD	2.21	0.70
1:H:56:GLY:O	1:H:69:TRP:NE1	2.22	0.69
1:H:329:LYS:NZ	2:H:523:HOH:O	2.25	0.69
1:D:181:SER:HB2	1:D:182:PRO:HD2	1.73	0.69
1:B:180:ASP:OD1	1:B:180:ASP:N	2.26	0.68
1:B:354:ASN:ND2	2:B:642:HOH:O	2.19	0.68
1:H:210:MET:HE3	1:H:388:HIS:HB2	1.74	0.68
1:H:132:SER:OG	1:H:134:ASN:OD1	2.09	0.67
1:F:45:ALA:O	1:F:49:ARG:HG3	1.95	0.66
1:E:106:LEU:HD22	1:E:246:ARG:O	1.95	0.66
1:B:280:GLN:OE1	1:F:409:GLN:HG3	1.96	0.66
1:F:99:THR:HG22	1:F:257:ILE:HD13	1.78	0.65
1:H:81:ARG:HH22	1:H:313:ASP:CG	2.03	0.65
1:C:158:THR:OG1	1:C:219:ASP:OD1	2.13	0.65
1:D:277:THR:HG23	2:D:580:HOH:O	1.96	0.65
1:G:181:SER:HB2	1:G:182:PRO:HD2	1.77	0.65
1:H:173:VAL:O	1:H:174:PHE:HD1	1.79	0.65
1:H:177:VAL:CG1	1:H:186:ALA:HB3	2.27	0.65
1:H:66:TYR:CE1	1:H:114:GLU:HA	2.32	0.64
1:H:380:ARG:NH2	2:H:553:HOH:O	2.27	0.64
1:H:155:LEU:HB2	1:H:223:VAL:HG23	1.79	0.64
1:F:113:GLU:O	1:F:117:TYR:HB2	1.98	0.64
1:H:82:GLU:OE2	1:H:82:GLU:HA	1.96	0.63
1:C:142:LYS:NZ	2:C:598:HOH:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:LEU:HD21	1:G:76:ALA:HB2	1.81	0.63
1:F:381:PHE:O	1:F:385:VAL:HG23	1.99	0.62
1:H:152:GLY:HA3	1:H:225:VAL:O	1.99	0.62
1:E:300:ARG:O	1:E:304:GLU:HG3	2.00	0.62
1:G:99:THR:HG22	1:G:257:ILE:HD12	1.82	0.62
1:H:132:SER:HB2	1:H:141:TRP:CH2	2.35	0.61
1:H:413:PRO:O	2:H:566:HOH:O	2.17	0.60
1:C:149:GLU:C	1:C:151:GLY:H	2.08	0.60
1:H:31:TRP:HZ2	1:H:51:ASP:HB2	1.66	0.59
1:A:48:GLU:OE2	2:A:649:HOH:O	2.15	0.59
1:F:207:ALA:HA	1:H:374:PRO:HD3	1.84	0.59
1:H:226:GLU:HB3	1:H:228:ASP:OD1	2.03	0.58
1:H:380:ARG:NH1	2:H:553:HOH:O	2.20	0.58
1:G:106:LEU:HD21	1:G:327:TRP:HZ3	1.69	0.58
1:B:92:HIS:HE1	2:B:651:HOH:O	1.85	0.58
1:F:105:GLU:HG2	1:F:246:ARG:HH12	1.68	0.58
1:B:226:GLU:HG2	1:B:229:GLU:OE1	2.04	0.58
1:C:144:ARG:HD2	1:C:178:GLN:HG2	1.86	0.57
1:D:200:THR:HB	1:D:219:ASP:HB2	1.85	0.57
1:F:317:ARG:NH2	2:F:558:HOH:O	2.37	0.57
1:H:177:VAL:HG13	1:H:186:ALA:HB3	1.87	0.57
1:A:49:ARG:NH2	2:A:542:HOH:O	2.05	0.57
1:E:34:THR:HG21	2:E:669:HOH:O	2.04	0.57
1:H:132:SER:HB2	1:H:141:TRP:HH2	1.69	0.57
1:E:375:ARG:NH1	2:E:579:HOH:O	2.36	0.57
1:H:180:ASP:HA	1:H:184:GLN:NE2	2.19	0.57
1:A:317:ARG:HD3	2:A:646:HOH:O	2.06	0.56
1:B:148:THR:HG22	1:B:152:GLY:N	2.20	0.56
1:E:18:ASN:N	2:E:525:HOH:O	2.38	0.56
1:F:38:ARG:HD3	1:F:48:GLU:CD	2.30	0.56
1:H:220:PHE:HD1	1:H:223:VAL:HG21	1.70	0.55
1:C:28:ALA:O	1:C:32:ARG:HD3	2.07	0.55
1:A:142:LYS:NZ	2:A:583:HOH:O	2.35	0.55
1:D:37:GLU:HB2	2:D:599:HOH:O	2.05	0.55
1:C:181:SER:HB2	1:C:182:PRO:HD2	1.88	0.55
1:E:174:PHE:HE2	1:E:415:PHE:CE1	2.25	0.55
1:H:100:ASN:OD1	1:H:129:ASN:HB3	2.07	0.55
1:H:35:ALA:HB1	2:H:555:HOH:O	2.06	0.55
1:F:105:GLU:CG	1:F:246:ARG:HH12	2.20	0.55
1:B:115:HIS:ND1	2:B:631:HOH:O	2.33	0.55
1:E:34:THR:HG23	1:E:38:ARG:HE	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LYS:HD3	2:B:697:HOH:O	2.05	0.54
1:F:31:TRP:HB3	1:F:38:ARG:NH1	2.22	0.54
1:H:173:VAL:C	1:H:174:PHE:HD1	2.15	0.54
1:C:37:GLU:OE2	1:C:40:ARG:NH1	2.40	0.54
1:F:39:ASP:O	1:F:211:ARG:NH1	2.40	0.54
1:G:100:ASN:HB2	1:G:127:THR:HG21	1.89	0.54
1:H:103:MET:HA	1:H:106:LEU:HD12	1.87	0.54
1:F:149:GLU:H	1:F:149:GLU:CD	2.15	0.54
1:H:38:ARG:HD3	1:H:48:GLU:HG2	1.90	0.54
1:D:235:ASN:O	1:D:239:LEU:HG	2.07	0.54
1:C:52:LEU:O	1:C:55:SER:OG	2.24	0.54
1:E:375:ARG:NH2	1:E:376:TYR:OH	2.40	0.54
1:C:146:THR:OG1	1:C:154:VAL:CG1	2.57	0.53
1:G:106:LEU:HD21	1:G:327:TRP:CZ3	2.43	0.53
1:C:376:TYR:OH	2:C:563:HOH:O	2.15	0.53
1:F:31:TRP:HB3	1:F:38:ARG:CZ	2.38	0.53
1:D:181:SER:HB2	1:D:182:PRO:CD	2.39	0.53
1:C:116:LEU:O	1:C:120:ILE:HG13	2.08	0.53
1:A:274:ARG:NH1	1:A:278:ARG:NH1	2.56	0.53
1:F:374:PRO:HG2	1:H:206:ALA:HB1	1.90	0.53
1:F:263:LEU:HD21	1:F:312:ALA:HB1	1.91	0.53
1:G:53:ARG:NH2	1:G:169:ASP:OD2	2.41	0.53
1:H:23:VAL:HG11	1:H:55:SER:HB2	1.89	0.53
1:B:116:LEU:O	1:B:120:ILE:HG13	2.09	0.52
1:G:119:GLN:O	1:G:123:ASN:HB2	2.09	0.52
1:G:100:ASN:OD1	1:G:127:THR:HG23	2.10	0.52
1:H:31:TRP:CZ2	1:H:51:ASP:HB2	2.45	0.52
1:A:109:SER:OG	2:A:636:HOH:O	2.18	0.52
1:B:181:SER:CB	1:B:182:PRO:HD2	2.34	0.52
1:D:174:PHE:HA	1:D:188:ILE:O	2.08	0.52
1:F:66:TYR:CE1	1:F:114:GLU:HG3	2.45	0.52
1:H:226:GLU:HB2	1:H:229:GLU:HG3	1.92	0.52
1:G:113:GLU:O	1:G:117:TYR:HB2	2.10	0.52
1:A:31:TRP:HH2	1:A:52:LEU:HG	1.76	0.51
1:B:72:ASP:HB2	1:B:324:GLN:OE1	2.09	0.51
1:D:358:ASN:HB2	2:D:642:HOH:O	2.10	0.51
1:G:99:THR:HG22	1:G:257:ILE:CD1	2.41	0.51
1:H:19:ASP:HB2	1:H:20:PRO:HD2	1.93	0.51
1:H:49:ARG:NH1	1:H:93:LEU:HD11	2.26	0.51
1:C:196:ARG:HG3	1:C:197:ALA:N	2.24	0.51
1:E:317:ARG:HD3	2:E:582:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ASN:N	1:E:18:ASN:HD21	2.10	0.50
1:H:173:VAL:HG13	1:H:190:ALA:HB3	1.93	0.50
1:H:283:PRO:HG3	1:H:290:GLN:O	2.11	0.50
1:C:354:ASN:ND2	2:C:584:HOH:O	2.45	0.50
1:E:101:ALA:O	1:E:104:ILE:HD12	2.12	0.50
1:C:146:THR:OG1	1:C:154:VAL:HG12	2.11	0.50
1:A:285:THR:N	1:A:286:PRO:CD	2.75	0.50
1:E:381:PHE:O	1:E:385:VAL:HG23	2.11	0.50
1:F:92:HIS:NE2	1:F:96:TYR:HD2	2.09	0.50
1:G:333:LEU:HD13	1:G:333:LEU:O	2.11	0.50
1:F:31:TRP:HB3	1:F:38:ARG:HH12	1.76	0.50
1:G:146:THR:O	1:G:153:TYR:HA	2.11	0.50
1:H:265:ILE:HG21	1:H:385:VAL:HG23	1.94	0.50
1:G:61:LEU:HD21	1:G:76:ALA:CB	2.42	0.49
1:F:95:GLY:O	1:F:99:THR:HG23	2.12	0.49
1:B:122:GLN:HG2	2:B:717:HOH:O	2.11	0.49
1:G:251:ALA:HB3	1:G:252:PRO:HD3	1.95	0.49
1:A:403:LYS:NZ	2:A:679:HOH:O	2.21	0.49
1:G:60:LEU:HD21	1:G:76:ALA:HA	1.94	0.49
1:E:333:LEU:HD13	1:E:333:LEU:O	2.13	0.49
1:A:74:PRO:O	1:A:78:GLU:HG2	2.12	0.49
1:H:23:VAL:CG1	1:H:55:SER:HB2	2.43	0.49
1:H:210:MET:CE	1:H:388:HIS:HB2	2.42	0.49
1:B:176:VAL:HG12	1:B:178:GLN:HG3	1.95	0.48
1:G:43:GLY:O	1:G:212:GLN:HG2	2.13	0.48
1:E:313:ASP:OD2	2:E:585:HOH:O	2.20	0.48
1:H:25:ARG:HG2	1:H:25:ARG:O	2.12	0.48
1:H:210:MET:HE3	1:H:388:HIS:CB	2.43	0.48
1:A:226:GLU:HG2	1:A:229:GLU:OE1	2.13	0.48
1:B:81:ARG:HH22	1:B:313:ASP:CG	2.22	0.48
1:C:92:HIS:HE1	2:C:615:HOH:O	1.95	0.48
1:E:174:PHE:CE2	1:E:415:PHE:CE1	3.01	0.48
1:F:149:GLU:CD	1:F:149:GLU:N	2.72	0.48
1:C:179:ASP:OD1	1:C:180:ASP:N	2.47	0.48
1:D:339:GLY:O	1:D:343:VAL:HG23	2.14	0.48
1:H:27:LEU:O	1:H:31:TRP:HB2	2.13	0.48
1:D:340:GLU:OE2	1:D:410:TYR:OH	2.25	0.48
1:F:274:ARG:NH2	1:F:275:GLU:OE1	2.47	0.48
1:B:45:ALA:O	1:B:49:ARG:HG3	2.14	0.47
1:H:162:CYS:O	1:H:215:SER:HA	2.15	0.47
1:A:144:ARG:NE	2:A:652:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:GLU:HG3	2:B:632:HOH:O	2.15	0.47
1:D:184:GLN:C	1:D:184:GLN:HE21	2.23	0.47
1:E:139:LEU:HD13	2:E:684:HOH:O	2.14	0.47
1:A:210:MET:HB3	1:A:213:THR:CG2	2.45	0.47
1:G:373:HIS:ND1	1:G:375:ARG:HG2	2.30	0.47
1:D:144:ARG:NH2	2:D:671:HOH:O	2.47	0.47
1:A:309:LEU:HG	1:A:359:ILE:CD1	2.46	0.46
1:H:213:THR:O	1:H:214:ASP:C	2.59	0.46
1:F:38:ARG:HD3	1:F:48:GLU:OE2	2.15	0.46
1:A:210:MET:HB3	1:A:213:THR:HG21	1.97	0.46
1:A:275:GLU:HG2	2:A:553:HOH:O	2.15	0.46
1:E:336:GLU:N	1:E:336:GLU:CD	2.74	0.46
1:G:40:ARG:NH1	2:G:595:HOH:O	2.48	0.46
1:H:40:ARG:NH1	2:H:512:HOH:O	2.48	0.46
1:H:179:ASP:O	1:H:184:GLN:NE2	2.48	0.46
1:B:99:THR:HG22	1:B:257:ILE:CD1	2.46	0.46
1:D:244:SER:HB3	1:D:335:PRO:HA	1.97	0.46
1:E:200:THR:OG1	1:E:219:ASP:HB2	2.16	0.46
1:H:101:ALA:HB3	1:H:102:PRO:CD	2.38	0.46
1:G:32:ARG:HH11	1:G:32:ARG:HB2	1.81	0.46
1:D:122:GLN:NE2	2:D:627:HOH:O	2.48	0.46
1:C:45:ALA:O	1:C:49:ARG:HG3	2.16	0.46
1:F:317:ARG:NH1	2:F:629:HOH:O	2.15	0.46
1:D:138:VAL:HA	1:D:141:TRP:CD1	2.51	0.45
1:F:179:ASP:HB3	1:F:181:SER:H	1.80	0.45
1:G:100:ASN:O	1:G:103:MET:HB3	2.16	0.45
1:G:407:ASN:HB2	1:G:409:GLN:HG3	1.96	0.45
1:H:180:ASP:HA	1:H:184:GLN:HE21	1.81	0.45
1:H:282:ARG:NE	2:H:570:HOH:O	2.49	0.45
1:B:181:SER:HB2	1:B:182:PRO:CD	2.35	0.45
1:E:112:GLN:O	1:E:113:GLU:C	2.57	0.45
1:E:142:LYS:O	1:E:157:GLY:HA3	2.16	0.45
1:H:73:TRP:HD1	1:H:324:GLN:OE1	1.99	0.45
1:F:146:THR:HA	1:F:147:PRO:HD3	1.86	0.45
1:H:199:VAL:HG22	1:H:220:PHE:CE1	2.52	0.45
1:H:403:LYS:HD2	2:H:564:HOH:O	2.17	0.45
1:F:66:TYR:HE1	1:F:114:GLU:HG3	1.81	0.45
1:F:49:ARG:HE	1:F:49:ARG:HB3	1.48	0.45
1:B:187:ILE:HD12	1:B:238:VAL:CG2	2.47	0.45
1:F:386:ARG:HA	1:F:386:ARG:NE	2.32	0.45
1:B:138:VAL:CG1	1:B:187:ILE:HD11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:VAL:HA	1:F:223:VAL:O	2.17	0.45
1:D:251:ALA:O	1:D:252:PRO:C	2.58	0.44
1:D:363:VAL:O	1:D:367:ILE:HG13	2.16	0.44
1:A:36:VAL:HB	2:A:658:HOH:O	2.18	0.44
1:G:196:ARG:NH1	1:G:224:LYS:O	2.49	0.44
1:H:78:GLU:OE1	1:H:78:GLU:HA	2.18	0.44
1:E:60:LEU:HD21	1:E:76:ALA:HA	1.98	0.44
1:H:22:ALA:O	1:H:26:GLY:N	2.48	0.44
1:B:31:TRP:HZ3	1:B:83:ILE:HG23	1.83	0.44
1:B:367:ILE:CG2	1:B:371:GLY:HA3	2.47	0.44
1:C:72:ASP:OD1	1:C:72:ASP:C	2.58	0.44
1:G:83:ILE:HD12	1:G:94:PHE:CD2	2.53	0.44
1:G:249:LEU:C	1:G:252:PRO:HD2	2.43	0.44
1:B:138:VAL:HG11	1:B:187:ILE:HD11	2.00	0.44
1:A:351:LEU:HG	1:D:307:ILE:CG2	2.48	0.44
1:E:220:PHE:HD2	1:E:223:VAL:HG21	1.82	0.44
1:B:24:ALA:HB2	1:B:79:VAL:HG13	1.99	0.43
1:C:24:ALA:HB2	1:C:79:VAL:HG13	1.99	0.43
1:D:338:ARG:HH22	1:D:417:SER:C	2.25	0.43
1:D:358:ASN:ND2	2:D:642:HOH:O	2.33	0.43
1:C:149:GLU:C	1:C:151:GLY:N	2.69	0.43
1:E:107:ILE:HD13	1:E:237:PHE:CE2	2.53	0.43
1:H:168:SER:O	1:H:194:THR:HB	2.18	0.43
1:H:173:VAL:HG22	1:H:174:PHE:N	2.32	0.43
1:B:188:ILE:HD13	1:B:188:ILE:N	2.32	0.43
1:C:179:ASP:OD1	1:C:179:ASP:C	2.61	0.43
1:H:101:ALA:CB	1:H:102:PRO:HD3	2.37	0.43
1:E:145:ALA:O	1:E:177:VAL:HA	2.17	0.43
1:F:149:GLU:N	1:F:149:GLU:OE1	2.37	0.43
1:H:62:VAL:HG13	1:H:117:TYR:CD2	2.42	0.43
1:H:125:TRP:HA	1:H:169:ASP:OD2	2.18	0.43
1:H:380:ARG:CZ	2:H:553:HOH:O	2.55	0.43
1:C:53:ARG:HA	1:C:58:LEU:HD12	2.00	0.43
1:D:131:SER:OG	1:D:132:SER:N	2.52	0.43
1:F:273:ALA:HA	1:F:367:ILE:HD11	2.01	0.43
1:H:97:HIS:CD2	1:H:98:LEU:HD23	2.54	0.43
1:D:144:ARG:HG3	1:D:178:GLN:HB2	2.00	0.43
1:E:146:THR:HA	1:E:147:PRO:HD3	1.91	0.43
1:B:18:ASN:N	1:E:18:ASN:ND2	2.67	0.42
1:G:274:ARG:NH1	1:G:278:ARG:NH1	2.66	0.42
1:D:336:GLU:O	1:D:340:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ASP:HB2	1:C:324:GLN:OE1	2.18	0.42
1:F:159:LYS:HG2	1:F:162:CYS:SG	2.59	0.42
1:E:25:ARG:NH1	1:E:82:GLU:OE2	2.52	0.42
1:F:263:LEU:HD13	1:F:313:ASP:OD1	2.20	0.42
1:G:32:ARG:HH11	1:G:32:ARG:CB	2.32	0.42
1:C:20:PRO:HG3	1:C:69:TRP:CE3	2.54	0.42
1:F:176:VAL:HB	1:F:178:GLN:NE2	2.34	0.42
1:G:131:SER:HB2	1:G:174:PHE:CE2	2.55	0.42
1:H:29:GLU:C	1:H:31:TRP:N	2.78	0.42
1:D:179:ASP:O	1:D:184:GLN:HG3	2.20	0.42
1:D:364:PHE:HB3	1:C:390:LEU:HD11	2.00	0.42
1:H:22:ALA:O	1:H:23:VAL:C	2.62	0.42
1:H:72:ASP:CG	1:H:74:PRO:HD2	2.44	0.42
1:B:263:LEU:HD23	1:B:263:LEU:HA	1.80	0.42
1:D:309:LEU:HG	1:D:359:ILE:CD1	2.50	0.42
1:H:97:HIS:O	1:H:100:ASN:HB2	2.19	0.42
1:H:150:ASP:OD2	1:H:227:PRO:HD3	2.20	0.42
1:D:208:ILE:HG13	1:D:209:GLY:N	2.34	0.42
1:C:40:ARG:CZ	1:C:40:ARG:HB3	2.47	0.42
1:C:283:PRO:HB2	1:C:289:ILE:O	2.20	0.42
1:C:367:ILE:CG2	1:C:371:GLY:HA3	2.50	0.42
1:E:177:VAL:HG23	1:E:188:ILE:HG12	2.01	0.42
1:E:181:SER:HB2	1:E:182:PRO:HD2	2.02	0.42
1:F:295:ASP:HB3	1:F:298:THR:HB	2.02	0.41
1:A:187:ILE:HD12	1:A:238:VAL:HG23	2.02	0.41
1:F:99:THR:CG2	1:F:257:ILE:HD13	2.48	0.41
1:H:258:PHE:CG	1:H:388:HIS:HE1	2.37	0.41
1:E:166:LYS:HE3	1:E:203:ASP:HB2	2.02	0.41
1:H:283:PRO:HB2	1:H:289:ILE:O	2.21	0.41
1:A:72:ASP:OD1	1:A:75:THR:CB	2.68	0.41
1:B:246:ARG:NE	1:B:330:GLY:HA2	2.35	0.41
1:B:273:ALA:CB	1:B:363:VAL:HB	2.51	0.41
1:F:102:PRO:O	1:F:103:MET:C	2.62	0.41
1:F:138:VAL:HG12	1:F:176:VAL:HG11	2.03	0.41
1:G:176:VAL:HG12	1:G:178:GLN:HG3	2.02	0.41
1:H:69:TRP:H	1:H:69:TRP:CD1	2.38	0.41
1:H:170:LEU:HD12	1:H:170:LEU:HA	1.94	0.41
1:A:187:ILE:HD12	1:A:238:VAL:CG2	2.50	0.41
1:D:265:ILE:HG21	1:D:385:VAL:HG23	2.01	0.41
1:D:373:HIS:CG	1:D:374:PRO:HD2	2.55	0.41
1:F:103:MET:HE3	1:F:103:MET:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:388:HIS:C	1:G:390:LEU:H	2.28	0.41
1:A:29:GLU:HG2	1:A:32:ARG:HH22	1.85	0.41
1:B:18:ASN:HA	2:B:661:HOH:O	2.19	0.41
1:C:198:GLY:O	1:C:221:HIS:N	2.38	0.41
1:G:66:TYR:HE1	1:G:114:GLU:HG2	1.86	0.41
1:C:192:ILE:HD13	1:C:192:ILE:HG21	1.79	0.41
1:E:119:GLN:NE2	2:E:590:HOH:O	2.54	0.41
1:F:31:TRP:CB	1:F:38:ARG:HH22	2.26	0.41
1:G:92:HIS:O	1:G:96:TYR:HB2	2.21	0.41
1:H:22:ALA:O	1:H:25:ARG:N	2.54	0.41
1:B:131:SER:O	1:B:159:LYS:HE2	2.21	0.41
1:C:154:VAL:HA	1:C:223:VAL:O	2.20	0.41
1:C:309:LEU:HG	1:C:359:ILE:CD1	2.51	0.41
1:F:228:ASP:OD1	1:F:228:ASP:N	2.51	0.41
1:F:354:ASN:HB2	2:F:600:HOH:O	2.21	0.41
1:H:48:GLU:CD	1:H:48:GLU:N	2.79	0.41
1:H:338:ARG:HD3	1:H:338:ARG:O	2.21	0.41
1:A:367:ILE:CG2	1:A:371:GLY:HA3	2.51	0.41
1:D:18:ASN:HB3	2:D:622:HOH:O	2.20	0.41
1:E:101:ALA:HB1	1:E:117:TYR:HE1	1.86	0.41
1:F:208:ILE:O	1:F:383:ARG:HD2	2.20	0.41
1:F:277:THR:HA	1:F:281:ALA:HB2	2.02	0.41
1:F:282:ARG:NH2	1:H:135:ASN:O	2.54	0.41
1:H:27:LEU:HD22	1:H:31:TRP:CH2	2.56	0.41
1:A:28:ALA:HB1	1:A:86:ALA:HB2	2.02	0.40
1:D:19:ASP:HA	1:D:20:PRO:HD2	1.92	0.40
1:C:101:ALA:HB1	1:C:117:TYR:CE1	2.57	0.40
1:G:62:VAL:HB	1:G:68:GLY:HA3	2.03	0.40
1:H:267:HIS:CD2	1:H:309:LEU:HD13	2.56	0.40
1:B:273:ALA:HB2	1:B:363:VAL:HB	2.04	0.40
1:H:80:VAL:O	1:H:80:VAL:HG12	2.21	0.40
1:H:250:PHE:C	1:H:250:PHE:CD1	2.99	0.40
1:H:390:LEU:O	1:H:391:HIS:C	2.61	0.40
1:B:32:ARG:NE	2:B:633:HOH:O	2.48	0.40
1:E:139:LEU:HD23	1:E:139:LEU:HA	1.94	0.40
1:E:162:CYS:O	1:E:215:SER:HA	2.21	0.40
1:B:27:LEU:HD22	1:B:51:ASP:HB3	2.02	0.40
1:C:179:ASP:CG	1:C:181:SER:H	2.30	0.40
1:H:73:TRP:CD1	1:H:324:GLN:OE1	2.73	0.40
1:A:127:THR:HA	1:A:170:LEU:O	2.21	0.40
1:D:18:ASN:O	1:D:20:PRO:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:SER:OG	1:E:338:ARG:HG3	2.22	0.40
1:F:116:LEU:HA	1:F:116:LEU:HD23	1.88	0.40
1:F:339:GLY:O	1:F:343:VAL:HG23	2.22	0.40
1:G:181:SER:CB	1:G:182:PRO:CD	2.96	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	398/417 (95%)	381 (96%)	17 (4%)	0	100	100
1	B	398/417 (95%)	388 (98%)	10 (2%)	0	100	100
1	C	398/417 (95%)	384 (96%)	13 (3%)	1 (0%)	36	36
1	D	398/417 (95%)	388 (98%)	9 (2%)	1 (0%)	36	36
1	E	398/417 (95%)	385 (97%)	12 (3%)	1 (0%)	36	36
1	F	398/417 (95%)	383 (96%)	12 (3%)	3 (1%)	16	12
1	G	398/417 (95%)	381 (96%)	16 (4%)	1 (0%)	36	36
1	H	398/417 (95%)	365 (92%)	29 (7%)	4 (1%)	12	8
All	All	3184/3336 (95%)	3055 (96%)	118 (4%)	11 (0%)	36	36

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	179	ASP
1	G	181	SER
1	H	131	SER
1	D	179	ASP
1	H	179	ASP
1	H	134	ASN

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Mol	Chain	Res	Type
1	H	408	GLY
1	F	35	ALA
1	F	179	ASP
1	F	374	PRO
1	E	233	ALA

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	308/323 (95%)	301 (98%)	7 (2%)	44	50
1	B	308/323 (95%)	302 (98%)	6 (2%)	50	57
1	C	308/323 (95%)	299 (97%)	9 (3%)	37	41
1	D	308/323 (95%)	302 (98%)	6 (2%)	50	57
1	E	308/323 (95%)	297 (96%)	11 (4%)	31	33
1	F	308/323 (95%)	292 (95%)	16 (5%)	21	19
1	G	308/323 (95%)	296 (96%)	12 (4%)	28	29
1	H	308/323 (95%)	285 (92%)	23 (8%)	12	9
All	All	2464/2584 (95%)	2374 (96%)	90 (4%)	30	31

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	144	ARG
1	A	163	SER
1	A	180	ASP
1	A	275	GLU
1	A	333	LEU
1	A	412	ILE
1	B	148	THR
1	B	180	ASP
1	B	219	ASP

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Mol	Chain	Res	Type
1	B	228	ASP
1	B	237	PHE
1	B	333	LEU
1	D	180	ASP
1	D	184	GLN
1	D	228	ASP
1	D	237	PHE
1	D	245	GLU
1	D	333	LEU
1	C	25	ARG
1	C	32	ARG
1	C	40	ARG
1	C	149	GLU
1	C	178	GLN
1	C	184	GLN
1	C	196	ARG
1	C	228	ASP
1	C	333	LEU
1	E	29	GLU
1	E	46	THR
1	E	50	GLU
1	E	96	TYR
1	E	102	PRO
1	E	105	GLU
1	E	226	GLU
1	E	228	ASP
1	E	275	GLU
1	E	333	LEU
1	E	344	LYS
1	F	29	GLU
1	F	36	VAL
1	F	39	ASP
1	F	46	THR
1	F	65	GLU
1	F	77	ILE
1	F	96	TYR
1	F	114	GLU
1	F	181	SER
1	F	226	GLU
1	F	228	ASP
1	F	257	ILE
1	F	285	THR

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Mol	Chain	Res	Type
1	F	291	GLN
1	F	333	LEU
1	F	344	LYS
1	G	29	GLU
1	G	30	LYS
1	G	40	ARG
1	G	50	GLU
1	G	144	ARG
1	G	154	VAL
1	G	173	VAL
1	G	179	ASP
1	G	184	GLN
1	G	208	ILE
1	G	228	ASP
1	G	333	LEU
1	H	36	VAL
1	H	51	ASP
1	H	52	LEU
1	H	69	TRP
1	H	78	GLU
1	H	82	GLU
1	H	132	SER
1	H	154	VAL
1	H	158	THR
1	H	169	ASP
1	H	177	VAL
1	H	194	THR
1	H	202	ASN
1	H	219	ASP
1	H	223	VAL
1	H	226	GLU
1	H	228	ASP
1	H	257	ILE
1	H	285	THR
1	H	333	LEU
1	H	375	ARG
1	H	387	THR
1	H	397	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	122	GLN
1	A	280	GLN
1	B	124	ASN
1	B	183	GLN
1	B	290	GLN
1	D	110	GLN
1	D	119	GLN
1	D	183	GLN
1	D	184	GLN
1	D	409	GLN
1	C	18	ASN
1	C	115	HIS
1	C	178	GLN
1	C	184	GLN
1	E	184	GLN
1	E	280	GLN
1	E	290	GLN
1	E	404	HIS
1	F	212	GLN
1	F	409	GLN
1	G	409	GLN
1	H	18	ASN
1	H	119	GLN
1	H	123	ASN
1	H	156	ASN
1	H	184	GLN
1	H	221	HIS
1	H	280	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 oligosaccharides 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	400/417 (95%)	-0.19	1 (0%) 90 91	17, 35, 56, 84	0
1	B	400/417 (95%)	-0.29	2 (0%) 87 89	16, 30, 54, 108	0
1	C	400/417 (95%)	-0.15	0 100 100	17, 34, 57, 104	0
1	D	400/417 (95%)	-0.18	3 (0%) 82 85	16, 33, 56, 95	0
1	E	400/417 (95%)	-0.15	2 (0%) 87 89	17, 34, 60, 105	0
1	F	400/417 (95%)	0.11	6 (1%) 72 74	19, 39, 67, 109	0
1	G	400/417 (95%)	0.04	4 (1%) 79 82	20, 40, 63, 101	0
1	H	400/417 (95%)	0.73	34 (8%) 16 18	20, 57, 94, 125	0
All	All	3200/3336 (95%)	-0.01	52 (1%) 70 73	16, 36, 72, 125	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	101	ALA	4.2
1	G	182	PRO	3.9
1	H	43	GLY	3.7
1	H	138	VAL	3.6
1	H	104	ILE	3.4
1	H	26	GLY	3.2
1	F	33	ALA	3.1
1	F	182	PRO	3.1
1	H	31	TRP	3.0
1	E	160	HIS	2.8
1	H	96	TYR	2.8
1	H	205	TRP	2.8
1	H	33	ALA	2.7
1	F	181	SER	2.6
1	H	42	GLY	2.6
1	H	41	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	206	ALA	2.6
1	B	181	SER	2.6
1	H	221	HIS	2.5
1	H	54	ALA	2.5
1	H	147	PRO	2.5
1	H	117	TYR	2.5
1	H	24	ALA	2.5
1	D	161	PHE	2.5
1	A	151	GLY	2.5
1	H	230	VAL	2.4
1	H	109	SER	2.4
1	G	18	ASN	2.4
1	H	157	GLY	2.3
1	H	28	ALA	2.3
1	F	203	ASP	2.3
1	H	125	TRP	2.3
1	D	183	GLN	2.3
1	H	182	PRO	2.2
1	G	121	ALA	2.2
1	H	250	PHE	2.2
1	H	213	THR	2.2
1	H	188	ILE	2.2
1	D	235	ASN	2.2
1	H	35	ALA	2.1
1	H	130	ALA	2.1
1	F	313	ASP	2.1
1	G	151	GLY	2.1
1	E	180	ASP	2.1
1	H	153	TYR	2.1
1	H	38	ARG	2.1
1	H	108	GLY	2.1
1	B	182	PRO	2.1
1	F	206	ALA	2.1
1	H	220	PHE	2.0
1	H	223	VAL	2.0
1	H	313	ASP	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 [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.