



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2023 – 12:45 am GMT

PDB ID : 2BP7  
Title : New crystal form of the Pseudomonas putida branched-chain dehydrogenase (E1)  
Authors : Frank, R.A.W.; Pratap, J.V.; Pei, X.Y.; Perham, R.N.; Luisi, B.F.  
Deposited on : 2005-04-18  
Resolution : 2.90 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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

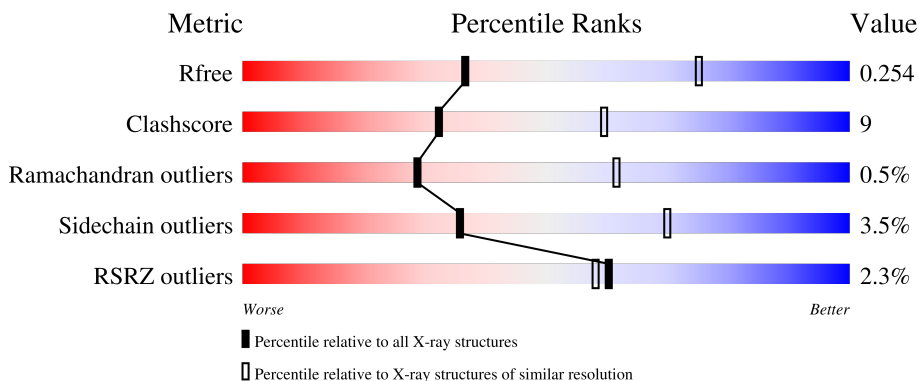
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



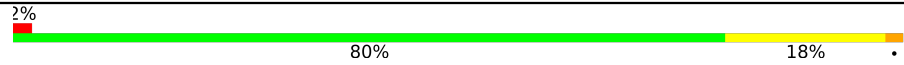

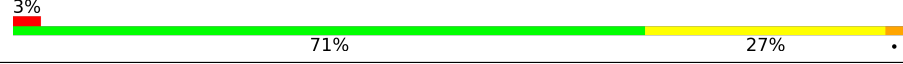
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	410	80% 18% ..
1	C	410	77% 21% ..
1	E	410	80% 18% ..
1	G	410	80% 18% ..
2	B	339	78% 20% .

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Mol	Chain	Length	Quality of chain
2	D	339	 2% 80% 18% •
2	F	339	 2% 75% 23% •
2	H	339	 3% 71% 27% •

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23118 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 2-OXOISOVALERATE DEHYDROGENASE ALPHA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	407	Total 3153	C 1983	N 568	O 598	S 4	0	0	0
1	C	407	Total 3153	C 1983	N 568	O 598	S 4	0	0	0
1	E	407	Total 3153	C 1983	N 568	O 598	S 4	0	0	0
1	G	407	Total 3153	C 1983	N 568	O 598	S 4	0	0	0

- Molecule 2 is a protein called 2-OXOISOVALERATE DEHYDROGENASE BETA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	338	Total 2592	C 1652	N 441	O 492	S 7	0	0	0
2	D	338	Total 2592	C 1652	N 441	O 492	S 7	0	0	0
2	F	338	Total 2592	C 1652	N 441	O 492	S 7	0	0	0
2	H	338	Total 2592	C 1652	N 441	O 492	S 7	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total 18	O 18	0	0
3	B	13	Total 13	O 13	0	0
3	C	25	Total 25	O 25	0	0

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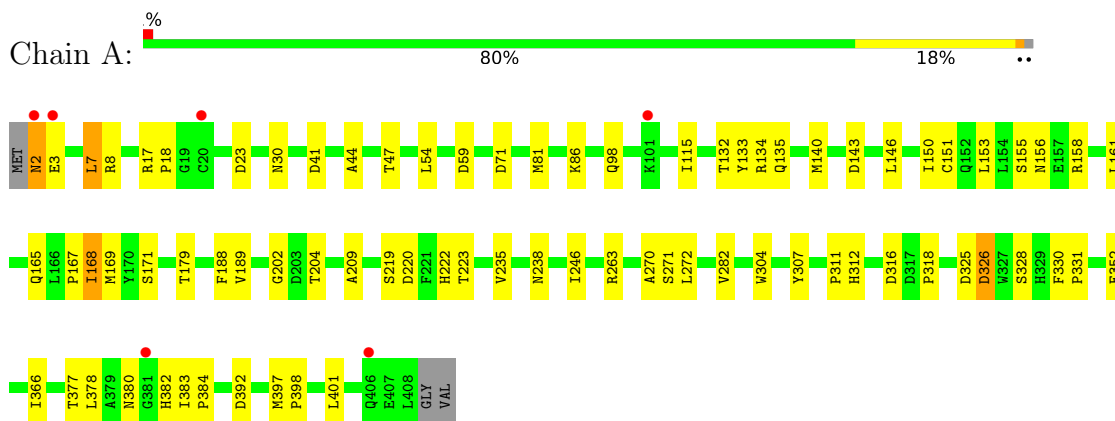
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	15	Total O 15 15	0	0
3	E	16	Total O 16 16	0	0
3	F	13	Total O 13 13	0	0
3	G	22	Total O 22 22	0	0
3	H	16	Total O 16 16	0	0

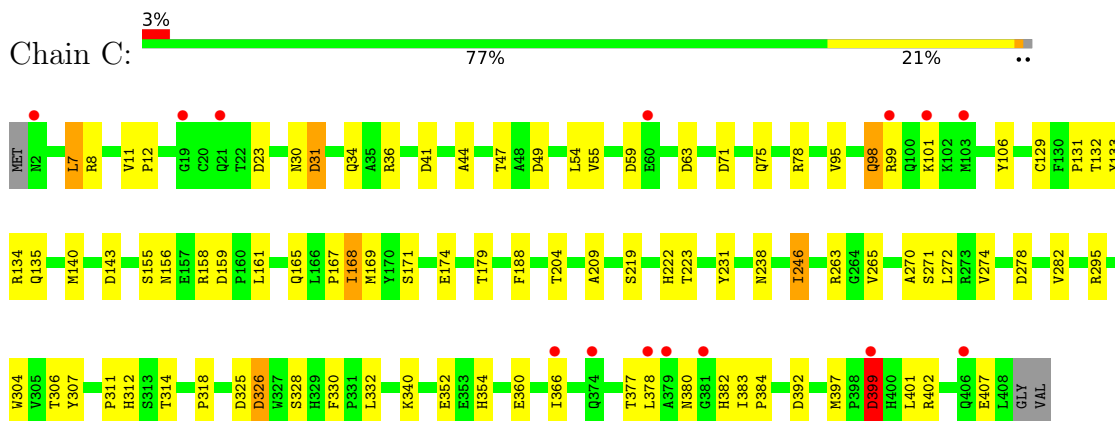
### 3 Residue-property plots [i](#)

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.

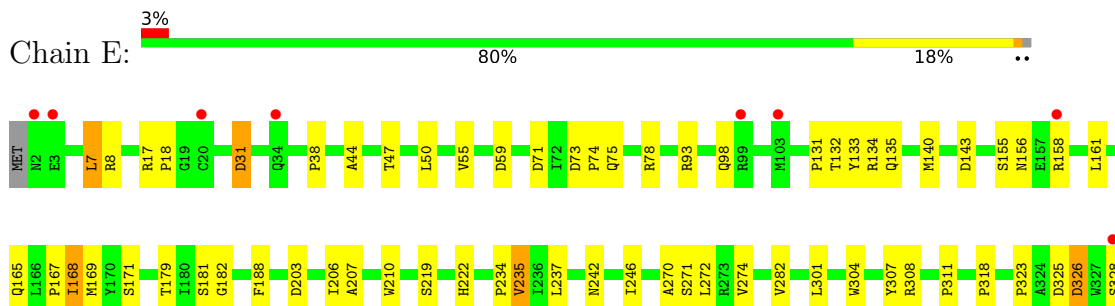
- Molecule 1: 2-OXOISOVALERATE DEHYDROGENASE ALPHA SUBUNIT

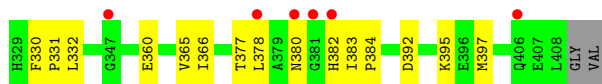


- Molecule 1: 2-OXOISOVALERATE DEHYDROGENASE ALPHA SUBUNIT

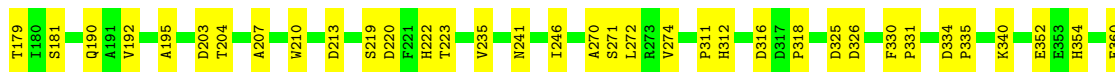
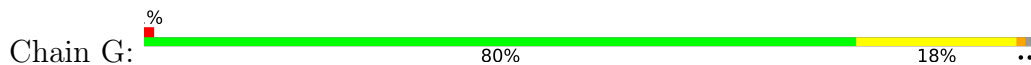


- Molecule 1: 2-OXOISOVALERATE DEHYDROGENASE ALPHA SUBUNIT

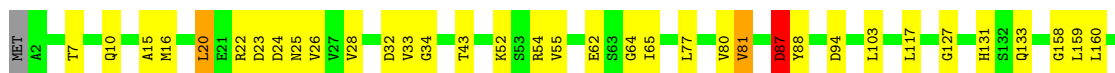
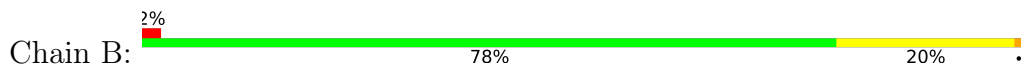




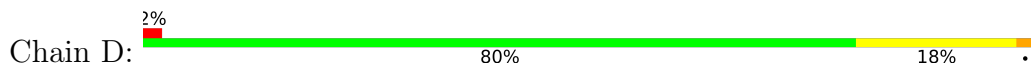
● Molecule 1: 2-OXOISOVALERATE DEHYDROGENASE ALPHA SUBUNIT



● Molecule 2: 2-OXOISOVALERATE DEHYDROGENASE BETA SUBUNIT

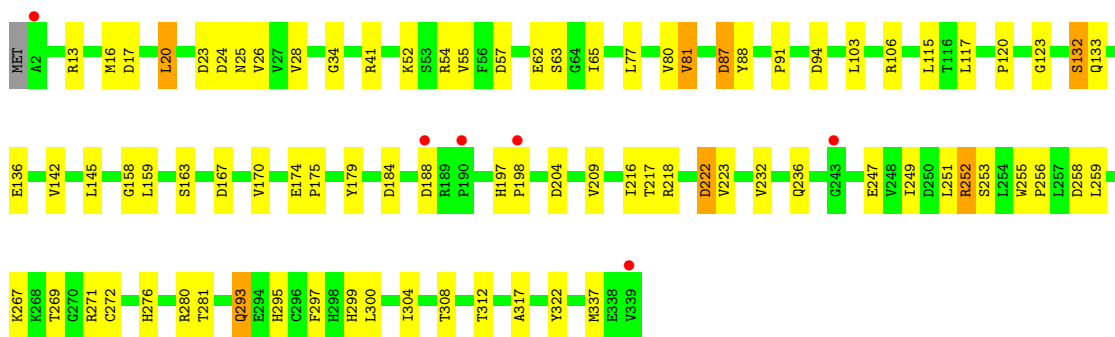


● Molecule 2: 2-OXOISOVALERATE DEHYDROGENASE BETA SUBUNIT

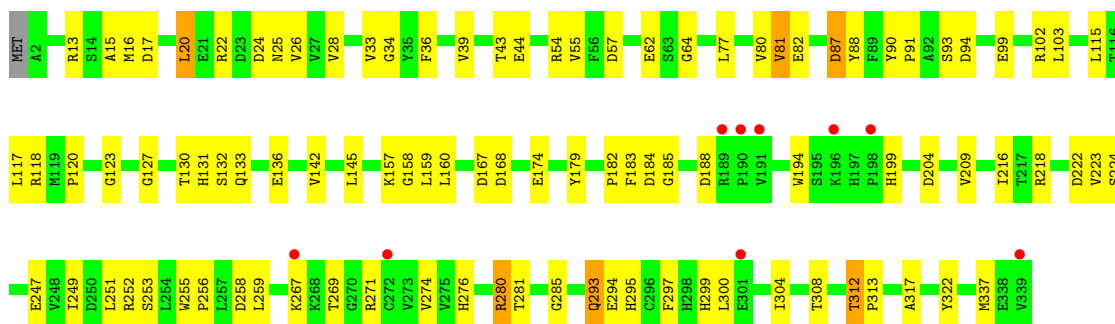


● Molecule 2: 2-OXOISOVALERATE DEHYDROGENASE BETA SUBUNIT





● Molecule 2: 2-OXOISOVALERATE DEHYDROGENASE BETA SUBUNIT





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.87Å 156.87Å 619.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	76.5 (20.00-2.90) 76.5 (19.99-2.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.88Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.227 , 0.254 0.227 , 0.254	Depositor DCC
$R_{free}$ test set	3870 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtrriage
Anisotropy	0.108	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 31.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	23118	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.34	0/3213	0.69	9/4367 (0.2%)
1	C	0.36	0/3213	0.70	10/4367 (0.2%)
1	E	0.35	0/3213	0.69	7/4367 (0.2%)
1	G	0.35	0/3213	0.69	7/4367 (0.2%)
2	B	0.32	0/2650	0.70	12/3618 (0.3%)
2	D	0.31	0/2650	0.70	10/3618 (0.3%)
2	F	0.32	0/2650	0.71	10/3618 (0.3%)
2	H	0.32	0/2650	0.70	11/3618 (0.3%)
All	All	0.33	0/23452	0.70	76/31940 (0.2%)

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	59	ASP	CB-CG-OD2	6.87	124.48	118.30
1	G	59	ASP	CB-CG-OD2	6.83	124.45	118.30
2	H	258	ASP	CB-CG-OD2	6.81	124.43	118.30
2	D	258	ASP	CB-CG-OD2	6.27	123.95	118.30
1	C	143	ASP	CB-CG-OD2	6.16	123.84	118.30
2	F	184	ASP	CB-CG-OD2	6.16	123.84	118.30
1	E	59	ASP	CB-CG-OD2	6.11	123.80	118.30
2	B	94	ASP	CB-CG-OD2	6.11	123.79	118.30
2	D	184	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	59	ASP	CB-CG-OD2	6.08	123.78	118.30
2	B	258	ASP	CB-CG-OD2	6.03	123.73	118.30
2	H	184	ASP	CB-CG-OD2	6.03	123.73	118.30
2	H	94	ASP	CB-CG-OD2	6.01	123.71	118.30
2	F	258	ASP	CB-CG-OD2	5.98	123.68	118.30
2	B	184	ASP	CB-CG-OD2	5.94	123.65	118.30
2	F	222	ASP	CB-CG-OD2	5.86	123.57	118.30
2	F	94	ASP	CB-CG-OD2	5.84	123.56	118.30
2	D	222	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	392	ASP	CB-CG-OD2	5.83	123.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	168	ASP	CB-CG-OD2	5.80	123.53	118.30
1	E	326	ASP	CB-CG-OD2	5.79	123.52	118.30
2	H	222	ASP	CB-CG-OD2	5.77	123.50	118.30
1	G	143	ASP	CB-CG-OD2	5.77	123.49	118.30
1	E	143	ASP	CB-CG-OD2	5.74	123.47	118.30
1	G	325	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	325	ASP	CB-CG-OD2	5.69	123.42	118.30
2	B	222	ASP	CB-CG-OD2	5.69	123.42	118.30
1	E	325	ASP	CB-CG-OD2	5.58	123.32	118.30
2	F	87	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	41	ASP	CB-CG-OD2	5.53	123.28	118.30
2	D	94	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	41	ASP	CB-CG-OD2	5.47	123.23	118.30
2	D	204	ASP	CB-CG-OD2	5.46	123.22	118.30
1	G	316	ASP	CB-CG-OD2	5.45	123.21	118.30
2	H	204	ASP	CB-CG-OD2	5.45	123.20	118.30
1	E	31	ASP	CB-CG-OD2	5.42	123.17	118.30
2	B	204	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	316	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	71	ASP	CB-CG-OD2	5.39	123.15	118.30
2	D	24	ASP	CB-CG-OD2	5.38	123.14	118.30
2	F	204	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	326	ASP	CB-CG-OD2	5.34	123.11	118.30
2	H	57	ASP	CB-CG-OD2	5.32	123.09	118.30
2	D	87	ASP	CB-CG-OD2	5.30	123.08	118.30
2	B	32	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	31	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	71	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	143	ASP	CB-CG-OD2	5.22	123.00	118.30
2	B	168	ASP	CB-CG-OD2	5.21	122.99	118.30
1	G	41	ASP	CB-CG-OD2	5.19	122.97	118.30
2	H	24	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	326	ASP	CB-CG-OD2	5.19	122.97	118.30
2	B	87	ASP	CB-CG-OD2	5.16	122.95	118.30
2	B	250	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	325	ASP	CB-CG-OD2	5.12	122.91	118.30
2	D	17	ASP	CB-CG-OD2	5.12	122.91	118.30
2	F	17	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	392	ASP	CB-CG-OD2	5.11	122.89	118.30
1	E	392	ASP	CB-CG-OD2	5.09	122.88	118.30
2	B	24	ASP	CB-CG-OD2	5.09	122.88	118.30
2	H	17	ASP	CB-CG-OD2	5.08	122.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	24	ASP	CB-CG-OD2	5.08	122.87	118.30
2	F	188	ASP	CB-CG-OD2	5.08	122.87	118.30
2	H	87	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	23	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	63	ASP	CB-CG-OD2	5.06	122.86	118.30
1	E	71	ASP	CB-CG-OD2	5.06	122.85	118.30
2	B	245	ASP	CB-CG-OD2	5.05	122.84	118.30
2	F	57	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	23	ASP	CB-CG-OD2	5.03	122.83	118.30
1	G	23	ASP	CB-CG-OD2	5.03	122.83	118.30
1	G	220	ASP	CB-CG-OD2	5.03	122.82	118.30
2	B	212	ASP	CB-CG-OD2	5.01	122.81	118.30
2	D	32	ASP	CB-CG-OD2	5.01	122.81	118.30
2	H	188	ASP	CB-CG-OD2	5.01	122.81	118.30
2	D	311	ASP	CB-CG-OD2	5.00	122.80	118.30

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	3153	0	3015	59	0
1	C	3153	0	3015	70	0
1	E	3153	0	3015	56	0
1	G	3153	0	3015	64	0
2	B	2592	0	2482	44	0
2	D	2592	0	2482	41	0
2	F	2592	0	2482	58	0
2	H	2592	0	2482	59	0
3	A	18	0	0	0	0
3	B	13	0	0	0	0
3	C	25	0	0	0	0
3	D	15	0	0	0	0
3	E	16	0	0	1	0
3	F	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	22	0	0	1	0
3	H	16	0	0	0	0
All	All	23118	0	21988	395	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 9.

All (395) 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:A:2:ASN:OD1	2:F:218:ARG:HA	1.60	1.02
1:G:47:THR:HG21	1:G:271:SER:H	1.33	0.94
1:A:219:SER:HB2	1:C:219:SER:HB2	1.50	0.93
1:C:295:ARG:NH1	2:F:198:PRO:HA	1.85	0.91
1:E:219:SER:HB2	1:G:219:SER:HB2	1.52	0.91
1:C:380:ASN:HB3	1:C:382:HIS:ND1	1.87	0.90
1:E:47:THR:HG21	1:E:271:SER:H	1.37	0.89
1:C:98:GLN:HG3	1:C:314:THR:HG21	1.56	0.85
2:F:280:ARG:HG3	2:F:308:THR:OG1	1.77	0.85
1:C:295:ARG:CZ	2:F:198:PRO:HA	2.07	0.84
2:F:87:ASP:OD1	2:F:133:GLN:HG2	1.76	0.83
1:G:377:THR:HG22	1:G:378:LEU:H	1.42	0.82
2:B:280:ARG:HG3	2:B:308:THR:OG1	1.80	0.82
2:D:280:ARG:HG3	2:D:308:THR:OG1	1.80	0.81
1:A:377:THR:HG22	1:A:378:LEU:H	1.44	0.80
1:A:156:ASN:HB3	1:A:158:ARG:H	1.45	0.80
1:A:47:THR:HG21	1:A:271:SER:H	1.44	0.79
2:F:271:ARG:HH11	2:F:337:MET:HA	1.46	0.78
1:G:156:ASN:HB3	1:G:158:ARG:H	1.47	0.78
2:H:271:ARG:HH11	2:H:337:MET:HA	1.48	0.77
1:C:167:PRO:O	1:C:168:ILE:HG12	1.84	0.77
1:C:47:THR:HG21	1:C:271:SER:H	1.50	0.76
1:A:167:PRO:O	1:A:168:ILE:HG12	1.86	0.76
1:A:140:MET:CE	1:A:140:MET:CG	2.64	0.76
1:C:263:ARG:HG3	1:C:263:ARG:HH11	1.51	0.75
1:E:377:THR:HG22	1:E:378:LEU:H	1.52	0.74
1:G:167:PRO:O	1:G:168:ILE:HG12	1.88	0.74
2:H:271:ARG:NH1	2:H:337:MET:HA	2.03	0.73
2:B:271:ARG:NH1	2:B:337:MET:HA	2.03	0.73
1:E:132:THR:H	1:E:135:GLN:NE2	1.87	0.72
1:E:156:ASN:HB3	1:E:158:ARG:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:ARG:HH11	2:B:337:MET:HA	1.56	0.71
2:D:218:ARG:O	2:D:247:GLU:HA	1.92	0.70
2:B:16:MET:O	2:B:20:LEU:HB2	1.93	0.69
1:G:181:SER:HB3	3:G:2010:HOH:O	1.92	0.69
2:B:317:ALA:HB2	1:C:155:SER:HB3	1.73	0.69
1:A:3:GLU:O	2:F:198:PRO:HB3	1.92	0.68
2:F:232:VAL:HG12	2:F:236:GLN:HE21	1.59	0.68
2:H:81:VAL:HG12	2:H:117:LEU:HD22	1.76	0.67
1:G:47:THR:HG21	1:G:271:SER:N	2.06	0.67
1:C:165:GLN:HG3	1:C:169:MET:HB3	1.76	0.67
1:E:140:MET:CG	1:E:140:MET:CE	2.73	0.66
2:F:16:MET:O	2:F:20:LEU:HB2	1.94	0.66
2:F:317:ALA:HB2	1:G:155:SER:HB3	1.76	0.66
1:G:47:THR:CG2	1:G:271:SER:H	2.08	0.66
1:C:340:LYS:HD2	1:C:354:HIS:CE1	2.31	0.66
1:C:377:THR:HG22	1:C:378:LEU:H	1.60	0.66
2:F:271:ARG:NH1	2:F:337:MET:HA	2.10	0.66
1:E:219:SER:HB2	1:G:219:SER:CB	2.23	0.65
1:E:155:SER:HB3	2:H:317:ALA:HB2	1.78	0.65
1:C:165:GLN:CG	1:C:169:MET:HB3	2.27	0.64
1:A:155:SER:HB3	2:D:317:ALA:HB2	1.78	0.64
1:C:36:ARG:HG2	1:C:36:ARG:HH11	1.62	0.64
2:H:218:ARG:O	2:H:247:GLU:HA	1.98	0.64
1:A:44:ALA:O	1:A:47:THR:HG22	1.98	0.64
1:A:263:ARG:HG3	1:A:263:ARG:HH11	1.62	0.64
2:F:13:ARG:HH22	2:F:41:ARG:HH21	1.46	0.64
1:E:47:THR:HG21	1:E:271:SER:N	2.10	0.63
2:H:16:MET:O	2:H:20:LEU:HB2	1.98	0.63
2:D:16:MET:O	2:D:20:LEU:HB2	1.97	0.63
2:B:26:VAL:O	2:B:54:ARG:NH1	2.31	0.63
1:G:140:MET:CG	1:G:140:MET:CE	2.76	0.63
2:H:267:LYS:HG3	2:H:299:HIS:ND1	2.14	0.63
1:G:377:THR:HG22	1:G:378:LEU:N	2.13	0.62
1:G:223:THR:HG21	2:H:64:GLY:HA2	1.81	0.62
1:G:223:THR:CG2	2:H:64:GLY:HA2	2.29	0.62
2:H:82:GLU:OE2	2:H:118:ARG:NH2	2.33	0.62
1:C:295:ARG:NH1	2:F:198:PRO:CA	2.62	0.61
1:G:397:MET:CE	1:G:397:MET:CG	2.78	0.61
1:G:195:ALA:CB	1:G:235:VAL:HG23	2.30	0.61
1:G:340:LYS:HD2	1:G:354:HIS:CE1	2.36	0.61
1:G:207:ALA:HB3	1:G:235:VAL:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:28:VAL:O	2:H:55:VAL:HA	2.01	0.60
1:E:397:MET:CE	1:E:397:MET:CG	2.79	0.60
2:F:269:THR:HG22	2:F:271:ARG:H	1.66	0.60
1:A:377:THR:HG22	1:A:378:LEU:N	2.15	0.60
1:E:311:PRO:HA	1:E:318:PRO:HG3	1.83	0.60
2:F:218:ARG:O	2:F:247:GLU:HA	2.00	0.60
1:E:222:HIS:HB2	1:G:222:HIS:CG	2.37	0.60
1:C:311:PRO:HA	1:C:318:PRO:HG3	1.85	0.59
2:D:259:LEU:HD21	2:D:295:HIS:HE1	1.68	0.59
2:D:223:VAL:HA	2:D:269:THR:HG21	1.85	0.59
1:A:380:ASN:HB3	1:A:382:HIS:ND1	2.18	0.59
1:E:167:PRO:O	1:E:168:ILE:HG12	2.01	0.59
1:C:140:MET:CE	1:C:140:MET:CG	2.81	0.59
1:G:192:VAL:HA	1:G:235:VAL:HG21	1.84	0.59
1:E:219:SER:CB	1:G:219:SER:HB2	2.29	0.58
1:A:3:GLU:O	2:F:198:PRO:CB	2.50	0.58
2:F:259:LEU:HD21	2:F:295:HIS:HE1	1.68	0.58
1:E:377:THR:HG22	1:E:378:LEU:N	2.19	0.58
2:F:251:LEU:O	2:F:253:SER:N	2.36	0.58
2:B:15:ALA:HB3	2:B:160:LEU:HD23	1.85	0.57
2:F:259:LEU:HD21	2:F:295:HIS:CE1	2.39	0.57
1:E:383:ILE:HB	1:E:384:PRO:CD	2.35	0.57
1:C:47:THR:CG2	1:C:271:SER:H	2.18	0.57
1:E:44:ALA:O	1:E:47:THR:HG22	2.04	0.57
2:F:158:GLY:HA3	2:F:209:VAL:HG23	1.85	0.57
1:A:204:THR:HA	1:C:7:LEU:HD22	1.86	0.57
2:F:28:VAL:O	2:F:55:VAL:HA	2.04	0.57
1:C:47:THR:HG21	1:C:271:SER:N	2.18	0.57
1:C:295:ARG:CZ	2:F:198:PRO:CA	2.81	0.57
2:D:259:LEU:HD21	2:D:295:HIS:CE1	2.39	0.57
1:E:93:ARG:HG3	1:E:365:VAL:HG11	1.85	0.57
1:C:263:ARG:HG3	1:C:263:ARG:NH1	2.21	0.56
2:D:271:ARG:NH1	2:D:337:MET:HA	2.21	0.56
2:H:183:PHE:CE2	2:H:185:GLY:HA2	2.41	0.56
1:E:55:VAL:HB	1:E:274:VAL:HG22	1.88	0.56
1:C:397:MET:CG	1:C:397:MET:CE	2.84	0.56
1:A:219:SER:CB	1:C:219:SER:HB2	2.29	0.56
1:E:47:THR:CG2	1:E:271:SER:H	2.16	0.56
1:A:223:THR:HG21	2:B:64:GLY:HA2	1.87	0.55
1:A:223:THR:CG2	2:B:64:GLY:HA2	2.36	0.55
1:C:407:GLU:O	1:C:407:GLU:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:TYR:HB2	1:G:168:ILE:HD12	1.88	0.55
2:H:294:GLU:HG2	2:H:295:HIS:HD2	1.72	0.55
1:C:47:THR:HG21	1:C:270:ALA:HA	1.89	0.55
1:E:165:GLN:HG2	1:E:169:MET:HB3	1.88	0.55
1:G:161:LEU:HD21	1:G:171:SER:HB3	1.88	0.55
2:B:218:ARG:O	2:B:247:GLU:HA	2.06	0.55
1:A:86:LYS:HE2	1:A:146:LEU:HD21	1.89	0.54
2:B:223:VAL:HA	2:B:269:THR:HG21	1.89	0.54
1:E:161:LEU:HD21	1:E:171:SER:HB3	1.89	0.54
1:G:17:ARG:HB3	1:G:18:PRO:CD	2.37	0.54
1:A:397:MET:CG	1:A:397:MET:CE	2.86	0.54
2:B:87:ASP:OD1	2:B:133:GLN:HG2	2.08	0.54
1:A:383:ILE:HB	1:A:384:PRO:HD2	1.89	0.54
1:E:132:THR:H	1:E:135:GLN:HE22	1.56	0.54
1:G:380:ASN:HB3	1:G:382:HIS:ND1	2.23	0.54
1:G:389:MET:CE	1:G:389:MET:CG	2.86	0.54
2:F:217:THR:HG21	2:F:236:GLN:NE2	2.23	0.53
2:D:7:THR:OG1	2:D:10:GLN:HG3	2.09	0.53
1:C:106:TYR:O	1:C:314:THR:HG23	2.09	0.53
1:C:159:ASP:OD1	1:C:161:LEU:N	2.36	0.53
1:A:134:ARG:NH2	1:A:312:HIS:O	2.43	0.52
2:D:232:VAL:HG12	2:D:236:GLN:HE21	1.74	0.52
2:D:120:PRO:HA	2:D:174:GLU:O	2.10	0.52
2:D:23:ASP:HB3	2:D:26:VAL:HG23	1.91	0.52
1:E:17:ARG:HB3	1:E:18:PRO:HD2	1.91	0.52
2:B:216:ILE:HD13	2:B:249:ILE:HG12	1.92	0.52
2:F:267:LYS:HG3	2:F:299:HIS:ND1	2.24	0.52
2:H:15:ALA:HB2	2:H:157:LYS:HG3	1.91	0.52
1:A:311:PRO:HA	1:A:318:PRO:HG3	1.92	0.52
1:C:44:ALA:O	1:C:47:THR:HG22	2.09	0.52
1:G:352:GLU:OE1	1:G:352:GLU:N	2.42	0.52
2:D:13:ARG:HH22	2:D:41:ARG:HH21	1.58	0.51
2:D:158:GLY:HA3	2:D:209:VAL:HG23	1.92	0.51
1:G:133:TYR:HE1	1:G:134:ARG:NH1	2.08	0.51
1:A:115:ILE:HA	1:A:282:VAL:HG11	1.92	0.51
2:B:251:LEU:O	2:B:253:SER:N	2.44	0.51
2:F:312:THR:HG22	2:F:322:TYR:HE1	1.75	0.51
1:G:132:THR:H	1:G:135:GLN:NE2	2.08	0.51
1:G:195:ALA:HB2	1:G:235:VAL:CG2	2.40	0.51
2:B:25:ASN:HB3	2:B:77:LEU:HA	1.93	0.51
2:B:270:GLY:HA2	2:B:299:HIS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ARG:HH22	2:F:198:PRO:HG3	1.75	0.51
1:E:181:SER:HB3	3:E:2009:HOH:O	2.11	0.51
1:A:383:ILE:HB	1:A:384:PRO:CD	2.40	0.51
2:B:255:TRP:HA	2:B:256:PRO:C	2.31	0.51
1:G:17:ARG:HB3	1:G:18:PRO:HD2	1.91	0.51
1:A:219:SER:HB2	1:C:219:SER:CB	2.33	0.51
2:H:62:GLU:HG2	2:H:88:TYR:O	2.10	0.51
2:H:259:LEU:HD21	2:H:295:HIS:CE1	2.47	0.50
2:H:26:VAL:O	2:H:54:ARG:NH1	2.44	0.50
1:A:398:PRO:HD2	1:A:401:LEU:HD12	1.93	0.50
2:B:28:VAL:O	2:B:55:VAL:HA	2.10	0.50
1:C:330:PHE:CE2	1:C:332:LEU:HB2	2.46	0.50
2:H:158:GLY:HA3	2:H:209:VAL:HG23	1.92	0.50
1:E:203:ASP:O	1:G:7:LEU:HB2	2.10	0.50
1:A:133:TYR:HB2	1:A:168:ILE:HD12	1.93	0.50
2:D:223:VAL:HA	2:D:269:THR:CG2	2.42	0.50
2:F:293:GLN:OE1	2:H:304:ILE:N	2.45	0.50
1:A:380:ASN:C	1:A:382:HIS:H	2.14	0.50
2:B:269:THR:HG22	2:B:271:ARG:H	1.77	0.50
2:H:280:ARG:HH21	2:H:308:THR:H	1.59	0.50
1:A:7:LEU:CD2	1:C:204:THR:HA	2.42	0.50
2:F:13:ARG:HH22	2:F:41:ARG:NH2	2.10	0.50
1:A:155:SER:OG	2:D:316:HIS:HD2	1.94	0.50
1:A:222:HIS:CG	1:C:222:HIS:HB2	2.47	0.50
2:B:62:GLU:HG2	2:B:88:TYR:O	2.10	0.50
2:D:146:ARG:HB3	2:D:170:VAL:HG22	1.94	0.50
1:E:7:LEU:HD22	1:G:204:THR:HA	1.94	0.50
1:E:133:TYR:HB2	1:E:168:ILE:HD12	1.93	0.49
1:E:156:ASN:O	1:E:384:PRO:HG3	2.12	0.49
1:E:380:ASN:HB3	1:E:382:HIS:ND1	2.26	0.49
1:G:167:PRO:O	1:G:168:ILE:CG1	2.58	0.49
1:C:377:THR:HG22	1:C:378:LEU:N	2.25	0.49
2:H:87:ASP:OD1	2:H:133:GLN:HG2	2.13	0.49
2:H:224:SER:N	2:H:269:THR:HG21	2.28	0.49
1:E:73:ASP:OD2	1:E:75:GLN:HB2	2.12	0.49
1:C:223:THR:HG21	2:D:64:GLY:CA	2.42	0.48
2:H:216:ILE:HD13	2:H:249:ILE:HG12	1.96	0.48
1:A:132:THR:H	1:A:135:GLN:NE2	2.11	0.48
1:A:352:GLU:OE1	1:A:352:GLU:N	2.43	0.48
1:C:156:ASN:C	1:C:158:ARG:H	2.14	0.48
1:E:165:GLN:CG	1:E:169:MET:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:HIS:CG	1:G:222:HIS:HB2	2.49	0.48
2:F:312:THR:HG22	2:F:322:TYR:CE1	2.49	0.48
2:B:281:THR:HG21	2:D:255:TRP:CE2	2.49	0.48
2:F:255:TRP:CE2	2:H:281:THR:HG21	2.49	0.48
2:D:28:VAL:O	2:D:55:VAL:HA	2.14	0.47
1:G:132:THR:H	1:G:135:GLN:HE21	1.62	0.47
1:G:223:THR:CG2	2:H:64:GLY:CA	2.92	0.47
2:B:65:ILE:HG23	2:B:81:VAL:CG2	2.43	0.47
2:D:223:VAL:CA	2:D:269:THR:HG21	2.44	0.47
2:F:223:VAL:HA	2:F:269:THR:HG21	1.96	0.47
2:H:123:GLY:HA2	2:H:132:SER:HB2	1.96	0.47
1:G:383:ILE:HB	1:G:384:PRO:CD	2.45	0.47
1:A:165:GLN:HG3	1:A:169:MET:HB2	1.97	0.47
1:G:383:ILE:HB	1:G:384:PRO:HD2	1.95	0.47
2:H:223:VAL:HA	2:H:269:THR:CG2	2.44	0.47
2:H:120:PRO:HA	2:H:174:GLU:O	2.15	0.47
1:A:222:HIS:HB2	1:C:222:HIS:CG	2.50	0.47
2:B:7:THR:OG1	2:B:10:GLN:HG3	2.15	0.47
1:E:282:VAL:HA	1:E:304:TRP:CZ3	2.50	0.47
2:H:276:HIS:O	2:H:308:THR:HA	2.15	0.47
1:A:17:ARG:HB3	1:A:18:PRO:HD2	1.96	0.47
2:H:142:VAL:HB	2:H:145:LEU:HD12	1.97	0.47
1:A:189:VAL:HG23	1:A:220:ASP:HB3	1.96	0.47
2:B:304:ILE:N	2:D:293:GLN:OE1	2.48	0.47
1:C:133:TYR:HE1	1:C:134:ARG:NH1	2.13	0.47
2:D:255:TRP:HA	2:D:256:PRO:C	2.34	0.47
1:E:133:TYR:HE1	1:E:134:ARG:NH1	2.12	0.47
1:A:156:ASN:O	1:A:384:PRO:HG3	2.14	0.47
2:B:81:VAL:HG12	2:B:117:LEU:HD22	1.97	0.47
2:B:232:VAL:HG12	2:B:236:GLN:HE21	1.79	0.47
1:A:47:THR:HG21	1:A:271:SER:N	2.22	0.46
1:G:91:ASP:O	1:G:95:VAL:HG23	2.15	0.46
1:A:167:PRO:O	1:A:168:ILE:CG1	2.60	0.46
1:E:330:PHE:CE2	1:E:332:LEU:HB2	2.50	0.46
1:G:156:ASN:O	1:G:384:PRO:HG3	2.15	0.46
1:A:47:THR:CG2	1:A:271:SER:H	2.21	0.46
1:G:151:CYS:SG	1:G:158:ARG:HB3	2.56	0.46
1:G:330:PHE:HA	1:G:331:PRO:HD3	1.81	0.46
2:B:312:THR:HG22	2:B:322:TYR:CE1	2.51	0.46
2:D:81:VAL:HG12	2:D:117:LEU:HD22	1.98	0.46
2:B:65:ILE:HG23	2:B:81:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:203:ASP:OD1	1:G:204:THR:N	2.44	0.46
1:C:55:VAL:HB	1:C:274:VAL:HG22	1.97	0.46
1:C:133:TYR:HB2	1:C:168:ILE:HD12	1.98	0.46
2:F:216:ILE:HD13	2:F:249:ILE:HG12	1.96	0.46
1:G:131:PRO:HA	1:G:210:TRP:HB2	1.98	0.46
1:G:134:ARG:NH2	1:G:312:HIS:O	2.49	0.46
1:C:282:VAL:HA	1:C:304:TRP:CZ3	2.51	0.46
1:C:399:ASP:O	1:C:402:ARG:HB2	2.15	0.46
2:D:26:VAL:O	2:D:54:ARG:NH1	2.49	0.46
1:E:237:LEU:O	1:E:301:LEU:HD12	2.15	0.46
1:A:156:ASN:CB	1:A:158:ARG:H	2.21	0.45
2:B:159:LEU:HD11	2:B:252:ARG:HG2	1.97	0.45
1:E:207:ALA:HB3	1:E:235:VAL:HG13	1.98	0.45
1:G:131:PRO:HG3	1:G:177:PHE:CE1	2.50	0.45
1:G:47:THR:HG21	1:G:270:ALA:HA	1.98	0.45
2:D:123:GLY:HA2	2:D:132:SER:HB2	1.99	0.45
2:H:36:PHE:HE2	2:H:39:VAL:HA	1.81	0.45
2:H:274:VAL:HG11	2:H:285:GLY:HA2	1.99	0.45
2:B:312:THR:HG22	2:B:322:TYR:HE1	1.82	0.45
1:C:47:THR:CG2	1:C:265:VAL:HG22	2.47	0.45
1:A:30:ASN:HB2	1:A:54:LEU:HB3	1.99	0.45
2:B:311:ASP:O	1:C:401:LEU:HD21	2.16	0.45
1:E:383:ILE:HB	1:E:384:PRO:HD2	1.99	0.45
2:B:255:TRP:CE2	2:D:281:THR:HG21	2.52	0.45
2:D:65:ILE:HG23	2:D:81:VAL:CG2	2.47	0.45
2:B:293:GLN:OE1	2:D:304:ILE:N	2.50	0.45
1:E:131:PRO:HA	1:E:210:TRP:HB2	1.98	0.45
2:F:81:VAL:HG12	2:F:117:LEU:HD22	1.98	0.45
2:B:267:LYS:HG3	2:B:299:HIS:ND1	2.32	0.45
1:C:30:ASN:HB2	1:C:54:LEU:HB3	1.99	0.45
1:C:134:ARG:NH2	1:C:312:HIS:O	2.51	0.44
1:C:156:ASN:C	1:C:158:ARG:N	2.70	0.44
1:G:55:VAL:HB	1:G:274:VAL:HG22	1.98	0.44
1:E:133:TYR:HE1	1:E:134:ARG:HH11	1.64	0.44
2:F:25:ASN:HB3	2:F:77:LEU:HA	2.00	0.44
2:F:232:VAL:HG12	2:F:236:GLN:NE2	2.31	0.44
2:D:82:GLU:OE2	2:D:118:ARG:NH2	2.51	0.44
1:E:330:PHE:HA	1:E:331:PRO:HD3	1.85	0.44
1:C:132:THR:H	1:C:135:GLN:NE2	2.14	0.44
1:E:182:GLY:HA3	2:H:130:THR:OG1	2.17	0.44
1:A:330:PHE:HA	1:A:331:PRO:HD3	1.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:297:PHE:HE1	2:H:300:LEU:HD23	1.82	0.44
2:H:28:VAL:HG22	2:H:80:VAL:HB	1.99	0.44
2:D:22:ARG:NH1	2:D:165:GLU:OE2	2.51	0.44
2:B:223:VAL:HA	2:B:269:THR:CG2	2.47	0.44
1:E:206:ILE:HG22	1:E:234:PRO:HB2	2.00	0.44
2:F:123:GLY:HA2	2:F:132:SER:HB3	1.99	0.44
1:C:99:ARG:C	1:C:101:LYS:H	2.21	0.44
1:C:246:ILE:HG12	1:C:312:HIS:CE1	2.53	0.44
2:F:62:GLU:HG2	2:F:88:TYR:O	2.18	0.44
1:G:155:SER:HA	1:G:159:ASP:OD2	2.18	0.44
2:H:127:GLY:O	2:H:131:HIS:HB2	2.17	0.44
2:H:223:VAL:HA	2:H:269:THR:HG21	2.00	0.44
1:A:223:THR:CG2	2:B:64:GLY:CA	2.95	0.43
2:F:23:ASP:HB3	2:F:26:VAL:HG23	2.00	0.43
2:H:25:ASN:HB3	2:H:77:LEU:HA	2.01	0.43
1:A:397:MET:HA	1:A:398:PRO:HD3	1.88	0.43
2:D:182:PRO:HD3	2:D:194:TRP:CE3	2.53	0.43
2:F:133:GLN:HE22	2:H:102:ARG:HH12	1.66	0.43
2:H:312:THR:HG22	2:H:322:TYR:CE1	2.53	0.43
2:B:127:GLY:O	2:B:131:HIS:HB2	2.18	0.43
1:C:231:TYR:OH	2:D:58:ALA:HA	2.18	0.43
1:G:311:PRO:HA	1:G:318:PRO:HG3	2.01	0.43
2:H:90:TYR:HB2	2:H:91:PRO:HD3	2.00	0.43
1:A:47:THR:HG21	1:A:270:ALA:HA	2.01	0.43
2:D:224:SER:O	2:D:272:CYS:HA	2.18	0.43
1:E:7:LEU:CD2	1:G:204:THR:HA	2.48	0.43
2:F:26:VAL:O	2:F:54:ARG:NH1	2.51	0.43
1:E:133:TYR:HB2	1:E:168:ILE:CD1	2.47	0.43
1:E:242:ASN:HB2	1:E:308:ARG:N	2.33	0.43
1:E:323:PRO:O	1:E:326:ASP:HB2	2.18	0.43
1:G:398:PRO:O	1:G:402:ARG:HG3	2.19	0.43
1:G:133:TYR:HB3	1:G:169:MET:CE	2.49	0.43
2:F:276:HIS:O	2:F:308:THR:HA	2.19	0.43
2:F:281:THR:HG21	2:H:255:TRP:CE2	2.53	0.43
2:B:33:VAL:HG13	2:B:43:THR:HG21	2.01	0.43
1:C:11:VAL:HA	1:C:12:PRO:HD3	1.88	0.43
2:D:87:ASP:OD1	2:D:133:GLN:HG2	2.19	0.43
2:D:146:ARG:HG3	2:D:256:PRO:HD2	2.00	0.43
1:G:213:ASP:HB3	1:G:241:ASN:HA	2.01	0.43
1:G:223:THR:HG21	2:H:64:GLY:CA	2.49	0.43
2:F:255:TRP:HA	2:F:256:PRO:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:THR:OG1	1:C:307:TYR:N	2.51	0.42
1:E:282:VAL:HA	1:E:304:TRP:HZ3	1.83	0.42
2:H:159:LEU:HD11	2:H:252:ARG:HG2	2.00	0.42
1:E:74:PRO:O	1:E:78:ARG:HG3	2.19	0.42
1:G:190:GLN:NE2	2:H:99:GLU:HG3	2.34	0.42
2:H:312:THR:HG23	2:H:313:PRO:O	2.19	0.42
1:C:352:GLU:OE1	1:C:352:GLU:N	2.49	0.42
2:D:65:ILE:HG23	2:D:81:VAL:HG21	2.00	0.42
2:F:163:SER:HB3	2:F:170:VAL:HG11	2.02	0.42
1:A:151:CYS:SG	1:A:158:ARG:HB3	2.60	0.42
2:B:23:ASP:HB3	2:B:26:VAL:HG23	2.01	0.42
1:A:307:TYR:OH	1:A:326:ASP:HB3	2.19	0.42
1:C:129:CYS:O	1:C:131:PRO:HD3	2.19	0.42
2:B:28:VAL:HA	2:B:80:VAL:O	2.19	0.42
1:C:133:TYR:HE1	1:C:134:ARG:HH11	1.68	0.42
1:E:156:ASN:CB	1:E:158:ARG:H	2.29	0.42
1:A:161:LEU:HD21	1:A:171:SER:HB3	2.01	0.42
1:C:95:VAL:O	1:C:98:GLN:HB3	2.20	0.42
1:C:307:TYR:OH	1:C:326:ASP:HB3	2.19	0.42
2:D:267:LYS:HG3	2:D:299:HIS:ND1	2.35	0.42
2:H:251:LEU:O	2:H:253:SER:N	2.52	0.42
1:C:278:ASP:O	1:C:282:VAL:HG23	2.20	0.42
2:F:304:ILE:N	2:H:293:GLN:OE1	2.53	0.42
2:H:182:PRO:HD3	2:H:194:TRP:CE3	2.55	0.42
1:A:132:THR:H	1:A:135:GLN:HE21	1.67	0.41
2:B:158:GLY:HA3	2:B:209:VAL:HG23	2.01	0.41
1:C:223:THR:CG2	2:D:64:GLY:CA	2.98	0.41
2:D:272:CYS:SG	2:D:304:ILE:HG23	2.60	0.41
1:E:38:PRO:HG3	1:E:50:LEU:HD11	2.02	0.41
2:F:63:SER:HB3	2:F:91:PRO:O	2.20	0.41
2:B:280:ARG:HH21	2:B:308:THR:H	1.68	0.41
1:C:75:GLN:NE2	1:C:78:ARG:HD3	2.36	0.41
1:E:181:SER:HB2	2:F:106:ARG:CZ	2.50	0.41
1:A:282:VAL:HA	1:A:304:TRP:CZ3	2.56	0.41
1:A:378:LEU:HD23	1:A:378:LEU:HA	1.95	0.41
1:C:31:ASP:O	1:C:34:GLN:HB2	2.20	0.41
2:H:15:ALA:HB3	2:H:160:LEU:HD23	2.02	0.41
1:C:311:PRO:HA	1:C:318:PRO:CG	2.48	0.41
1:G:116:GLY:HA3	1:G:137:SER:OG	2.20	0.41
2:H:255:TRP:HA	2:H:256:PRO:C	2.41	0.41
2:D:224:SER:N	2:D:269:THR:HG21	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:HIS:O	2:B:308:THR:HA	2.20	0.41
1:A:202:GLY:HA2	1:C:7:LEU:O	2.19	0.41
1:C:383:ILE:HB	1:C:384:PRO:CD	2.51	0.41
2:H:267:LYS:HG3	2:H:299:HIS:CE1	2.55	0.41
1:A:81:MET:CG	1:A:81:MET:CE	2.99	0.41
1:C:36:ARG:HG2	1:C:36:ARG:NH1	2.31	0.41
1:C:161:LEU:HD21	1:C:171:SER:HB3	2.02	0.41
1:C:165:GLN:HG2	1:C:169:MET:HB3	2.02	0.41
1:E:47:THR:HG21	1:E:270:ALA:HA	2.03	0.41
2:F:159:LEU:HD11	2:F:252:ARG:HG2	2.03	0.41
2:F:174:GLU:HA	2:F:175:PRO:HD3	1.91	0.41
1:G:44:ALA:O	1:G:47:THR:HG22	2.20	0.41
2:H:81:VAL:CG1	2:H:117:LEU:HD22	2.46	0.41
2:H:88:TYR:O	2:H:91:PRO:HD2	2.21	0.41
1:A:209:ALA:O	1:A:238:ASN:HB2	2.21	0.41
2:F:300:LEU:HD23	2:H:297:PHE:HE1	1.86	0.41
1:G:395:LYS:HD2	2:H:167:ASP:HB2	2.03	0.41
2:H:33:VAL:HG13	2:H:43:THR:HG21	2.03	0.41
1:C:209:ALA:O	1:C:238:ASN:HB2	2.21	0.40
1:E:307:TYR:OH	1:E:326:ASP:HB3	2.21	0.40
2:F:65:ILE:HG23	2:F:81:VAL:CG2	2.51	0.40
1:G:195:ALA:CB	1:G:235:VAL:CG2	2.96	0.40
1:G:334:ASP:HA	1:G:335:PRO:HD2	1.86	0.40
2:F:197:HIS:HB3	2:F:198:PRO:HD2	2.03	0.40
2:F:222:ASP:O	2:F:269:THR:HG23	2.21	0.40
2:F:120:PRO:HA	2:F:174:GLU:O	2.21	0.40
2:H:90:TYR:O	2:H:93:SER:HB2	2.22	0.40
2:F:28:VAL:HA	2:F:80:VAL:O	2.21	0.40
2:F:142:VAL:HB	2:F:145:LEU:HD12	2.03	0.40
1:G:165:GLN:CG	1:G:169:MET:CB	3.00	0.40
2:H:13:ARG:NH1	2:H:44:GLU:HB2	2.37	0.40
1:A:150:ILE:HA	1:A:153:LEU:HD12	2.03	0.40
1:A:263:ARG:HG3	1:A:263:ARG:NH1	2.33	0.40
2:B:224:SER:N	2:B:269:THR:HG21	2.37	0.40
1:E:395:LYS:HD2	2:F:167:ASP:HB2	2.04	0.40
1:G:165:GLN:HG3	1:G:169:MET:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	405/410 (99%)	382 (94%)	21 (5%)	2 (0%)	29	61
1	C	405/410 (99%)	381 (94%)	21 (5%)	3 (1%)	22	54
1	E	405/410 (99%)	384 (95%)	19 (5%)	2 (0%)	29	61
1	G	405/410 (99%)	384 (95%)	18 (4%)	3 (1%)	22	54
2	B	336/339 (99%)	316 (94%)	19 (6%)	1 (0%)	41	71
2	D	336/339 (99%)	319 (95%)	16 (5%)	1 (0%)	41	71
2	F	336/339 (99%)	317 (94%)	17 (5%)	2 (1%)	25	58
2	H	336/339 (99%)	315 (94%)	19 (6%)	2 (1%)	25	58
All	All	2964/2996 (99%)	2798 (94%)	150 (5%)	16 (0%)	29	61

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	ILE
1	C	168	ILE
1	E	168	ILE
1	G	168	ILE
1	A	246	ILE
1	C	246	ILE
1	G	246	ILE
1	C	399	ASP
1	E	246	ILE
1	G	382	HIS
2	H	199	HIS
2	F	252	ARG
2	B	34	GLY
2	D	34	GLY
2	F	34	GLY
2	H	34	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	314/328 (96%)	304 (97%)	10 (3%)	39	73
1	C	314/328 (96%)	302 (96%)	12 (4%)	33	67
1	E	314/328 (96%)	303 (96%)	11 (4%)	36	70
1	G	314/328 (96%)	305 (97%)	9 (3%)	42	76
2	B	269/280 (96%)	258 (96%)	11 (4%)	30	64
2	D	269/280 (96%)	261 (97%)	8 (3%)	41	75
2	F	269/280 (96%)	259 (96%)	10 (4%)	34	68
2	H	269/280 (96%)	259 (96%)	10 (4%)	34	68
All	All	2332/2432 (96%)	2251 (96%)	81 (4%)	36	70

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	7	LEU
1	A	8	ARG
1	A	98	GLN
1	A	179	THR
1	A	188	PHE
1	A	235	VAL
1	A	272	LEU
1	A	328	SER
1	A	366	ILE
2	B	20	LEU
2	B	22	ARG
2	B	52	LYS
2	B	81	VAL
2	B	87	ASP
2	B	103	LEU
2	B	179	TYR
2	B	272	CYS
2	B	280	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	293	GLN
2	B	312	THR
1	C	7	LEU
1	C	8	ARG
1	C	49	ASP
1	C	98	GLN
1	C	174	GLU
1	C	179	THR
1	C	188	PHE
1	C	272	LEU
1	C	328	SER
1	C	360	GLU
1	C	366	ILE
1	C	399	ASP
2	D	81	VAL
2	D	103	LEU
2	D	146	ARG
2	D	179	TYR
2	D	272	CYS
2	D	280	ARG
2	D	293	GLN
2	D	312	THR
1	E	7	LEU
1	E	8	ARG
1	E	31	ASP
1	E	98	GLN
1	E	179	THR
1	E	188	PHE
1	E	235	VAL
1	E	272	LEU
1	E	328	SER
1	E	360	GLU
1	E	366	ILE
2	F	20	LEU
2	F	52	LYS
2	F	81	VAL
2	F	103	LEU
2	F	115	LEU
2	F	132	SER
2	F	136	GLU
2	F	179	TYR
2	F	272	CYS

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Mol	Chain	Res	Type
2	F	293	GLN
1	G	7	LEU
1	G	8	ARG
1	G	47	THR
1	G	134	ARG
1	G	179	THR
1	G	272	LEU
1	G	326	ASP
1	G	360	GLU
1	G	366	ILE
2	H	20	LEU
2	H	22	ARG
2	H	81	VAL
2	H	103	LEU
2	H	115	LEU
2	H	136	GLU
2	H	179	TYR
2	H	280	ARG
2	H	293	GLN
2	H	312	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	135	GLN
1	A	222	HIS
1	A	369	GLN
2	B	141	GLN
2	B	236	GLN
2	B	295	HIS
2	B	316	HIS
1	C	75	GLN
1	C	98	GLN
1	C	124	ASN
1	C	135	GLN
1	C	183	ASN
1	C	369	GLN
2	D	84	GLN
2	D	236	GLN
2	D	295	HIS
2	D	316	HIS

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Mol	Chain	Res	Type
1	E	98	GLN
1	E	135	GLN
1	E	369	GLN
2	F	199	HIS
2	F	236	GLN
2	F	295	HIS
2	F	316	HIS
2	F	318	GLN
1	G	98	GLN
1	G	135	GLN
1	G	165	GLN
1	G	222	HIS
1	G	369	GLN
2	H	199	HIS
2	H	236	GLN
2	H	295	HIS
2	H	316	HIS

### 5.3.3 RNA [i](#)

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 monosaccharides 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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	407/410 (99%)	-0.28	6 (1%) 73 73	15, 28, 54, 87	0
1	C	407/410 (99%)	-0.21	14 (3%) 45 40	15, 28, 54, 87	0
1	E	407/410 (99%)	-0.15	14 (3%) 45 40	15, 28, 54, 87	0
1	G	407/410 (99%)	-0.31	5 (1%) 79 79	15, 28, 54, 87	0
2	B	338/339 (99%)	-0.22	6 (1%) 68 67	19, 36, 70, 107	0
2	D	338/339 (99%)	-0.26	8 (2%) 59 56	19, 36, 70, 107	0
2	F	338/339 (99%)	-0.15	6 (1%) 68 67	19, 36, 70, 107	0
2	H	338/339 (99%)	-0.16	9 (2%) 54 50	19, 36, 70, 107	0
All	All	2980/2996 (99%)	-0.22	68 (2%) 60 58	15, 32, 64, 107	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ASN	10.3
1	G	2	ASN	8.3
2	F	198	PRO	5.7
2	B	339	VAL	5.7
2	D	339	VAL	5.4
2	F	339	VAL	5.2
1	C	2	ASN	4.8
1	E	2	ASN	4.8
2	H	189	ARG	4.7
1	C	381	GLY	4.5
2	D	2	ALA	4.4
1	C	406	GLN	3.5
2	B	198	PRO	3.4
1	A	381	GLY	3.4
2	D	189	ARG	3.4
1	G	381	GLY	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	382	HIS	3.3
2	H	339	VAL	3.3
2	F	2	ALA	3.2
2	H	190	PRO	3.2
1	E	378	LEU	3.0
2	F	188	ASP	3.0
1	G	3	GLU	2.9
1	C	374	GLN	2.9
2	H	272	CYS	2.9
2	B	196	LYS	2.9
1	E	380	ASN	2.8
2	B	189	ARG	2.8
1	E	381	GLY	2.8
2	F	190	PRO	2.8
1	E	328	SER	2.8
2	D	188	ASP	2.7
2	H	198	PRO	2.7
2	B	267	LYS	2.7
1	A	406	GLN	2.7
2	D	190	PRO	2.7
1	C	379	ALA	2.7
1	G	380	ASN	2.6
1	E	3	GLU	2.6
1	C	19	GLY	2.5
2	F	243	GLY	2.5
2	D	243	GLY	2.5
2	D	191	VAL	2.4
1	C	399	ASP	2.3
1	E	99	ARG	2.3
1	G	379	ALA	2.3
2	H	301	GLU	2.3
1	E	20	CYS	2.3
1	C	366	ILE	2.3
2	H	191	VAL	2.3
2	H	267	LYS	2.3
1	A	20	CYS	2.3
1	E	34	GLN	2.3
2	D	221	ASN	2.3
1	A	101	LYS	2.2
1	C	21	GLN	2.2
1	C	378	LEU	2.2
1	A	3	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	99	ARG	2.2
1	C	103	MET	2.2
2	B	190	PRO	2.1
1	E	406	GLN	2.1
1	C	101	LYS	2.1
1	C	60	GLU	2.1
1	E	103	MET	2.1
1	E	347	GLY	2.1
1	E	158	ARG	2.0
2	H	196	LYS	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 monosaccharides 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.