



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:30 PM UTC

PDB ID : 7AE7 / pdb_00007ae7
Title : Structure of Sedimentibacter hydroxybenzoicus vanillic acid decarboxylase (ShVdcCD) in open form, with truncated ShVdcD (V59X)
Authors : Marshall, S.A.; Leys, D.
Deposited on : 2020-09-17
Resolution : 2.66 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

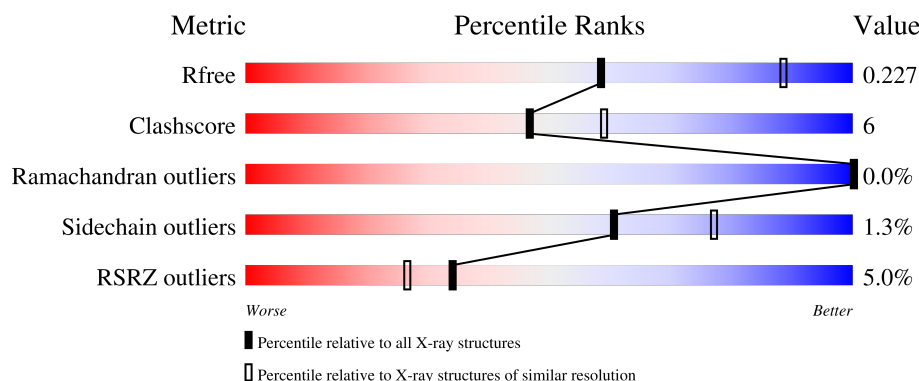
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	3% 86% 11% .
1	B	480	7% 80% 18% .
1	C	480	7% 80% 18% .
1	D	480	% 85% 14% .
1	E	480	4% 82% 14% ..

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Mol	Chain	Length	Quality of chain
1	F	480	6% 81% 16%
2	a	58	93%
2	b	58	31% 72% 10% 17%
2	c	58	2% 78% 19%
2	d	58	86% 12%
2	e	58	3% 93% 5%
2	f	58	5% 84% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24349 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	A	467	Total	C	N	O	S	0	0	0
			3608	2315	608	670	15			
1	B	468	Total	C	N	O	S	0	0	0
			3508	2252	590	652	14			
1	C	471	Total	C	N	O	S	0	0	0
			3534	2268	596	656	14			
1	D	475	Total	C	N	O	S	0	0	0
			3675	2352	617	691	15			
1	E	461	Total	C	N	O	S	0	0	0
			3491	2238	584	655	14			
1	F	471	Total	C	N	O	S	0	0	0
			3565	2286	601	663	15			

- Molecule 2 is a protein called Protein ShdD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	57	Total	C	N	O	S	0	0	0
			454	280	79	86	9			
2	b	48	Total	C	N	O	S	0	0	0
			286	179	50	53	4			
2	c	57	Total	C	N	O	S	0	0	0
			415	259	74	74	8			
2	d	57	Total	C	N	O	S	0	0	0
			441	275	77	80	9			
2	e	57	Total	C	N	O	S	0	0	0
			406	257	72	68	9			
2	f	57	Total	C	N	O	S	0	0	0
			419	262	74	74	9			

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	E	1	Total Na 1 1	0	0
3	F	1	Total Na 1 1	0	0

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

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

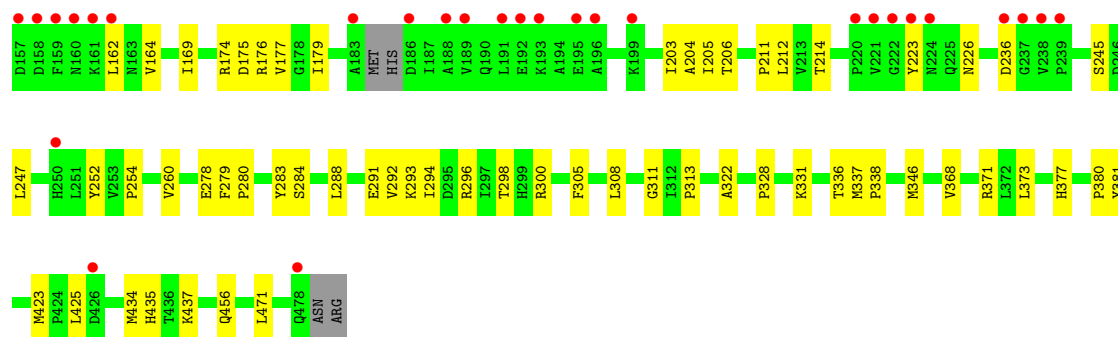
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	139	Total O 139 139	0	0
5	B	74	Total O 74 74	0	0
5	C	60	Total O 60 60	0	0
5	D	92	Total O 92 92	0	0
5	E	65	Total O 65 65	0	0
5	F	67	Total O 67 67	0	0
5	a	21	Total O 21 21	0	0

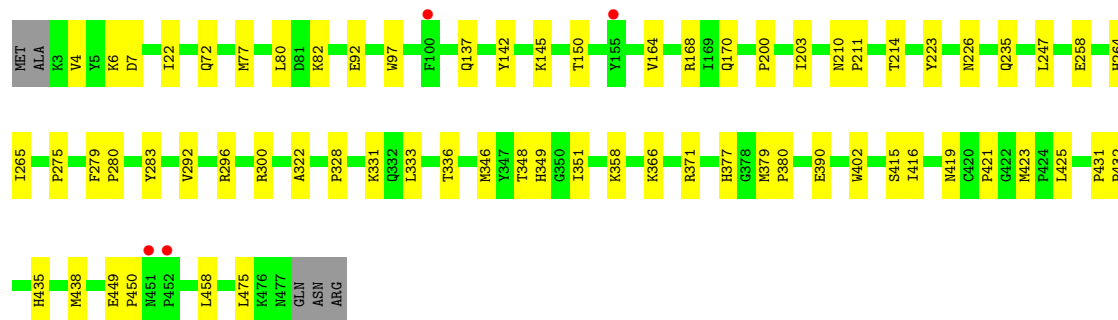
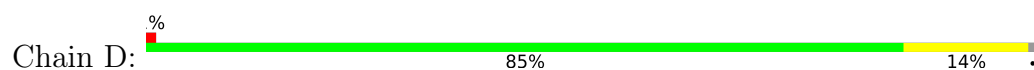
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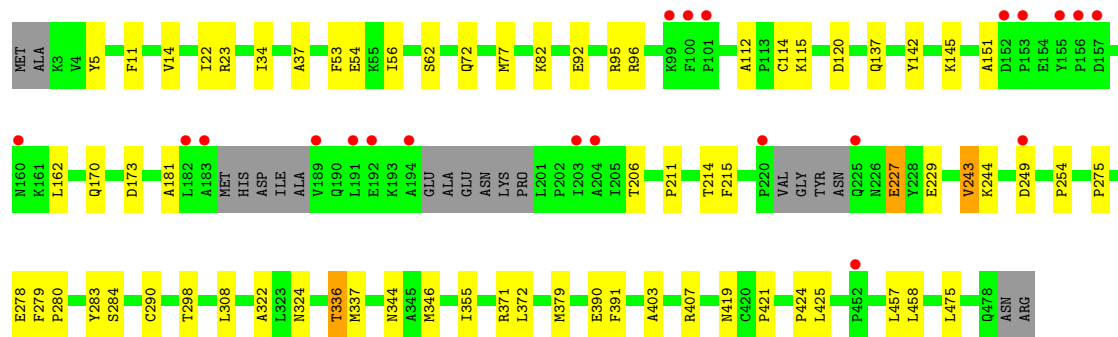
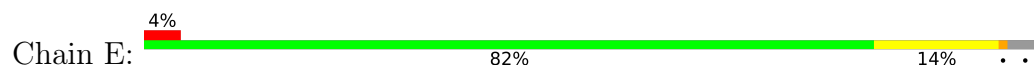
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	c	3	Total 3	O 3	0	0
5	d	6	Total 6	O 6	0	0
5	e	3	Total 3	O 3	0	0
5	f	6	Total 6	O 6	0	0



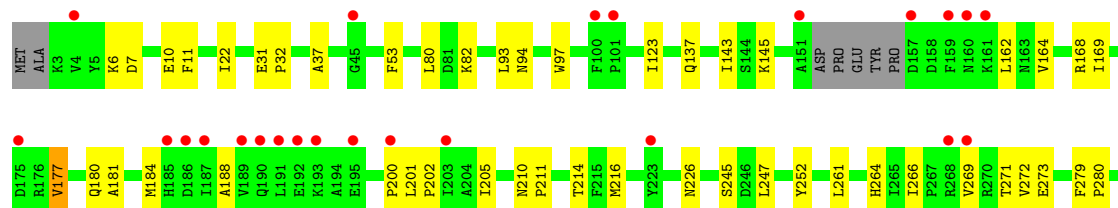
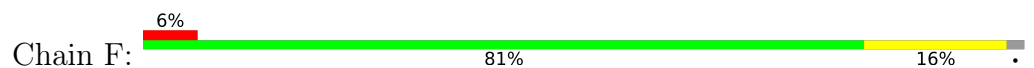
● Molecule 1: Phenolic acid decarboxylase

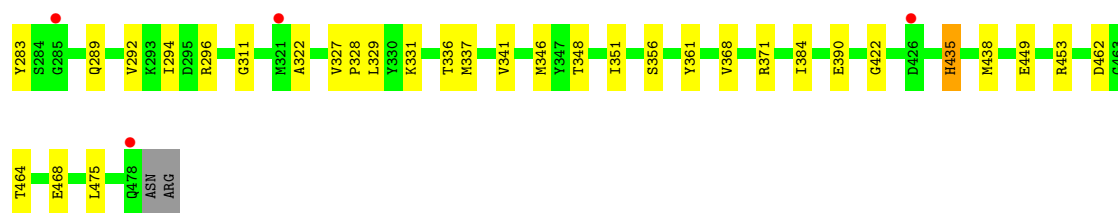


● Molecule 1: Phenolic acid decarboxylase



● Molecule 1: Phenolic acid decarboxylase





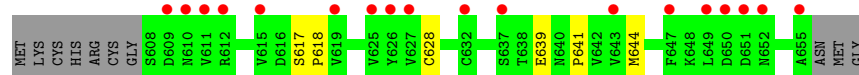
● Molecule 2: Protein ShdD

Chain a: 93%



● Molecule 2: Protein ShdD

Chain b: 31% 72% 10% 17%



● Molecule 2: Protein ShdD

Chain c: 2% 78% 19%



● Molecule 2: Protein ShdD

Chain d: 86% 12%



● Molecule 2: Protein ShdD

Chain e: 3% 93% 5%



● Molecule 2: Protein ShdD

Chain f: 5% 84% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.55Å 200.94Å 201.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.42 – 2.66 71.42 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.5 (71.42-2.66) 99.9 (71.42-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.180 , 0.227 0.180 , 0.227	Depositor DCC
R_{free} test set	5824 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24349	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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, NA

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	0.15	0/3697	0.40	0/5048
1	B	0.17	0/3598	0.39	0/4930
1	C	0.14	0/3620	0.39	0/4961
1	D	0.14	0/3768	0.38	0/5153
1	E	0.15	0/3577	0.36	0/4898
1	F	0.15	0/3654	0.37	0/5003
2	a	0.11	0/463	0.33	0/623
2	b	0.12	0/292	0.39	0/406
2	c	0.12	0/424	0.32	0/577
2	d	0.12	0/450	0.33	0/606
2	e	0.10	0/415	0.27	0/564
2	f	0.10	0/428	0.33	0/581
All	All	0.15	0/24386	0.38	0/33350

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	3608	0	3544	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3508	0	3326	51	0
1	C	3534	0	3379	53	0
1	D	3675	0	3573	42	0
1	E	3491	0	3338	42	0
1	F	3565	0	3416	46	0
2	a	454	0	426	2	0
2	b	286	0	186	2	0
2	c	415	0	362	7	0
2	d	441	0	412	4	0
2	e	406	0	357	2	0
2	f	419	0	371	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	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	139	0	0	1	0
5	B	74	0	0	2	0
5	C	60	0	0	1	0
5	D	92	0	0	1	0
5	E	65	0	0	1	0
5	F	67	0	0	2	0
5	a	21	0	0	1	0
5	c	3	0	0	1	0
5	d	6	0	0	0	0
5	e	3	0	0	0	0
5	f	6	0	0	0	0
All	All	24349	0	22690	266	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 (266) 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:456:GLN:HG3	2:b:644:MET:HE1	1.54	0.88
1:F:322:ALA:HB1	1:F:346:MET:HG2	1.62	0.81
1:E:77:MET:HG3	1:E:211:PRO:HB2	1.63	0.80
1:A:322:ALA:HB1	1:A:346:MET:HG2	1.64	0.80
1:B:112:ALA:HB2	1:B:243:VAL:HG11	1.69	0.73
1:F:289:GLN:NE2	5:F:601:HOH:O	2.24	0.69
1:E:112:ALA:HB2	1:E:243:VAL:HG11	1.75	0.68
1:C:288:LEU:HG	2:c:657:MET:HB3	1.76	0.68
1:A:6:LYS:NZ	5:A:601:HOH:O	2.26	0.67
1:C:145:LYS:HE2	1:C:214:THR:HG21	1.77	0.67
1:F:6:LYS:N	1:F:10:GLU:OE2	2.23	0.66
2:a:615:VAL:HG12	2:a:625:VAL:HB	1.77	0.66
1:C:63:VAL:HG12	1:C:305:PHE:HB3	1.77	0.64
1:C:423:MET:HB3	1:C:425:LEU:HD23	1.79	0.64
1:B:355:ILE:HD11	1:B:372:LEU:HD13	1.78	0.64
1:D:333:LEU:HD22	1:D:371:ARG:HG3	1.79	0.64
1:A:407:ARG:HH22	1:A:457:LEU:HD21	1.63	0.63
1:E:92:GLU:OE2	1:E:95:ARG:NH2	2.31	0.63
2:d:654:ILE:HA	2:d:657:MET:HE3	1.80	0.63
1:C:18:GLU:HB3	1:C:82:LYS:HD3	1.81	0.62
1:C:119:ILE:HG22	1:C:123:ILE:HD13	1.80	0.62
1:E:22:ILE:HD11	1:F:475:LEU:HG	1.80	0.62
1:B:143:ILE:HB	1:B:169:ILE:HB	1.82	0.62
1:A:150:THR:HG21	1:A:187:ILE:HD11	1.81	0.61
1:F:336:THR:HG21	1:F:371:ARG:HH21	1.64	0.61
1:B:344:ASN:OD1	1:B:346:MET:HG3	2.01	0.61
1:E:344:ASN:OD1	1:E:346:MET:HG3	2.01	0.61
1:C:206:THR:HG21	1:C:254:PRO:HD2	1.83	0.60
1:D:150:THR:HG22	1:D:203:ILE:HG22	1.83	0.60
1:F:266:ILE:HB	1:F:269:VAL:HG11	1.84	0.60
2:d:615:VAL:HG12	2:d:625:VAL:HB	1.84	0.60
1:F:337:MET:HE1	1:F:368:VAL:HA	1.84	0.60
1:C:22:ILE:HG12	1:D:475:LEU:HD13	1.83	0.59
1:E:115:LYS:HD3	1:E:298:THR:HG21	1.83	0.59
1:C:118:VAL:HG13	1:C:298:THR:HG22	1.84	0.59
1:C:247:LEU:HD11	1:C:296:ARG:HE	1.67	0.59
2:e:613:LYS:NZ	2:e:616:ASP:OD1	2.35	0.59
1:B:261:LEU:HD12	1:B:297:ILE:HD12	1.84	0.58
1:C:456:GLN:HG2	2:d:644:MET:HE1	1.85	0.58
1:F:216:MET:O	1:F:226:ASN:ND2	2.37	0.57
1:B:4:VAL:HG22	1:B:235:GLN:HB3	1.85	0.57
1:B:396:ASN:OD1	1:B:398:GLU:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:PRO:HA	1:B:156:PRO:HG3	1.85	0.57
1:F:200:PRO:HB3	1:F:264:HIS:CD2	2.40	0.57
2:c:614:MET:HE3	2:c:627:VAL:HG22	1.86	0.56
1:A:167:TYR:CZ	1:A:184:MET:HG2	2.40	0.56
1:F:271:THR:HG1	2:f:632:CYS:HG	1.47	0.56
1:A:475:LEU:HG	1:B:22:ILE:HD11	1.87	0.56
1:E:322:ALA:HB1	1:E:346:MET:SD	2.46	0.56
1:E:355:ILE:HD11	1:E:372:LEU:HD13	1.88	0.56
1:F:181:ALA:N	5:F:601:HOH:O	2.37	0.56
1:E:120:ASP:OD1	1:E:120:ASP:N	2.39	0.56
2:c:610:ASN:ND2	5:c:801:HOH:O	2.39	0.56
1:D:366:LYS:NZ	1:D:415:SER:OG	2.38	0.56
1:D:258:GLU:HA	1:D:300:ARG:HD2	1.87	0.56
1:B:150:THR:HG22	1:B:203:ILE:HD13	1.87	0.55
1:F:162:LEU:HD11	1:F:252:TYR:H	1.72	0.55
2:f:613:LYS:HE2	2:f:624:GLU:HG2	1.88	0.55
1:E:244:LYS:HE2	1:E:249:ASP:HA	1.88	0.54
1:D:142:TYR:CZ	1:D:170:GLN:HB2	2.43	0.54
1:B:97:TRP:CZ2	1:B:328:PRO:HG3	2.43	0.54
1:C:381:TYR:CZ	1:C:423:MET:HE2	2.42	0.54
1:A:449:GLU:HB2	1:C:434:MET:HE2	1.90	0.54
1:A:137:GLN:HB2	1:A:283:TYR:CZ	2.42	0.53
1:F:384:ILE:HG12	1:F:438:MET:HE3	1.89	0.53
1:B:321:MET:HG3	1:B:349:HIS:CE1	2.43	0.53
1:A:164:VAL:H	1:A:227:GLU:HG3	1.72	0.53
1:F:247:LEU:HD21	1:F:296:ARG:NH1	2.23	0.53
1:C:206:THR:HG22	1:C:260:VAL:HG22	1.90	0.53
1:B:77:MET:HG3	1:B:211:PRO:HB2	1.89	0.53
1:F:145:LYS:HE2	1:F:214:THR:HG21	1.91	0.52
1:A:37:ALA:HB3	1:A:53:PHE:HZ	1.73	0.52
1:A:184:MET:HE1	1:A:203:ILE:HD11	1.92	0.52
1:C:435:HIS:HB3	1:C:437:LYS:HD3	1.92	0.52
1:E:137:GLN:HB2	1:E:283:TYR:CZ	2.45	0.51
1:A:142:TYR:CZ	1:A:170:GLN:HB2	2.46	0.51
1:A:200:PRO:HB3	1:A:264:HIS:CD2	2.45	0.51
1:A:219:THR:HG23	1:A:220:PRO:HD2	1.92	0.51
1:C:37:ALA:HB3	1:C:53:PHE:HZ	1.74	0.51
1:D:223:TYR:CZ	1:D:328:PRO:HB2	2.46	0.51
1:F:143:ILE:HB	1:F:169:ILE:HB	1.92	0.51
1:B:171:VAL:HA	1:B:177:VAL:HG12	1.92	0.51
1:C:137:GLN:HB2	1:C:283:TYR:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ASP:OD1	1:C:98:ASP:N	2.43	0.50
1:B:266:ILE:HD11	1:B:293:LYS:CB	2.42	0.50
1:E:142:TYR:CZ	1:E:170:GLN:HB2	2.47	0.50
1:F:97:TRP:HB3	1:F:331:LYS:HE2	1.94	0.50
1:D:247:LEU:HD11	1:D:296:ARG:HB2	1.93	0.50
2:c:650:ASP:O	2:c:654:ILE:HG13	2.12	0.50
1:A:423:MET:HB3	1:A:425:LEU:HD22	1.94	0.49
1:F:168:ARG:NH2	1:F:273:GLU:OE1	2.45	0.49
1:B:93:LEU:HB3	1:B:327:VAL:HG21	1.95	0.49
1:B:371:ARG:NH2	5:B:606:HOH:O	2.45	0.49
1:C:336:THR:O	1:C:338:PRO:HD3	2.11	0.49
1:F:97:TRP:CZ2	1:F:328:PRO:HG3	2.48	0.49
1:F:94:ASN:OD1	1:F:331:LYS:NZ	2.37	0.49
1:F:137:GLN:HB2	1:F:283:TYR:CZ	2.48	0.49
1:B:168:ARG:NH1	1:B:276:PHE:HB3	2.27	0.49
1:A:99:LYS:NZ	1:A:236:ASP:OD1	2.43	0.49
1:D:97:TRP:CZ2	1:D:328:PRO:HG3	2.48	0.49
1:D:416:ILE:HD13	1:D:438:MET:HG3	1.94	0.49
1:E:11:PHE:CG	1:E:211:PRO:HG3	2.48	0.48
1:E:23:ARG:NH1	1:E:54:GLU:OE2	2.46	0.48
1:E:475:LEU:HD13	1:F:22:ILE:HG12	1.95	0.48
1:F:37:ALA:HB3	1:F:53:PHE:HZ	1.78	0.48
1:C:2:ALA:HB1	1:C:79:GLY:HA3	1.95	0.48
1:C:149:VAL:HG22	1:C:164:VAL:HG22	1.94	0.48
1:E:5:TYR:HE1	1:E:14:VAL:HG21	1.77	0.48
1:C:162:LEU:HD21	1:C:252:TYR:H	1.78	0.48
2:a:646:LYS:NZ	5:a:803:HOH:O	2.40	0.48
1:D:390:GLU:CD	1:D:390:GLU:H	2.21	0.48
1:C:97:TRP:CZ2	1:C:328:PRO:HG3	2.48	0.48
1:B:142:TYR:HE2	1:B:168:ARG:HG2	1.78	0.48
1:C:11:PHE:CG	1:C:211:PRO:HG3	2.49	0.48
1:B:125:LEU:HG	1:B:174:ARG:O	2.14	0.47
1:F:279:PHE:CG	1:F:280:PRO:HD3	2.48	0.47
1:E:151:ALA:HA	1:E:162:LEU:HD23	1.96	0.47
1:E:173:ASP:OD2	2:e:612:ARG:NH2	2.38	0.47
1:F:341:VAL:HG21	1:F:390:GLU:HB2	1.96	0.47
1:C:164:VAL:O	1:C:226:ASN:ND2	2.48	0.47
2:f:643:VAL:HG12	2:f:648:LYS:HG2	1.96	0.47
1:B:11:PHE:CG	1:B:211:PRO:HG3	2.50	0.47
1:B:135:ASN:ND2	5:B:602:HOH:O	2.28	0.47
1:C:175:ASP:OD2	1:C:293:LYS:HE3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:GLN:HG3	1:E:82:LYS:HG3	1.95	0.47
1:B:299:HIS:ND1	1:B:300:ARG:O	2.37	0.47
1:D:322:ALA:HB1	1:D:346:MET:HG2	1.95	0.47
1:D:7:ASP:OD2	1:D:300:ARG:NH2	2.48	0.47
1:B:148:VAL:HG22	1:B:205:ILE:HG12	1.98	0.46
1:C:175:ASP:OD1	1:C:175:ASP:N	2.47	0.46
1:D:421:PRO:O	1:D:435:HIS:HB2	2.15	0.46
2:d:613:LYS:HE3	2:d:624:GLU:HG2	1.97	0.46
1:B:382:SER:O	1:B:437:LYS:NZ	2.46	0.46
1:C:97:TRP:HB3	1:C:331:LYS:HE3	1.98	0.46
1:E:37:ALA:HB3	1:E:53:PHE:HZ	1.80	0.46
1:B:205:ILE:HB	1:B:261:LEU:HB2	1.97	0.46
1:B:202:PRO:HB3	1:B:248:TYR:CE2	2.51	0.46
2:c:605:ARG:NH2	2:c:631:CYS:O	2.45	0.46
1:B:360:ARG:HG2	1:B:361:TYR:CD2	2.51	0.46
1:E:424:PRO:O	1:F:453:ARG:NH1	2.49	0.46
1:C:203:ILE:HD11	1:C:292:VAL:HG11	1.98	0.45
1:F:348:THR:O	1:F:351:ILE:HG13	2.15	0.45
1:D:348:THR:O	1:D:351:ILE:HG13	2.17	0.45
1:A:104:PRO:HD3	1:A:229:GLU:HG2	1.97	0.45
1:C:176:ARG:HD2	1:C:291:GLU:OE1	2.17	0.45
1:F:123:ILE:HD13	1:F:294:ILE:HG22	1.98	0.45
1:F:205:ILE:HB	1:F:261:LEU:HB2	1.97	0.45
1:B:269:VAL:O	1:B:270:ARG:NH1	2.50	0.45
1:D:358:LYS:HA	1:D:390:GLU:HG3	1.98	0.45
1:A:216:MET:HE3	1:A:216:MET:HB3	1.80	0.45
1:E:336:THR:HG23	1:E:337:MET:HG3	1.99	0.45
1:B:275:PRO:HB3	1:B:284:SER:O	2.17	0.45
1:D:4:VAL:HG22	1:D:235:GLN:HB3	1.97	0.45
1:F:7:ASP:OD1	1:F:10:GLU:HG3	2.16	0.44
1:F:266:ILE:HB	1:F:269:VAL:CG1	2.47	0.44
1:D:137:GLN:O	1:D:275:PRO:HG2	2.17	0.44
1:F:184:MET:O	1:F:188:ALA:N	2.51	0.44
1:B:142:TYR:CE2	1:B:168:ARG:HG2	2.51	0.44
1:B:173:ASP:OD1	1:B:174:ARG:N	2.44	0.44
1:D:279:PHE:CG	1:D:280:PRO:HD3	2.52	0.44
1:B:120:ASP:OD1	1:B:120:ASP:N	2.46	0.44
1:E:379:MET:HG2	1:E:421:PRO:HG2	2.00	0.44
1:F:464:THR:O	1:F:468:GLU:HG3	2.18	0.44
1:E:227:GLU:HG3	1:E:229:GLU:HB3	2.00	0.44
1:D:137:GLN:HB2	1:D:283:TYR:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:HE3	1:A:199:LYS:HB2	1.66	0.43
1:B:132:TYR:OH	1:B:307:ASN:HB3	2.18	0.43
1:D:336:THR:OG1	1:D:371:ARG:NH1	2.51	0.43
1:F:11:PHE:CG	1:F:211:PRO:HG3	2.53	0.43
1:F:201:LEU:HD12	1:F:202:PRO:HD2	2.00	0.43
1:B:279:PHE:CG	1:B:280:PRO:HD3	2.53	0.43
1:C:131:LEU:O	2:c:636:ARG:NH2	2.47	0.43
1:E:403:ALA:O	1:E:407:ARG:HB2	2.19	0.43
1:C:125:LEU:HD11	1:C:294:ILE:HD13	2.01	0.43
1:C:174:ARG:HD2	5:C:642:HOH:O	2.18	0.43
1:C:279:PHE:CG	1:C:280:PRO:HD3	2.53	0.43
1:D:77:MET:HG3	1:D:211:PRO:HB2	1.99	0.43
1:C:169:ILE:HG23	1:C:177:VAL:HB	2.00	0.43
1:E:206:THR:HG21	1:E:254:PRO:HD2	2.00	0.43
1:C:75:ALA:HB2	1:C:89:GLN:NE2	2.34	0.43
1:E:419:ASN:ND2	5:E:611:HOH:O	2.52	0.43
1:A:29:ASN:O	1:A:33:ASP:HB2	2.19	0.43
1:F:422:GLY:HA2	1:F:435:HIS:ND1	2.33	0.43
1:A:168:ARG:HD2	1:A:276:PHE:CD2	2.54	0.43
1:B:168:ARG:NH2	1:B:180:GLN:OE1	2.52	0.43
1:C:113:PRO:O	1:C:300:ARG:HG2	2.19	0.43
1:D:200:PRO:HB3	1:D:264:HIS:CD2	2.54	0.43
1:F:177:VAL:HG12	1:F:292:VAL:HB	2.00	0.43
1:B:296:ARG:O	1:B:297:ILE:HD13	2.18	0.43
1:E:215:PHE:CZ	1:E:324:ASN:HB3	2.54	0.43
1:A:75:ALA:HB2	1:A:89:GLN:NE2	2.34	0.43
1:D:145:LYS:HE2	1:D:214:THR:HG21	2.00	0.43
1:A:279:PHE:CG	1:A:280:PRO:HD3	2.53	0.42
1:A:22:ILE:HD11	1:B:475:LEU:HD13	2.00	0.42
1:C:13:GLU:O	1:C:17:GLN:HG3	2.18	0.42
1:B:359:VAL:HG13	1:B:364:TYR:HB3	2.00	0.42
1:E:77:MET:HE2	1:E:77:MET:HB3	1.96	0.42
1:A:6:LYS:NZ	1:A:241:ASP:H	2.17	0.42
1:A:317:ILE:HD12	1:A:317:ILE:HA	1.90	0.42
1:E:458:LEU:HD13	1:F:311:GLY:HA2	2.02	0.42
1:C:373:LEU:HD22	1:C:437:LYS:HE3	2.00	0.42
1:D:265:ILE:HG12	1:D:292:VAL:HG22	2.02	0.42
1:D:97:TRP:HB3	1:D:331:LYS:HE3	2.01	0.42
1:A:436:THR:HG22	1:B:410:PRO:HB2	2.01	0.42
1:B:206:THR:HG21	1:B:254:PRO:HD2	2.01	0.42
1:C:336:THR:HG21	1:C:371:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:HIS:O	1:C:380:PRO:HD2	2.20	0.42
1:D:72:GLN:HG3	1:D:82:LYS:HG3	2.01	0.42
1:E:145:LYS:HE2	1:E:214:THR:HG21	2.02	0.42
1:C:77:MET:HG3	1:C:211:PRO:HB2	2.01	0.42
1:C:223:TYR:CZ	1:C:328:PRO:HB2	2.55	0.42
1:C:337:MET:HE2	1:C:368:VAL:HA	2.00	0.42
1:E:279:PHE:CG	1:E:280:PRO:HD3	2.54	0.42
1:A:455:THR:HG21	1:B:427:PRO:HB3	2.02	0.41
1:E:34:ILE:HD11	1:E:56:ILE:HG12	2.02	0.41
1:E:53:PHE:O	1:E:62:SER:HB2	2.20	0.41
1:F:31:GLU:HA	1:F:32:PRO:HA	1.88	0.41
1:B:113:PRO:O	1:B:300:ARG:HG2	2.20	0.41
1:D:416:ILE:CD1	1:D:438:MET:HG3	2.51	0.41
1:E:336:THR:HG21	1:E:371:ARG:HE	1.86	0.41
1:F:93:LEU:HB3	1:F:327:VAL:HG21	2.02	0.41
1:C:322:ALA:HB1	1:C:346:MET:HG2	2.02	0.41
1:D:431:PRO:HA	1:D:432:PRO:HD3	1.98	0.41
2:c:617:SER:OG	2:c:623:TRP:N	2.44	0.41
1:D:168:ARG:HD3	5:D:552:HOH:O	2.21	0.41
1:D:419:ASN:HD21	1:F:449:GLU:CD	2.28	0.41
1:E:11:PHE:CD2	1:E:211:PRO:HG3	2.56	0.41
1:C:169:ILE:HD13	1:C:205:ILE:HD13	2.02	0.41
1:C:471:LEU:HD22	1:D:22:ILE:HD11	2.03	0.41
1:F:164:VAL:O	1:F:226:ASN:HB3	2.20	0.41
1:A:339:GLU:OE2	1:A:360:ARG:HD3	2.21	0.41
1:A:310:LEU:HD13	1:A:317:ILE:HG21	2.03	0.41
1:D:6:LYS:HA	1:D:6:LYS:HD2	1.76	0.41
1:D:80:LEU:HD21	1:D:92:GLU:HG2	2.03	0.41
1:D:164:VAL:O	1:D:226:ASN:HB3	2.21	0.41
1:D:380:PRO:HB2	1:D:423:MET:HE2	2.03	0.41
1:E:137:GLN:O	1:E:275:PRO:HG2	2.20	0.41
1:F:329:LEU:HD23	1:F:329:LEU:HA	1.94	0.41
1:A:413:ASP:HB3	1:A:441:ASP:O	2.22	0.41
1:B:134:ILE:HG22	1:B:135:ASN:ND2	2.36	0.41
1:C:149:VAL:HB	1:C:204:ALA:HB3	2.03	0.41
1:C:311:GLY:HA2	1:D:458:LEU:HD13	2.03	0.41
1:C:313:PRO:HG2	1:D:402:TRP:CD1	2.55	0.41
1:D:425:LEU:HD23	1:D:425:LEU:HA	1.75	0.41
1:D:349:HIS:CE1	1:D:377:HIS:HE1	2.40	0.40
1:E:181:ALA:HB2	1:E:290:CYS:SG	2.61	0.40
2:b:639:GLU:O	2:b:641:PRO:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:VAL:O	1:B:226:ASN:HB3	2.21	0.40
1:C:212:LEU:HD23	1:C:212:LEU:HA	1.89	0.40
1:D:449:GLU:HA	1:D:450:PRO:HD3	1.97	0.40
1:E:278:GLU:CD	1:E:284:SER:HB3	2.46	0.40
1:E:390:GLU:HG2	1:E:391:PHE:N	2.35	0.40
1:E:457:LEU:HD23	1:E:457:LEU:HA	1.91	0.40
1:B:37:ALA:HB3	1:B:53:PHE:HZ	1.84	0.40
1:B:137:GLN:HB2	1:B:283:TYR:CE1	2.56	0.40
1:B:313:PRO:HA	1:B:314:TRP:HA	1.80	0.40
1:B:322:ALA:HB1	1:B:346:MET:SD	2.60	0.40
1:C:85:SER:O	1:C:89:GLN:HG3	2.21	0.40
1:D:379:MET:HE3	1:F:361:TYR:OH	2.21	0.40
1:E:92:GLU:O	1:E:96:ARG:HG3	2.22	0.40
1:F:272:VAL:HG13	2:f:657:MET:HE1	2.04	0.40
1:A:113:PRO:O	1:A:116:GLU:HG3	2.21	0.40
1:B:85:SER:O	1:B:89:GLN:HG3	2.22	0.40
1:B:168:ARG:HG3	1:B:276:PHE:CD2	2.56	0.40
1:C:278:GLU:OE2	1:C:284:SER:HB3	2.20	0.40
1:F:180:GLN:HA	1:F:289:GLN:NE2	2.36	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	463/480 (96%)	446 (96%)	17 (4%)	0	100	100
1	B	462/480 (96%)	453 (98%)	9 (2%)	0	100	100
1	C	465/480 (97%)	455 (98%)	10 (2%)	0	100	100
1	D	473/480 (98%)	464 (98%)	9 (2%)	0	100	100
1	E	453/480 (94%)	439 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	467/480 (97%)	456 (98%)	11 (2%)	0	100	100
2	a	55/58 (95%)	54 (98%)	1 (2%)	0	100	100
2	b	46/58 (79%)	43 (94%)	2 (4%)	1 (2%)	5	9
2	c	55/58 (95%)	53 (96%)	2 (4%)	0	100	100
2	d	55/58 (95%)	55 (100%)	0	0	100	100
2	e	55/58 (95%)	54 (98%)	1 (2%)	0	100	100
2	f	55/58 (95%)	53 (96%)	2 (4%)	0	100	100
All	All	3104/3228 (96%)	3025 (98%)	78 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	618	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	386/419 (92%)	384 (100%)	2 (0%)	81	91
1	B	358/419 (85%)	354 (99%)	4 (1%)	65	80
1	C	362/419 (86%)	357 (99%)	5 (1%)	59	76
1	D	394/419 (94%)	393 (100%)	1 (0%)	86	94
1	E	364/419 (87%)	358 (98%)	6 (2%)	55	74
1	F	369/419 (88%)	361 (98%)	8 (2%)	45	67
2	a	52/53 (98%)	51 (98%)	1 (2%)	50	71
2	b	16/53 (30%)	14 (88%)	2 (12%)	4	6
2	c	41/53 (77%)	39 (95%)	2 (5%)	22	38
2	d	48/53 (91%)	48 (100%)	0	100	100
2	e	38/53 (72%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	f	42/53 (79%)	40 (95%)	2 (5%)	23	39
All	All	2470/2832 (87%)	2437 (99%)	33 (1%)	61	77

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	ILE
1	A	435	HIS
1	B	210	ASN
1	B	245	SER
1	B	417	ILE
1	B	435	HIS
1	C	98	ASP
1	C	179	ILE
1	C	236	ASP
1	C	245	SER
1	C	308	LEU
1	D	210	ASN
1	E	114	CYS
1	E	227	GLU
1	E	243	VAL
1	E	308	LEU
1	E	336	THR
1	E	425	LEU
1	F	80	LEU
1	F	82	LYS
1	F	177	VAL
1	F	210	ASN
1	F	245	SER
1	F	356	SER
1	F	435	HIS
1	F	462	ASP
2	a	615	VAL
2	b	617	SER
2	b	628	CYS
2	c	613	LYS
2	c	617	SER
2	f	608	SER
2	f	628	CYS

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

Mol	Chain	Res	Type
1	A	29	ASN
1	A	225	GLN
1	A	456	GLN
1	A	477	ASN
1	B	17	GLN
1	B	29	ASN
1	B	135	ASN
1	B	163	ASN
1	C	17	GLN
1	C	20	GLN
1	C	209	ASN
1	C	226	ASN
1	C	349	HIS
1	D	377	HIS
1	E	47	ASN
1	E	66	ASN
1	E	163	ASN
1	E	377	HIS
1	E	419	ASN
1	E	451	ASN
1	F	17	GLN
1	F	47	ASN
1	F	225	GLN
1	F	289	GLN
1	F	349	HIS
2	c	610	ASN
2	d	604	HIS
2	f	604	HIS

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

Of 11 ligands modelled in this entry, 11 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

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	467/480 (97%)	-0.24	14 (2%)	52	45	16, 27, 76, 119	0
1	B	468/480 (97%)	0.28	33 (7%)	22	16	16, 46, 96, 128	0
1	C	471/480 (98%)	0.27	34 (7%)	21	16	19, 50, 90, 113	0
1	D	475/480 (98%)	-0.22	4 (0%)	82	79	20, 37, 67, 110	0
1	E	461/480 (96%)	0.05	21 (4%)	37	29	20, 44, 82, 118	0
1	F	471/480 (98%)	0.20	28 (5%)	28	21	21, 44, 88, 113	0
2	a	57/58 (98%)	-0.10	0	100	100	21, 30, 71, 85	0
2	b	48/58 (82%)	1.58	18 (37%)	1	0	58, 79, 94, 104	0
2	c	57/58 (98%)	0.56	1 (1%)	67	63	47, 60, 91, 101	0
2	d	57/58 (98%)	-0.10	0	100	100	30, 41, 60, 75	0
2	e	57/58 (98%)	0.55	2 (3%)	47	38	46, 60, 87, 102	0
2	f	57/58 (98%)	0.52	3 (5%)	32	25	43, 58, 83, 96	0
All	All	3146/3228 (97%)	0.10	158 (5%)	34	26	16, 43, 86, 128	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	194	ALA	5.6
1	E	100	PHE	5.0
1	B	184	MET	4.9
1	A	188	ALA	4.9
1	F	100	PHE	4.8
1	C	2	ALA	4.8
1	F	101	PRO	4.6
1	A	223	TYR	4.5
1	E	452	PRO	4.3
1	B	194	ALA	4.3
1	F	159	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	157	ASP	4.1
1	D	100	PHE	3.9
1	C	157	ASP	3.9
2	e	650	ASP	3.8
1	C	183	ALA	3.8
1	E	220	PRO	3.8
1	F	186	ASP	3.7
1	C	100	PHE	3.7
1	B	31	GLU	3.7
1	C	152	ASP	3.6
1	E	183	ALA	3.6
1	C	158	ASP	3.6
1	C	160	ASN	3.5
1	C	221	VAL	3.5
1	A	221	VAL	3.5
1	B	187	ILE	3.5
1	F	191	LEU	3.5
1	A	225	GLN	3.4
1	E	101	PRO	3.4
2	b	652	ASN	3.4
1	E	225	GLN	3.4
1	C	151	ALA	3.3
1	E	99	LYS	3.3
1	F	151	ALA	3.3
1	B	200	PRO	3.2
1	E	155	TYR	3.2
1	B	201	LEU	3.2
1	E	156	PRO	3.2
1	A	192	GLU	3.1
1	C	101	PRO	3.1
1	A	160	ASN	3.1
1	E	153	PRO	3.1
2	b	637	SER	3.1
1	B	191	LEU	3.1
1	C	186	ASP	3.1
1	C	478	GLN	3.1
1	C	250	HIS	3.0
1	B	152	ASP	3.0
1	E	157	ASP	3.0
1	C	162	LEU	3.0
1	B	160	ASN	3.0
1	B	183	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	161	LYS	2.9
1	F	478	GLN	2.9
2	b	647	PHE	2.9
1	B	156	PRO	2.9
1	C	192	GLU	2.9
1	B	157	ASP	2.9
1	B	271	THR	2.9
2	b	650	ASP	2.8
1	C	159	PHE	2.8
1	F	195	GLU	2.8
1	B	190	GLN	2.8
1	C	224	ASN	2.8
1	B	153	PRO	2.7
1	F	200	PRO	2.7
1	E	189	VAL	2.7
1	C	220	PRO	2.7
1	C	223	TYR	2.7
1	C	191	LEU	2.7
1	F	223	TYR	2.7
1	B	286	ALA	2.7
1	C	426	ASP	2.7
1	E	152	ASP	2.7
2	b	609	ASP	2.7
1	F	321	MET	2.7
2	b	611	VAL	2.6
2	b	632	CYS	2.6
1	A	224	ASN	2.6
1	C	188	ALA	2.6
1	F	269	VAL	2.6
2	c	652	ASN	2.6
2	e	651	ASP	2.6
2	b	626	TYR	2.6
1	C	237	GLY	2.6
1	F	45	GLY	2.6
1	F	4	VAL	2.6
1	A	222	GLY	2.5
1	B	98	ASP	2.5
1	C	222	GLY	2.5
2	b	625	VAL	2.5
1	A	226	ASN	2.5
2	b	649	LEU	2.5
1	B	223	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	239	PRO	2.5
1	A	189	VAL	2.5
2	b	619	VAL	2.5
1	B	122	ASP	2.4
1	B	155	TYR	2.4
2	b	643	VAL	2.4
1	E	160	ASN	2.4
1	F	187	ILE	2.4
1	F	426	ASP	2.4
1	D	452	PRO	2.4
1	B	225	GLN	2.4
1	C	189	VAL	2.4
1	C	196	ALA	2.4
1	B	267	PRO	2.4
1	F	268	ARG	2.4
1	C	236	ASP	2.3
2	f	651	ASP	2.3
1	A	452	PRO	2.3
1	F	203	ILE	2.3
1	F	193	LYS	2.3
1	D	155	TYR	2.3
1	E	192	GLU	2.3
1	B	154	GLU	2.2
1	F	190	GLN	2.2
1	B	292	VAL	2.2
1	E	191	LEU	2.2
1	F	189	VAL	2.2
1	A	185	HIS	2.2
1	A	220	PRO	2.2
1	F	285	GLY	2.2
1	B	171	VAL	2.2
1	C	199	LYS	2.2
1	E	249	ASP	2.2
1	B	189	VAL	2.2
1	F	192	GLU	2.1
1	B	268	ARG	2.1
2	b	610	ASN	2.1
1	F	185	HIS	2.1
2	b	615	VAL	2.1
2	b	655	ALA	2.1
1	B	275	PRO	2.1
1	C	193	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	451	ASN	2.1
1	C	16	GLU	2.1
1	C	195	GLU	2.1
1	C	161	LYS	2.1
1	F	161	LYS	2.1
1	B	139	GLY	2.1
1	B	285	GLY	2.1
2	f	650	ASP	2.1
1	B	166	THR	2.1
1	F	160	ASN	2.1
1	C	238	VAL	2.1
1	F	175	ASP	2.0
2	b	612	ARG	2.0
2	b	651	ASP	2.0
1	E	204	ALA	2.0
1	B	172	LYS	2.0
1	B	123	ILE	2.0
2	b	627	VAL	2.0
2	f	621	ASP	2.0
1	E	182	LEU	2.0
1	E	203	ILE	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
4	ZN	b	701	1/1	0.85	0.10	84,84,84,84	0
3	NA	A	501	1/1	0.90	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	E	501	1/1	0.91	0.11	41,41,41,41	0
3	NA	F	501	1/1	0.92	0.11	43,43,43,43	0
3	NA	C	501	1/1	0.93	0.10	31,31,31,31	0
3	NA	B	501	1/1	0.97	0.09	28,28,28,28	0
4	ZN	c	701	1/1	0.97	0.17	100,100,100,100	0
4	ZN	d	701	1/1	0.98	0.10	56,56,56,56	0
4	ZN	e	701	1/1	0.98	0.05	69,69,69,69	0
4	ZN	a	701	1/1	0.99	0.05	28,28,28,28	0
4	ZN	f	701	1/1	0.99	0.03	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.