



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:13 PM UTC

PDB ID : 7AE5 / pdb_00007ae5
Title : Structure of Sedimentibacter hydroxybenzoicus vanillic acid decarboxylase (ShVdcCD) in open form
Authors : Marshall, S.A.; Leys, D.
Deposited on : 2020-09-17
Resolution : 2.19 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

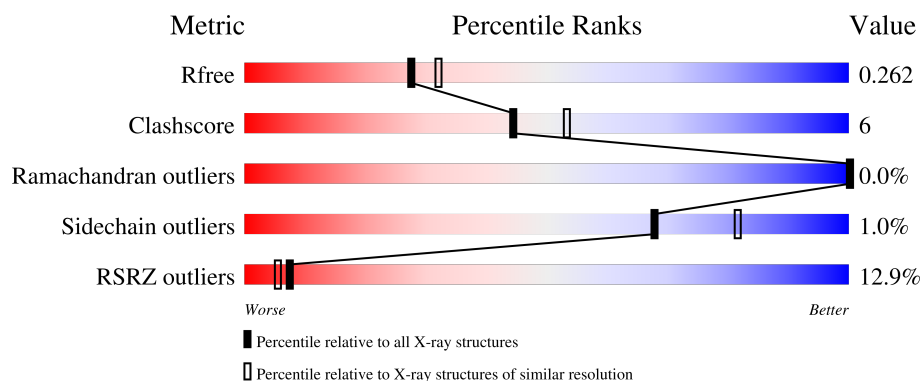
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	480	9% 82% 14% .
1	B	480	8% 82% 15% .
1	C	480	6% 84% 14% .
1	D	480	12% 84% 15% .
1	E	480	10% 85% 13% .

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Mol	Chain	Length	Quality of chain
1	F	480	
2	a	68	
2	b	68	
2	c	68	
2	d	68	
2	e	68	
2	f	68	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	RB	D	502	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25337 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 Phenolic acid decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	465	Total	C	N	O	S	0	1	0
			3606	2309	609	674	14			
1	C	469	Total	C	N	O	S	0	0	0
			3655	2339	616	685	15			
1	D	476	Total	C	N	O	S	0	1	0
			3688	2362	627	684	15			
1	E	470	Total	C	N	O	S	0	0	0
			3625	2318	614	679	14			
1	F	462	Total	C	N	O	S	0	0	0
			3528	2258	593	663	14			
1	A	466	Total	C	N	O	S	0	0	0
			3585	2302	605	664	14			

- Molecule 2 is a protein called Protein ShdD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	b	65	Total	C	N	O	S	0	0	0
			497	311	86	91	9			
2	c	67	Total	C	N	O	S	0	0	0
			520	327	89	95	9			
2	d	67	Total	C	N	O	S	0	0	0
			516	322	89	96	9			
2	e	64	Total	C	N	O	S	0	0	0
			460	289	81	82	8			
2	f	58	Total	C	N	O	S	0	0	0
			377	235	68	67	7			
2	a	63	Total	C	N	O	S	0	0	0
			458	286	80	83	9			

- Molecule 3 is RUBIDIUM ION (CCD ID: RB) (formula: Rb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Rb 2	0	0
3	C	2	Total 2	Rb 2	0	0
3	D	2	Total 2	Rb 2	0	0
3	E	2	Total 2	Rb 2	0	0
3	F	2	Total 2	Rb 2	0	0
3	A	2	Total 2	Rb 2	0	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	b	1	Total 1	Zn 1	0	0
4	c	1	Total 1	Zn 1	0	0
4	d	1	Total 1	Zn 1	0	0
4	e	1	Total 1	Zn 1	0	0
4	f	1	Total 1	Zn 1	0	0
4	a	1	Total 1	Zn 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	122	Total 122	O 122	0	0
5	C	145	Total 145	O 145	0	0
5	D	132	Total 132	O 132	0	0
5	E	136	Total 136	O 136	0	0
5	F	114	Total 114	O 114	0	0
5	A	101	Total 101	O 101	0	0

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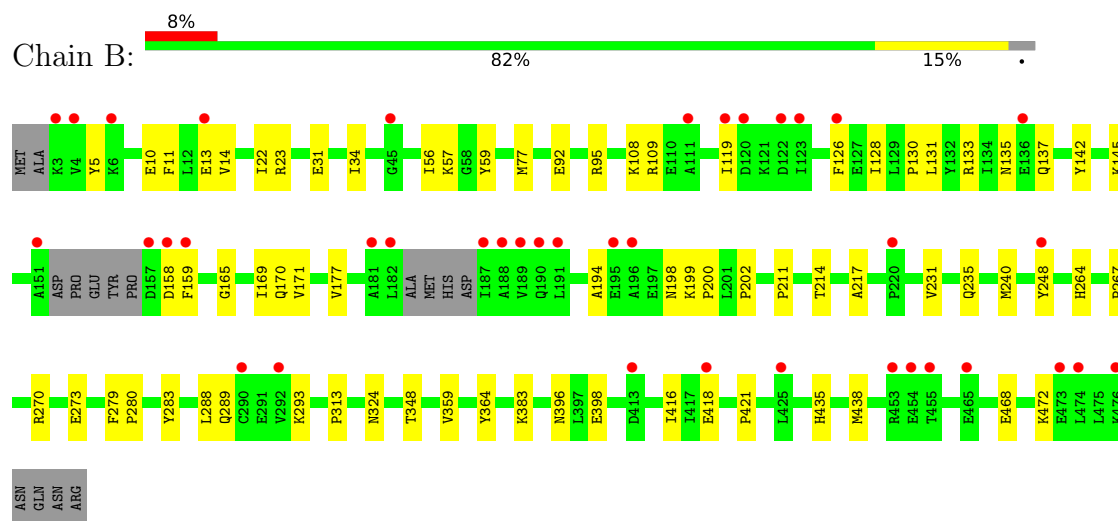
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	b	15	Total 15	O 15	0	0
5	c	7	Total 7	O 7	0	0
5	d	6	Total 6	O 6	0	0
5	e	9	Total 9	O 9	0	0
5	f	3	Total 3	O 3	0	0
5	a	14	Total 14	O 14	0	0

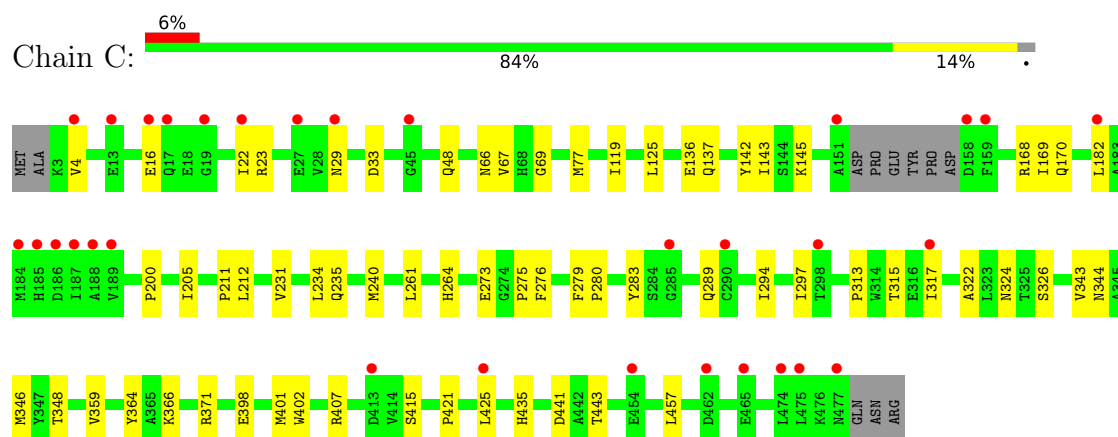
3 Residue-property plots [i](#)

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.

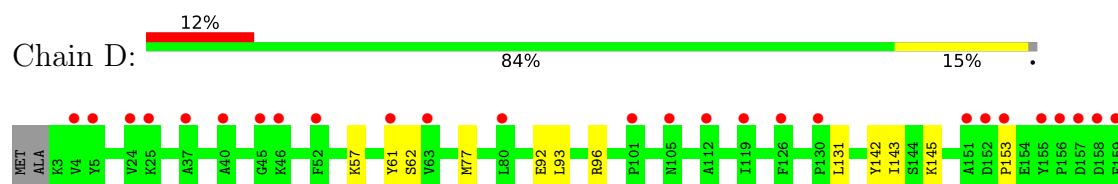
• Molecule 1: Phenolic acid decarboxylase

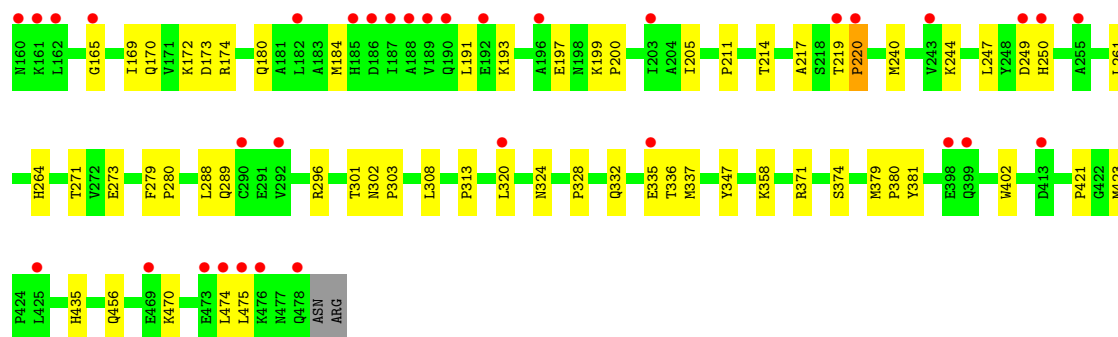


• Molecule 1: Phenolic acid decarboxylase

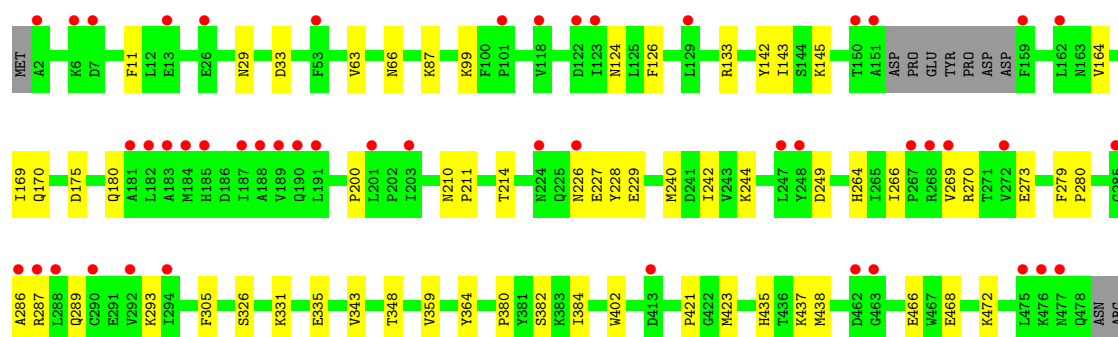
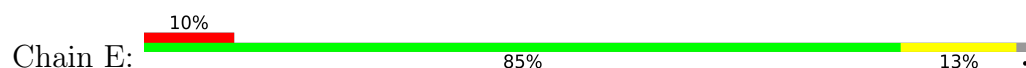


• Molecule 1: Phenolic acid decarboxylase

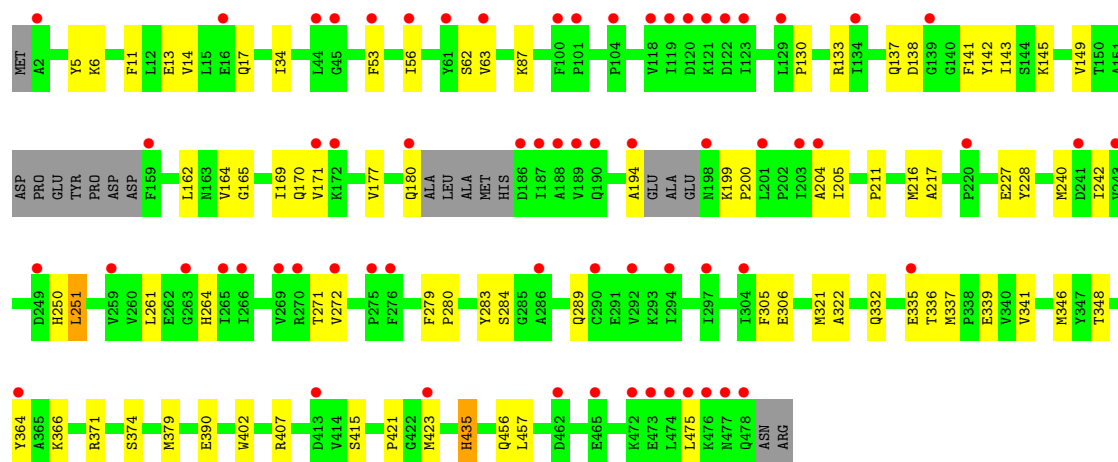
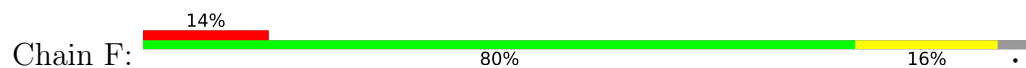




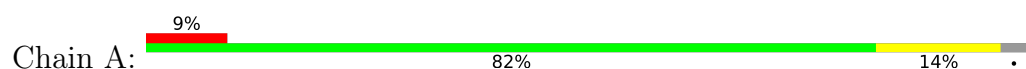
• Molecule 1: Phenolic acid decarboxylase

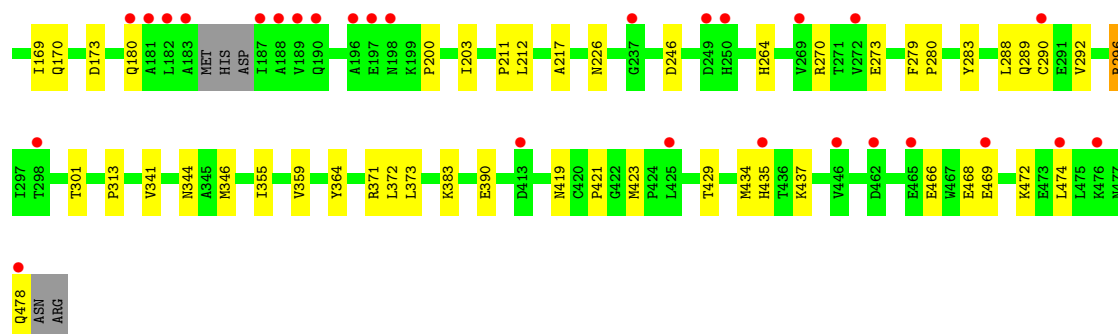


• Molecule 1: Phenolic acid decarboxylase

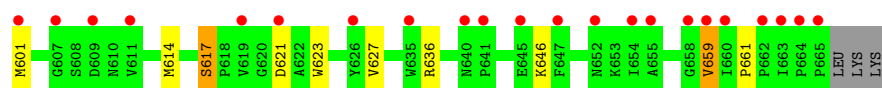
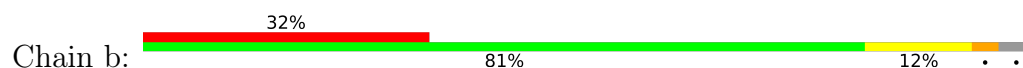


• Molecule 1: Phenolic acid decarboxylase

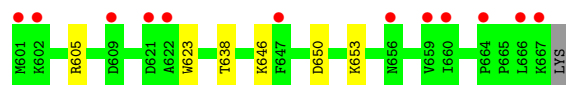
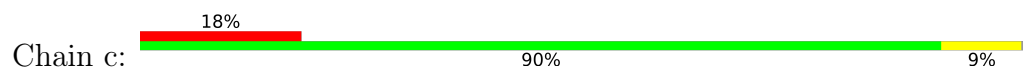




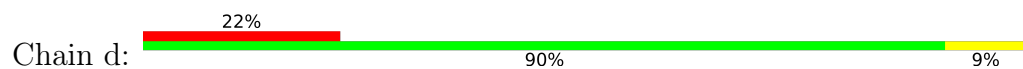
• Molecule 2: Protein ShdD



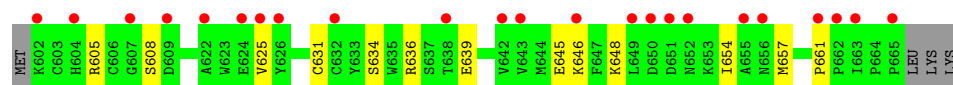
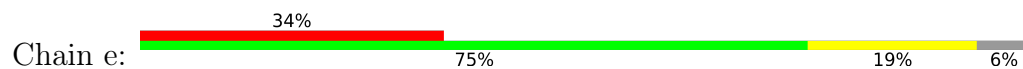
• Molecule 2: Protein ShdD



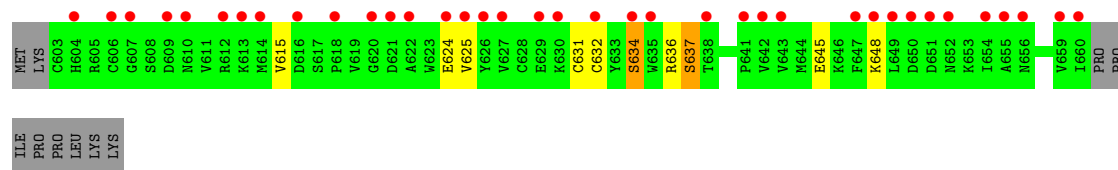
• Molecule 2: Protein ShdD



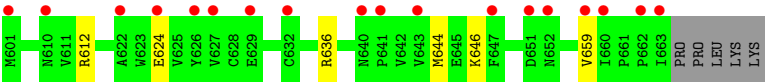
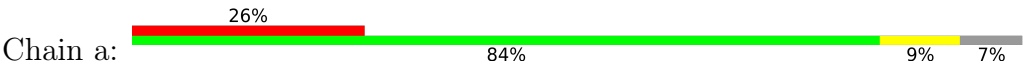
• Molecule 2: Protein ShdD



• Molecule 2: Protein ShdD



• Molecule 2: Protein ShdD



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	98.23Å 108.30Å 111.42Å 117.72° 101.32° 91.80°	Depositor
Resolution (Å)	70.14 – 2.19 70.14 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.0 (70.14-2.19) 97.1 (70.14-2.19)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.223 , 0.263 0.223 , 0.262	Depositor DCC
R_{free} test set	9812 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,k,-k-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25337	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.39% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, RB

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	0.12	0/3673	0.32	0/5016
1	B	0.12	0/3694	0.33	0/5040
1	C	0.15	0/3745	0.33	0/5109
1	D	0.17	0/3779	0.37	0/5157
1	E	0.12	0/3715	0.33	0/5070
1	F	0.15	0/3615	0.34	0/4936
2	a	0.18	0/469	0.36	0/637
2	b	0.14	0/510	0.30	0/692
2	c	0.10	0/533	0.27	0/722
2	d	0.12	0/529	0.31	0/718
2	e	0.13	0/473	0.32	0/647
2	f	0.11	0/384	0.37	0/526
All	All	0.14	0/25119	0.33	0/34270

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3585	0	3494	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3606	0	3515	46	0
1	C	3655	0	3583	42	0
1	D	3688	0	3630	48	0
1	E	3625	0	3517	37	0
1	F	3528	0	3379	57	0
2	a	458	0	400	5	0
2	b	497	0	464	10	0
2	c	520	0	499	5	0
2	d	516	0	483	6	0
2	e	460	0	395	9	0
2	f	377	0	298	8	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	a	1	0	0	0	0
4	b	1	0	0	0	0
4	c	1	0	0	0	0
4	d	1	0	0	0	0
4	e	1	0	0	0	0
4	f	1	0	0	0	0
5	A	101	0	0	4	0
5	B	122	0	0	1	0
5	C	145	0	0	3	0
5	D	132	0	0	1	0
5	E	136	0	0	2	0
5	F	114	0	0	1	0
5	a	14	0	0	0	0
5	b	15	0	0	0	0
5	c	7	0	0	0	0
5	d	6	0	0	1	0
5	e	9	0	0	0	0
5	f	3	0	0	0	0
All	All	25337	0	23657	287	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 6.

All (287) 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:B:108:LYS:HD2	1:B:109:ARG:H	1.47	0.78
2:e:646:LYS:H	2:e:646:LYS:HD2	1.50	0.77
2:f:645:GLU:HA	2:f:648:LYS:HD2	1.64	0.77
1:C:22:ILE:HD11	1:D:475:LEU:HG	1.68	0.76
2:f:625:VAL:HG12	2:f:636:ARG:HG3	1.70	0.73
1:F:407:ARG:HH22	1:F:457:LEU:HD21	1.54	0.72
2:d:653:LYS:NZ	5:d:801:HOH:O	2.22	0.72
1:F:171:VAL:HA	1:F:177:VAL:HG12	1.71	0.71
1:B:31:GLU:HG2	1:B:133:ARG:HB3	1.75	0.69
1:E:244:LYS:HE2	1:E:249:ASP:HA	1.77	0.66
1:D:205:ILE:HB	1:D:261:LEU:HB2	1.78	0.65
1:F:133:ARG:NH2	2:f:634:SER:O	2.28	0.64
1:F:63:VAL:HG12	1:F:305:PHE:HB3	1.79	0.64
1:B:119:ILE:HD12	1:B:128:ILE:HD11	1.81	0.63
1:F:366:LYS:NZ	1:F:415:SER:OG	2.30	0.62
1:F:142:TYR:CZ	1:F:170:GLN:HB2	2.35	0.62
1:A:468:GLU:O	1:A:472:LYS:HG3	2.00	0.62
1:A:143:ILE:HB	1:A:169:ILE:HB	1.83	0.61
1:B:92:GLU:OE2	1:B:95:ARG:NH2	2.30	0.61
1:C:407:ARG:HH22	1:C:457:LEU:HD21	1.66	0.61
1:D:379:MET:HB3	1:D:380:PRO:HD3	1.82	0.61
1:E:468:GLU:O	1:E:472:LYS:HG3	2.00	0.61
1:F:180:GLN:HA	1:F:289:GLN:HE21	1.65	0.60
1:F:200:PRO:HB3	1:F:264:HIS:ND1	2.16	0.60
1:C:401:MET:HG2	1:D:347:TYR:CG	2.37	0.60
1:B:396:ASN:OD1	1:B:398[A]:GLU:HG2	2.02	0.60
1:D:273:GLU:HB3	1:D:289:GLN:HG3	1.82	0.60
1:B:468:GLU:O	1:B:472:LYS:HG2	2.01	0.59
1:D:374:SER:HA	1:D:379:MET:HE3	1.85	0.59
1:A:26:GLU:OE1	1:A:26:GLU:N	2.34	0.59
1:F:137:GLN:HB2	1:F:283:TYR:CZ	2.37	0.59
1:D:244:LYS:NZ	1:D:249:ASP:OD1	2.36	0.59
1:A:109:ARG:HH22	1:A:118:VAL:HG21	1.68	0.59
1:E:133:ARG:NH2	2:e:634:SER:O	2.30	0.59
2:d:625:VAL:HG22	2:d:636:ARG:HG3	1.84	0.59
1:E:99:LYS:NZ	5:E:604:HOH:O	2.32	0.58
1:E:143:ILE:HB	1:E:169:ILE:HB	1.85	0.58
2:c:650:ASP:OD1	2:c:653:LYS:HD2	2.03	0.58
1:A:137:GLN:HB2	1:A:283:TYR:CZ	2.39	0.58
2:a:644:MET:HB3	2:a:646:LYS:HZ3	1.67	0.58
1:B:22:ILE:HD11	1:F:475:LEU:HG	1.86	0.58
1:A:341:VAL:HG21	1:A:390:GLU:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:645:GLU:HA	2:e:648:LYS:HD2	1.86	0.58
1:F:63:VAL:HG13	1:F:130:PRO:HG2	1.86	0.57
1:B:198:ASN:O	1:B:198:ASN:ND2	2.38	0.57
1:B:137:GLN:HB2	1:B:283:TYR:CZ	2.40	0.57
1:C:137:GLN:HB2	1:C:283:TYR:CZ	2.39	0.57
1:A:273:GLU:HB3	1:A:289:GLN:HG3	1.86	0.57
2:e:625:VAL:HG22	2:e:636:ARG:HG3	1.87	0.57
1:B:31:GLU:OE2	2:b:636:ARG:NH2	2.36	0.57
1:C:441:ASP:OD1	1:C:443:THR:OG1	2.23	0.56
2:b:617:SER:OG	2:b:623:TRP:O	2.24	0.56
1:F:322:ALA:HB1	1:F:346:MET:HG2	1.87	0.56
1:B:77:MET:HG3	1:B:211:PRO:HB2	1.88	0.56
1:D:143:ILE:HB	1:D:169:ILE:HB	1.87	0.56
1:A:466:GLU:H	1:A:466:GLU:CD	2.13	0.55
1:B:273:GLU:HB3	1:B:289:GLN:HG3	1.87	0.55
2:a:644:MET:HB3	2:a:646:LYS:NZ	2.22	0.55
1:D:379:MET:HE1	1:F:337:MET:HE1	1.87	0.55
1:D:131:LEU:O	2:d:636:ARG:NH2	2.32	0.55
1:A:77:MET:HG3	1:A:211:PRO:HB2	1.89	0.54
1:D:379:MET:HE1	1:F:337:MET:CE	2.37	0.54
1:C:344:ASN:OD1	1:C:346:MET:HG3	2.07	0.54
1:D:328:PRO:O	1:D:332:GLN:HG3	2.07	0.54
1:D:57:LYS:HE3	2:d:622:ALA:HB1	1.89	0.54
1:A:246:ASP:HB3	1:A:296:ARG:HH21	1.73	0.54
1:B:200:PRO:HB3	1:B:264:HIS:CD2	2.43	0.54
1:E:66:ASN:ND2	5:E:608:HOH:O	2.39	0.54
1:F:13:GLU:O	1:F:17:GLN:HG3	2.09	0.53
1:F:137:GLN:NE2	5:F:606:HOH:O	2.41	0.53
1:F:143:ILE:HB	1:F:169:ILE:HB	1.91	0.53
1:B:11:PHE:CG	1:B:211:PRO:HG3	2.44	0.53
1:F:149:VAL:HG13	1:F:162:LEU:HD21	1.91	0.53
1:B:142:TYR:CZ	1:B:170:GLN:HB2	2.44	0.53
1:E:180:GLN:HE21	1:E:289:GLN:HE22	1.57	0.53
1:B:34:ILE:HD11	1:B:56:ILE:HG12	1.90	0.52
1:B:23:ARG:NH2	5:B:607:HOH:O	2.42	0.52
1:D:193:LYS:O	1:D:197:GLU:HG2	2.09	0.52
1:C:142:TYR:CZ	1:C:170:GLN:HB2	2.45	0.52
1:F:250:HIS:CE1	1:F:251:LEU:HD13	2.45	0.52
1:A:180:GLN:HE21	1:A:289:GLN:HE22	1.56	0.52
1:A:45:GLY:C	1:A:46:LYS:HD2	2.35	0.52
1:F:180:GLN:HG3	1:F:289:GLN:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:VAL:HG22	1:E:305:PHE:HB3	1.92	0.52
1:E:331:LYS:O	1:E:335:GLU:HG3	2.10	0.52
1:A:117:ASN:HD21	1:A:301:THR:HG22	1.75	0.51
1:F:335:GLU:HG3	1:F:336:THR:HG23	1.90	0.51
1:C:200:PRO:HB3	1:C:264:HIS:CD2	2.45	0.51
1:D:371:ARG:HD2	1:F:371:ARG:NH1	2.26	0.51
1:E:226:ASN:OD1	1:E:229:GLU:HB2	2.11	0.51
1:A:200:PRO:HB3	1:A:264:HIS:CD2	2.45	0.51
1:A:373:LEU:HD22	1:A:437:LYS:HE3	1.91	0.51
1:D:374:SER:HA	1:D:379:MET:CE	2.40	0.51
1:D:142:TYR:CZ	1:D:170:GLN:HB2	2.46	0.51
1:D:335:GLU:HG3	1:D:336:THR:HG23	1.92	0.51
2:e:605:ARG:NH2	2:e:631:CYS:O	2.43	0.51
2:f:615:VAL:HG12	2:f:625:VAL:HG22	1.93	0.51
1:A:355:ILE:HD11	1:A:372:LEU:HD13	1.93	0.51
1:C:168:ARG:HD2	1:C:276:PHE:CD2	2.45	0.51
1:A:344:ASN:OD1	1:A:346:MET:HG3	2.11	0.51
1:F:272:VAL:HG11	2:f:631:CYS:O	2.10	0.50
1:A:6:LYS:HB2	1:A:10:GLU:OE2	2.11	0.50
1:F:56:ILE:HD11	1:F:63:VAL:HG22	1.94	0.50
1:B:126:PHE:HE1	2:b:614:MET:HE2	1.76	0.50
1:A:142:TYR:CZ	1:A:170:GLN:HB2	2.46	0.50
1:D:200:PRO:HB3	1:D:264:HIS:CD2	2.47	0.49
1:A:160:ASN:HA	1:A:226:ASN:ND2	2.27	0.49
1:B:421:PRO:O	1:B:435:HIS:HB2	2.12	0.49
1:C:371:ARG:NH2	5:C:611:HOH:O	2.41	0.49
1:E:142:TYR:CZ	1:E:170:GLN:HB2	2.48	0.49
1:A:371:ARG:NH2	5:A:611:HOH:O	2.43	0.49
1:C:322:ALA:HB1	1:C:346:MET:SD	2.53	0.49
1:B:416:ILE:HD13	1:B:438:MET:HG3	1.94	0.49
1:E:124:ASN:C	1:E:124:ASN:HD22	2.20	0.49
1:E:170:GLN:OE1	1:E:273:GLU:HG2	2.13	0.49
1:F:34:ILE:HD13	1:F:63:VAL:HG21	1.95	0.49
1:A:466:GLU:OE1	1:A:466:GLU:N	2.35	0.49
1:E:286:ALA:C	1:E:287:ARG:HD3	2.38	0.48
2:e:646:LYS:H	2:e:646:LYS:CD	2.24	0.48
1:F:341:VAL:HG21	1:F:390:GLU:HB2	1.94	0.48
1:B:145:LYS:HE2	1:B:214:THR:HG21	1.96	0.48
2:c:650:ASP:CG	2:c:653:LYS:HD2	2.38	0.48
2:d:659:VAL:C	2:d:660:ILE:HD13	2.39	0.48
1:B:313:PRO:HG2	1:F:402:TRP:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:GLU:OE1	1:C:23:ARG:HD2	2.14	0.48
1:F:374:SER:HA	1:F:379:MET:HE3	1.96	0.48
1:B:270:ARG:NH2	2:b:661:PRO:HD2	2.29	0.47
1:D:61:TYR:CE2	1:D:303:PRO:HD2	2.49	0.47
1:C:77:MET:HG3	1:C:211:PRO:HB2	1.96	0.47
1:D:371:ARG:NH1	1:F:371:ARG:HD2	2.28	0.47
1:B:231:VAL:O	1:B:235:GLN:HG3	2.13	0.47
1:C:48:GLN:NE2	5:C:602:HOH:O	2.40	0.47
1:F:133:ARG:NH1	1:F:138:ASP:O	2.47	0.47
1:F:194:ALA:HB1	1:F:199:LYS:O	2.14	0.47
1:A:116:GLU:OE2	1:A:301:THR:HG23	2.15	0.47
1:C:359:VAL:HG13	1:C:364:TYR:HB3	1.97	0.47
1:C:398:GLU:OE1	5:C:601:HOH:O	2.20	0.47
1:D:180:GLN:O	1:D:184:MET:HG3	2.14	0.47
1:B:199:LYS:C	1:B:267:PRO:HG3	2.40	0.47
1:D:358:LYS:NZ	5:D:608:HOH:O	2.36	0.47
1:F:205:ILE:HB	1:F:261:LEU:HB2	1.96	0.47
1:E:466:GLU:OE1	1:E:466:GLU:N	2.39	0.47
1:A:288:LEU:HD12	2:a:659:VAL:HG22	1.95	0.47
2:e:646:LYS:HD2	2:e:646:LYS:N	2.24	0.47
1:E:200:PRO:HB3	1:E:264:HIS:CD2	2.50	0.47
1:A:150:THR:HG22	1:A:203:ILE:HG22	1.97	0.47
1:D:336:THR:HG21	1:D:371:ARG:HH21	1.79	0.46
1:F:279:PHE:CG	1:F:280:PRO:HD3	2.50	0.46
2:f:624:GLU:H	2:f:637:SER:HB3	1.80	0.46
1:D:145:LYS:HE2	1:D:214:THR:HG21	1.97	0.46
1:E:359:VAL:HG13	1:E:364:TYR:HB3	1.96	0.46
1:F:11:PHE:CG	1:F:211:PRO:HG3	2.50	0.46
1:A:203:ILE:HD11	1:A:292:VAL:HG11	1.97	0.46
1:C:143:ILE:HB	1:C:169:ILE:HB	1.98	0.46
1:A:31:GLU:OE2	2:a:636:ARG:NH2	2.33	0.46
1:A:109:ARG:NH2	1:A:118:VAL:HG21	2.30	0.46
1:C:231:VAL:O	1:C:235:GLN:HG3	2.16	0.46
1:D:197:GLU:HG3	1:D:199:LYS:HG3	1.97	0.46
1:F:332:GLN:O	1:F:335:GLU:HG2	2.16	0.46
1:C:313:PRO:HG2	1:D:402:TRP:CD1	2.51	0.46
1:F:63:VAL:CG1	1:F:130:PRO:HG2	2.46	0.46
1:E:421:PRO:O	1:E:435:HIS:HB2	2.16	0.46
2:f:624:GLU:O	2:f:637:SER:N	2.46	0.46
1:B:202:PRO:HB3	1:B:248:TYR:CD1	2.51	0.45
1:D:381:TYR:CZ	1:D:423:MET:HE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:MET:HE3	1:D:240:MET:HB2	1.81	0.45
1:E:124:ASN:HD22	1:E:126:PHE:H	1.63	0.45
1:A:474:LEU:O	1:A:478:GLN:HG2	2.16	0.45
1:E:279:PHE:CG	1:E:280:PRO:HD3	2.52	0.45
1:C:324:ASN:OD1	1:C:324:ASN:N	2.50	0.45
1:E:380:PRO:HB2	1:E:423:MET:HE3	1.98	0.45
1:D:470:LYS:O	1:D:474:LEU:HD13	2.17	0.45
1:B:324:ASN:OD1	1:B:324:ASN:N	2.49	0.45
1:A:421:PRO:O	1:A:435:HIS:HB2	2.17	0.45
1:C:4:VAL:HG11	1:C:235:GLN:HB3	1.99	0.45
1:E:266:ILE:HD11	1:E:293:LYS:HB2	1.97	0.45
1:B:171:VAL:HG12	2:b:614:MET:HE1	1.99	0.44
1:D:77:MET:HG3	1:D:211:PRO:HB2	1.99	0.44
1:F:6:LYS:HD2	1:F:6:LYS:N	2.32	0.44
1:A:173:ASP:CG	2:a:612:ARG:HH22	2.25	0.44
1:D:324:ASN:OD1	1:D:324:ASN:N	2.44	0.44
1:E:240:MET:HE3	1:E:240:MET:HB2	1.72	0.44
1:A:434:MET:HG2	5:A:604:HOH:O	2.17	0.44
1:B:169:ILE:HG23	1:B:177:VAL:HB	1.99	0.44
1:B:200:PRO:HB3	1:B:264:HIS:CG	2.53	0.44
1:B:279:PHE:CG	1:B:280:PRO:HD3	2.52	0.44
1:E:11:PHE:CG	1:E:211:PRO:HG3	2.52	0.44
1:E:228:TYR:CD2	1:E:242:ILE:HG21	2.52	0.44
1:D:456:GLN:OE1	2:c:646:LYS:NZ	2.46	0.44
1:F:145:LYS:NZ	1:F:306:GLU:OE2	2.50	0.44
1:F:423:MET:HA	1:F:423:MET:HE2	2.00	0.44
1:C:402:TRP:CD1	1:D:313:PRO:HG2	2.53	0.44
1:D:93:LEU:HD23	1:D:93:LEU:HA	1.73	0.44
1:F:240:MET:HE3	1:F:240:MET:HB2	1.64	0.44
1:A:466:GLU:HA	1:A:469:GLU:OE2	2.16	0.44
1:B:5:TYR:HE1	1:B:14:VAL:HG21	1.83	0.44
1:C:275:PRO:HD3	2:c:605:ARG:NH1	2.33	0.44
1:F:216:MET:SD	1:F:227:GLU:HB3	2.58	0.44
1:F:339:GLU:OE1	1:F:364:TYR:OH	2.33	0.44
1:D:173:ASP:OD1	1:D:174:ARG:N	2.46	0.43
1:B:359:VAL:HG13	1:B:364:TYR:HB3	2.00	0.43
1:F:165:GLY:HA2	1:F:217:ALA:O	2.17	0.43
1:A:11:PHE:CG	1:A:211:PRO:HG3	2.53	0.43
1:A:419:ASN:OD1	5:A:601:HOH:O	2.21	0.43
1:A:279:PHE:CG	1:A:280:PRO:HD3	2.53	0.43
1:B:194:ALA:HB1	1:B:199:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:ARG:HH21	2:e:661:PRO:HG2	1.84	0.43
2:e:654:ILE:HA	2:e:657:MET:HE3	1.99	0.43
1:C:407:ARG:NH2	1:C:457:LEU:HD11	2.33	0.43
1:E:286:ALA:O	1:E:287:ARG:HD3	2.19	0.43
1:F:271:THR:OG1	2:f:632:CYS:SG	2.77	0.43
1:A:429:THR:HG22	1:A:435:HIS:HD2	1.84	0.43
1:D:288:LEU:HB2	2:d:659:VAL:HA	2.01	0.43
1:E:29:ASN:O	1:E:33:ASP:HB2	2.19	0.43
2:c:623:TRP:HB3	2:c:638:THR:HG23	2.00	0.43
1:A:165:GLY:HA2	1:A:217:ALA:O	2.19	0.43
1:C:77:MET:HE3	1:C:212:LEU:HD23	2.01	0.43
1:C:273:GLU:HB3	1:C:289:GLN:HG3	2.00	0.43
1:A:17:GLN:NE2	1:A:18:GLU:OE2	2.51	0.43
1:B:10:GLU:O	1:B:13:GLU:HG2	2.19	0.42
1:B:59:TYR:CD1	1:B:130:PRO:HA	2.54	0.42
1:E:326:SER:HB3	1:E:343:VAL:O	2.19	0.42
1:D:336:THR:HG21	1:D:371:ARG:NH2	2.34	0.42
1:A:359:VAL:HG13	1:A:364:TYR:HB3	2.01	0.42
1:C:212:LEU:HD22	1:C:234:LEU:HB3	2.01	0.42
1:E:269:VAL:O	1:E:270:ARG:HD3	2.20	0.42
1:C:279:PHE:CG	1:C:280:PRO:HD3	2.54	0.42
1:C:326:SER:HB3	1:C:343:VAL:O	2.20	0.42
1:E:402:TRP:CD1	1:A:313:PRO:HG2	2.54	0.42
1:A:65:THR:HG21	5:A:608:HOH:O	2.19	0.42
1:C:315:THR:OG1	1:C:317:ILE:HG22	2.20	0.42
1:C:67:VAL:HB	1:C:145:LYS:NZ	2.34	0.42
1:A:270:ARG:NH1	1:A:290:CYS:SG	2.92	0.42
1:A:383:LYS:HB2	1:A:435:HIS:CE1	2.54	0.42
1:F:141:PHE:O	1:F:171:VAL:HG22	2.19	0.42
1:F:228:TYR:CD2	1:F:242:ILE:HG21	2.55	0.42
1:B:57:LYS:HE3	1:B:57:LYS:HB3	1.83	0.42
1:B:108:LYS:CD	1:B:109:ARG:H	2.26	0.42
1:B:165:GLY:HA2	1:B:217:ALA:O	2.19	0.42
1:C:66:ASN:OD1	1:C:69:GLY:HA3	2.20	0.42
1:D:279:PHE:CG	1:D:280:PRO:HD3	2.55	0.42
1:D:247:LEU:HD21	1:D:296:ARG:HE	1.84	0.42
1:D:337:MET:CE	1:F:379:MET:HE1	2.50	0.42
1:B:131:LEU:HD13	1:B:171:VAL:HG21	2.01	0.41
1:C:119:ILE:HB	1:C:297:ILE:HB	2.02	0.41
1:D:301:THR:HG22	1:D:302:ASN:HD22	1.84	0.41
2:b:614:MET:HB2	2:b:627:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:646:LYS:HE2	2:b:646:LYS:HB2	1.83	0.41
1:E:382:SER:O	1:E:437:LYS:NZ	2.47	0.41
1:A:423:MET:HA	1:A:423:MET:HE2	2.03	0.41
1:B:383:LYS:HB2	1:B:435:HIS:CE1	2.55	0.41
1:C:366:LYS:NZ	1:C:415:SER:OG	2.42	0.41
1:D:92:GLU:O	1:D:96:ARG:HG3	2.20	0.41
1:E:175:ASP:OD2	1:E:293:LYS:NZ	2.42	0.41
1:F:5:TYR:HE1	1:F:14:VAL:HG21	1.85	0.41
1:B:158:ASP:OD1	1:B:159:PHE:N	2.50	0.41
1:C:182:LEU:HD12	1:C:182:LEU:O	2.20	0.41
1:E:164:VAL:HG23	1:E:227:GLU:HG3	2.03	0.41
1:F:421:PRO:O	1:F:435:HIS:HB2	2.20	0.41
1:B:126:PHE:CE1	2:b:614:MET:HE2	2.54	0.41
1:E:145:LYS:HE2	1:E:214:THR:HG21	2.03	0.41
1:F:87:LYS:HE2	1:F:87:LYS:HB3	1.92	0.41
1:D:153:PRO:HA	1:D:250:HIS:CD2	2.56	0.41
1:F:180:GLN:HA	1:F:289:GLN:NE2	2.34	0.41
1:B:240:MET:HE3	1:B:240:MET:HB2	1.91	0.41
1:C:205:ILE:HB	1:C:261:LEU:HB2	2.03	0.41
1:F:149:VAL:HB	1:F:204:ALA:HB3	2.02	0.41
1:F:164:VAL:N	1:F:227:GLU:HG3	2.36	0.41
1:F:456:GLN:OE1	2:b:646:LYS:NZ	2.46	0.41
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.92	0.41
1:B:288:LEU:HB2	2:b:659:VAL:HA	2.03	0.41
1:C:29:ASN:O	1:C:33:ASP:HB2	2.21	0.41
1:F:53:PHE:O	1:F:62:SER:HB2	2.21	0.41
1:B:135:ASN:HB3	1:B:283:TYR:OH	2.21	0.40
1:C:240:MET:HE3	1:C:240:MET:HB2	1.71	0.40
1:D:165:GLY:HA2	1:D:217:ALA:O	2.20	0.40
1:D:421:PRO:O	1:D:435:HIS:HB2	2.21	0.40
1:C:125:LEU:HD21	1:C:294:ILE:HD13	2.03	0.40
1:F:279:PHE:HB2	1:F:321:MET:HE1	2.03	0.40
1:D:219:THR:HA	1:D:220:PRO:HD3	1.78	0.40
1:E:87:LYS:HE2	1:E:87:LYS:HB3	1.93	0.40
1:C:371:ARG:HA	1:C:371:ARG:HD2	1.68	0.40
1:E:384:ILE:HG12	1:E:438:MET:HE3	2.04	0.40
1:C:136:GLU:HG3	1:C:137:GLN:HG2	2.02	0.40
1:C:421:PRO:O	1:C:435:HIS:HB2	2.22	0.40
1:D:172:LYS:NZ	1:D:271:THR:OG1	2.55	0.40
1:F:336:THR:HG21	1:F:371:ARG:HH21	1.86	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	460/480 (96%)	444 (96%)	16 (4%)	0	100	100
1	B	460/480 (96%)	448 (97%)	12 (3%)	0	100	100
1	C	465/480 (97%)	452 (97%)	13 (3%)	0	100	100
1	D	475/480 (99%)	455 (96%)	19 (4%)	1 (0%)	43	51
1	E	466/480 (97%)	454 (97%)	12 (3%)	0	100	100
1	F	454/480 (95%)	436 (96%)	18 (4%)	0	100	100
2	a	61/68 (90%)	60 (98%)	1 (2%)	0	100	100
2	b	63/68 (93%)	62 (98%)	1 (2%)	0	100	100
2	c	65/68 (96%)	64 (98%)	1 (2%)	0	100	100
2	d	65/68 (96%)	64 (98%)	1 (2%)	0	100	100
2	e	62/68 (91%)	56 (90%)	6 (10%)	0	100	100
2	f	56/68 (82%)	53 (95%)	3 (5%)	0	100	100
All	All	3152/3288 (96%)	3048 (97%)	103 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	220	PRO

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	378/419 (90%)	376 (100%)	2 (0%)	81	90
1	B	384/419 (92%)	381 (99%)	3 (1%)	73	85
1	C	394/419 (94%)	392 (100%)	2 (0%)	81	90
1	D	394/419 (94%)	390 (99%)	4 (1%)	68	81
1	E	383/419 (91%)	381 (100%)	2 (0%)	81	90
1	F	368/419 (88%)	364 (99%)	4 (1%)	65	79
2	a	45/63 (71%)	44 (98%)	1 (2%)	45	61
2	b	55/63 (87%)	51 (93%)	4 (7%)	13	15
2	c	59/63 (94%)	59 (100%)	0	100	100
2	d	58/63 (92%)	58 (100%)	0	100	100
2	e	44/63 (70%)	42 (96%)	2 (4%)	24	33
2	f	30/63 (48%)	28 (93%)	2 (7%)	15	17
All	All	2592/2892 (90%)	2566 (99%)	26 (1%)	68	81

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	293	LYS
1	B	348	THR
1	B	418	GLU
1	C	348	THR
1	C	425	LEU
1	D	62	SER
1	D	191	LEU
1	D	308	LEU
1	D	320	LEU
1	E	210	ASN
1	E	348	THR
1	F	251	LEU
1	F	284	SER
1	F	348	THR
1	F	435	HIS
1	A	93	LEU
1	A	296	ARG
2	b	601	MET
2	b	617	SER
2	b	621	ASP
2	b	659	VAL
2	e	608	SER

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Mol	Chain	Res	Type
2	e	639	GLU
2	f	634	SER
2	f	637	SER
2	a	624	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	20	GLN
1	B	105	ASN
1	B	419	ASN
1	C	135	ASN
1	C	396	ASN
1	C	419	ASN
1	D	163	ASN
1	D	302	ASN
1	D	377	HIS
1	E	124	ASN
1	E	235	GLN
1	E	289	GLN
1	E	478	GLN
1	F	29	ASN
1	F	180	GLN
1	F	289	GLN
1	A	17	GLN
1	A	20	GLN
1	A	83	ASN
1	A	117	ASN
1	A	180	GLN
1	A	226	ASN
1	A	349	HIS
1	A	435	HIS
2	b	610	ASN
2	b	656	ASN
2	d	610	ASN
2	d	656	ASN

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](#)

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	466/480 (97%)	0.92	42 (9%)	15 12	28, 54, 93, 124	0
1	B	465/480 (96%)	0.81	39 (8%)	17 14	22, 52, 87, 125	1 (0%)
1	C	469/480 (97%)	0.70	31 (6%)	24 21	27, 45, 74, 110	0
1	D	476/480 (99%)	0.97	60 (12%)	8 6	20, 53, 94, 129	1 (0%)
1	E	470/480 (97%)	0.87	48 (10%)	12 9	29, 50, 89, 143	0
1	F	462/480 (96%)	0.99	66 (14%)	6 4	28, 55, 93, 130	0
2	a	63/68 (92%)	1.60	18 (28%)	1 1	50, 69, 99, 114	0
2	b	65/68 (95%)	1.57	22 (33%)	1 0	49, 70, 97, 114	0
2	c	67/68 (98%)	1.15	12 (17%)	3 3	41, 57, 82, 117	0
2	d	67/68 (98%)	1.43	15 (22%)	2 1	39, 64, 92, 122	0
2	e	64/68 (94%)	1.90	23 (35%)	1 0	58, 81, 115, 126	0
2	f	58/68 (85%)	2.34	37 (63%)	0 0	70, 96, 111, 117	0
All	All	3192/3288 (97%)	0.97	413 (12%)	7 5	20, 53, 96, 143	2 (0%)

All (413) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	f	649	LEU	6.4
1	D	187	ILE	5.5
2	a	663	ILE	5.4
1	E	187	ILE	5.4
1	D	155	TYR	5.3
1	A	187	ILE	5.3
1	A	159	PHE	5.2
1	E	2	ALA	5.0
2	c	601	MET	5.0
1	C	187	ILE	4.8
1	A	183	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	181	ALA	4.7
2	f	660	ILE	4.7
1	B	181	ALA	4.6
1	D	188	ALA	4.5
1	F	297	ILE	4.5
1	A	413	ASP	4.4
1	D	220	PRO	4.4
1	E	475	LEU	4.4
2	d	622	ALA	4.3
1	B	182	LEU	4.3
1	E	191	LEU	4.3
1	F	123	ILE	4.3
2	b	663	ILE	4.3
1	E	294	ILE	4.2
1	D	156	PRO	4.2
1	C	159	PHE	4.2
1	D	152	ASP	4.2
2	a	659	VAL	4.1
1	D	153	PRO	4.1
1	F	119	ILE	4.1
1	F	187	ILE	4.1
1	D	159	PHE	4.1
2	a	601	MET	4.1
2	f	621	ASP	4.0
1	F	194	ALA	4.0
2	f	655	ALA	4.0
1	F	198	ASN	3.9
2	d	601	MET	3.9
2	a	640	ASN	3.8
1	F	294	ILE	3.8
2	e	663	ILE	3.8
2	f	656	ASN	3.8
1	A	298	THR	3.8
1	F	186	ASP	3.8
2	b	665	PRO	3.7
2	b	601	MET	3.7
1	B	159	PHE	3.7
2	d	667	LYS	3.7
1	C	475	LEU	3.7
1	A	45	GLY	3.6
2	d	663	ILE	3.6
2	f	652	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	4	VAL	3.6
1	E	159	PHE	3.6
1	F	203	ILE	3.6
1	A	151	ALA	3.6
2	e	665	PRO	3.6
2	e	602	LYS	3.6
1	D	24	VAL	3.6
2	f	650	ASP	3.6
1	F	243	VAL	3.5
2	a	662	PRO	3.5
1	F	475	LEU	3.5
2	e	661	PRO	3.4
1	B	151	ALA	3.4
2	b	607	GLY	3.4
2	d	621	ASP	3.4
1	B	476	LYS	3.4
1	E	182	LEU	3.4
1	D	165	GLY	3.4
1	B	188	ALA	3.4
1	B	290	CYS	3.4
2	a	632	CYS	3.4
1	F	423	MET	3.4
1	F	276	PHE	3.4
1	C	17	GLN	3.3
1	B	191	LEU	3.3
1	F	159	PHE	3.3
1	C	454	GLU	3.3
1	A	197	GLU	3.3
1	C	186	ASP	3.3
1	F	122	ASP	3.3
2	e	607	GLY	3.3
1	B	4	VAL	3.3
1	D	250	HIS	3.3
1	D	5	TYR	3.2
1	A	160	ASN	3.2
2	b	660	ILE	3.2
1	E	184	MET	3.2
2	f	625	VAL	3.2
1	D	46	LYS	3.2
1	F	2	ALA	3.2
2	c	666	LEU	3.2
1	E	476	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	183	ALA	3.2
1	D	413	ASP	3.2
1	D	290	CYS	3.2
2	e	656	ASN	3.2
1	D	190	GLN	3.2
2	f	659	VAL	3.1
2	f	641	PRO	3.1
1	B	189	VAL	3.1
1	D	112	ALA	3.1
1	D	186	ASP	3.1
1	C	13	GLU	3.1
2	f	614	MET	3.1
1	F	462	ASP	3.1
1	F	44	LEU	3.1
2	f	630	LYS	3.1
1	D	101	PRO	3.1
1	F	476	LYS	3.1
1	A	478	GLN	3.1
1	E	101	PRO	3.0
2	c	609	ASP	3.0
1	A	188	ALA	3.0
1	B	187	ILE	3.0
1	F	265	ILE	3.0
1	B	157	ASP	3.0
2	f	616	ASP	3.0
1	F	290	CYS	3.0
1	F	129	LEU	3.0
1	A	189	VAL	3.0
1	C	29	ASN	3.0
2	e	652	ASN	3.0
1	F	335	GLU	3.0
1	D	158	ASP	3.0
1	E	122	ASP	3.0
1	F	272	VAL	3.0
2	d	666	LEU	3.0
1	D	398	GLU	3.0
1	F	465	GLU	3.0
1	F	304	ILE	3.0
2	c	621	ASP	3.0
1	D	126	PHE	3.0
2	c	647	PHE	3.0
1	D	335	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	f	610	ASN	2.9
1	A	269	VAL	2.9
2	f	651	ASP	2.9
1	F	477	ASN	2.9
2	b	652	ASN	2.9
1	A	425	LEU	2.9
1	D	45	GLY	2.9
1	B	123	ILE	2.9
1	D	219	THR	2.9
2	f	647	PHE	2.9
1	F	263	GLY	2.9
1	D	189	VAL	2.9
2	e	643	VAL	2.9
2	e	650	ASP	2.9
2	f	618	PRO	2.9
2	c	622	ALA	2.9
1	D	182	LEU	2.8
2	a	651	ASP	2.8
2	b	659	VAL	2.8
1	F	266	ILE	2.8
1	B	195	GLU	2.8
1	B	454	GLU	2.8
1	D	425	LEU	2.8
1	E	201	LEU	2.8
1	B	122	ASP	2.8
1	E	413	ASP	2.8
1	D	151	ALA	2.8
2	e	655	ALA	2.8
2	e	625	VAL	2.8
1	F	292	VAL	2.8
2	b	611	VAL	2.8
2	d	627	VAL	2.8
1	E	203	ILE	2.8
1	F	270	ARG	2.7
2	a	610	ASN	2.7
1	B	45	GLY	2.7
2	d	665	PRO	2.7
1	E	118	VAL	2.7
2	f	613	LYS	2.7
1	A	182	LEU	2.7
1	B	13	GLU	2.7
1	B	292	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	473	GLU	2.7
1	E	292	VAL	2.7
1	F	118	VAL	2.7
1	F	189	VAL	2.7
2	f	642	VAL	2.7
1	B	190	GLN	2.7
2	f	629	GLU	2.7
2	f	626	TYR	2.7
1	E	189	VAL	2.7
1	F	249	ASP	2.7
1	F	413	ASP	2.7
1	C	45	GLY	2.7
1	C	425	LEU	2.6
1	E	162	LEU	2.6
2	e	642	VAL	2.6
2	f	627	VAL	2.6
1	F	45	GLY	2.6
1	A	44	LEU	2.6
2	b	647	PHE	2.6
1	D	157	ASP	2.6
1	F	172	LYS	2.6
2	e	609	ASP	2.6
1	D	243	VAL	2.6
1	F	180	GLN	2.6
1	A	58	GLY	2.6
2	d	620	GLY	2.6
2	f	624	GLU	2.6
1	D	105	ASN	2.6
1	C	151	ALA	2.6
1	C	298	THR	2.6
1	E	151	ALA	2.6
2	f	638	THR	2.6
1	B	6	LYS	2.6
1	E	267	PRO	2.6
2	b	664	PRO	2.6
2	e	651	ASP	2.6
1	A	190	GLN	2.6
1	A	272	VAL	2.6
2	b	640	ASN	2.6
1	A	161	LYS	2.6
1	B	474	LEU	2.6
2	e	649	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	63	VAL	2.5
1	E	272	VAL	2.5
1	C	184	MET	2.5
1	A	237	GLY	2.5
1	C	290	CYS	2.5
1	E	290	CYS	2.5
1	F	204	ALA	2.5
2	a	622	ALA	2.5
2	a	629	GLU	2.5
1	F	63	VAL	2.5
2	f	620	GLY	2.5
1	D	161	LYS	2.5
1	F	364	TYR	2.5
1	A	476	LYS	2.5
1	B	465	GLU	2.5
1	D	320	LEU	2.5
1	D	475	LEU	2.5
1	B	3	LYS	2.5
1	E	287	ARG	2.5
1	F	56	ILE	2.5
1	F	134	ILE	2.5
1	A	290	CYS	2.5
1	C	158	ASP	2.5
1	F	478	GLN	2.5
2	d	638	THR	2.5
1	F	100	PHE	2.5
1	C	4	VAL	2.4
1	F	120	ASP	2.4
1	B	248	TYR	2.4
1	D	196	ALA	2.4
1	C	182	LEU	2.4
1	D	162	LEU	2.4
1	A	3	LYS	2.4
1	C	27	GLU	2.4
1	D	478	GLN	2.4
1	F	190	GLN	2.4
1	B	120	ASP	2.4
2	a	627	VAL	2.4
1	B	455	THR	2.4
1	B	111	ALA	2.4
2	c	602	LYS	2.4
1	E	129	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	247	LEU	2.4
1	C	317	ILE	2.4
2	b	626	TYR	2.4
1	C	185	HIS	2.4
1	D	37	ALA	2.4
1	E	188	ALA	2.4
1	F	201	LEU	2.4
1	A	465	GLU	2.4
2	b	645	GLU	2.4
1	A	180	GLN	2.4
1	B	158	ASP	2.4
1	E	462	ASP	2.4
1	F	472	LYS	2.4
2	c	667	LYS	2.4
1	B	220	PRO	2.4
2	f	632	CYS	2.4
2	f	635	TRP	2.4
1	F	61	TYR	2.3
2	a	626	TYR	2.3
1	B	136	GLU	2.3
1	E	286	ALA	2.3
1	D	80	LEU	2.3
1	E	190	GLN	2.3
1	F	53	PHE	2.3
1	D	473	GLU	2.3
1	F	275	PRO	2.3
1	A	196	ALA	2.3
1	D	160	ASN	2.3
1	C	462	ASP	2.3
1	B	453	ARG	2.3
1	B	126	PHE	2.3
2	f	654	ILE	2.3
1	D	192	GLU	2.3
1	F	473	GLU	2.3
2	a	643	VAL	2.3
1	C	477	ASN	2.3
1	E	268	ARG	2.3
1	E	463	GLY	2.3
1	F	139	GLY	2.3
1	A	474	LEU	2.3
2	f	609	ASP	2.3
2	e	604	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	53	PHE	2.3
2	c	660	ILE	2.3
1	C	189	VAL	2.3
2	f	643	VAL	2.3
1	D	130	PRO	2.3
1	F	104	PRO	2.3
2	f	606	CYS	2.3
1	A	462	ASP	2.3
2	b	609	ASP	2.3
1	D	469	GLU	2.2
1	F	16	GLU	2.2
1	F	101	PRO	2.2
1	F	220	PRO	2.2
2	b	662	PRO	2.2
2	c	659	VAL	2.2
2	f	612	ARG	2.2
1	D	25	LYS	2.2
1	B	413	ASP	2.2
1	C	413	ASP	2.2
1	B	196	ALA	2.2
1	C	188	ALA	2.2
1	D	474	LEU	2.2
1	B	418	GLU	2.2
1	E	248	TYR	2.2
1	A	59	TYR	2.2
1	A	469	GLU	2.2
1	E	150	THR	2.2
1	F	171	VAL	2.2
2	e	662	PRO	2.2
1	D	249	ASP	2.2
1	C	285	GLY	2.2
1	C	16	GLU	2.2
1	E	13	GLU	2.2
2	b	655	ALA	2.2
2	d	639	GLU	2.2
2	e	626	TYR	2.2
2	d	662	PRO	2.2
1	E	269	VAL	2.2
2	b	658	GLY	2.2
1	D	399	GLN	2.2
2	f	634	SER	2.2
1	A	46	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	e	646	LYS	2.2
1	A	249	ASP	2.2
1	E	123	ILE	2.1
1	A	126	PHE	2.1
2	a	647	PHE	2.1
1	F	269	VAL	2.1
1	A	446	VAL	2.1
2	d	611	VAL	2.1
2	f	607	GLY	2.1
1	A	435	HIS	2.1
1	D	40	ALA	2.1
1	C	474	LEU	2.1
1	E	288	LEU	2.1
1	F	474	LEU	2.1
2	e	632	CYS	2.1
1	D	476	LYS	2.1
1	E	226	ASN	2.1
1	A	198	ASN	2.1
1	F	241	ASP	2.1
2	e	624	GLU	2.1
1	A	65	THR	2.1
2	c	664	PRO	2.1
2	d	661	PRO	2.1
1	D	52	PHE	2.1
1	D	119	ILE	2.1
1	A	134	ILE	2.1
1	D	292	VAL	2.1
2	f	648	LYS	2.1
1	E	26	GLU	2.1
2	a	624	GLU	2.1
1	E	7	ASP	2.1
1	A	122	ASP	2.1
2	b	641	PRO	2.1
2	e	638	THR	2.1
1	B	119	ILE	2.1
1	C	19	GLY	2.1
2	b	619	VAL	2.1
2	f	622	ALA	2.1
1	D	61	TYR	2.1
1	D	185	HIS	2.1
1	A	250	HIS	2.1
2	d	626	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	f	604	HIS	2.1
2	a	641	PRO	2.1
1	F	121	LYS	2.1
2	b	654	ILE	2.1
2	a	660	ILE	2.1
1	F	259	VAL	2.1
1	D	255	ALA	2.1
1	F	188	ALA	2.1
1	A	181	ALA	2.1
2	e	622	ALA	2.1
1	B	425	LEU	2.0
2	a	652	ASN	2.0
1	E	6	LYS	2.0
1	C	22	ILE	2.0
1	D	203	ILE	2.0
1	C	465	GLU	2.0
1	F	286	ALA	2.0
2	b	635	TRP	2.0
1	E	224	ASN	2.0
1	E	477	ASN	2.0
2	c	656	ASN	2.0
2	b	621	ASP	2.0
1	E	185	HIS	2.0
1	E	285	GLY	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	RB	D	502	1/1	0.11	0.41	367,367,367,367	0
3	RB	C	502	1/1	0.92	0.09	60,60,60,60	0
3	RB	B	502	1/1	0.93	0.11	75,75,75,75	0
3	RB	F	501	1/1	0.94	0.09	63,63,63,63	0
3	RB	A	501	1/1	0.94	0.10	67,67,67,67	0
3	RB	F	502	1/1	0.95	0.09	75,75,75,75	0
3	RB	A	502	1/1	0.96	0.07	64,64,64,64	0
3	RB	E	501	1/1	0.97	0.08	47,47,47,47	0
3	RB	D	501	1/1	0.98	0.08	48,48,48,48	0
3	RB	E	502	1/1	0.98	0.06	47,47,47,47	0
3	RB	B	501	1/1	0.98	0.08	45,45,45,45	0
3	RB	C	501	1/1	0.99	0.10	44,44,44,44	0
4	ZN	f	701	1/1	0.99	0.04	87,87,87,87	0
4	ZN	a	701	1/1	0.99	0.02	55,55,55,55	0
4	ZN	d	701	1/1	1.00	0.01	40,40,40,40	0
4	ZN	e	701	1/1	1.00	0.03	68,68,68,68	0
4	ZN	b	701	1/1	1.00	0.02	51,51,51,51	0
4	ZN	c	701	1/1	1.00	0.02	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.