Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2021 – 02:19 pm BST

PDB ID	:	7AE5
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 following versions of software and data (see references ①) were used in the production of this report:

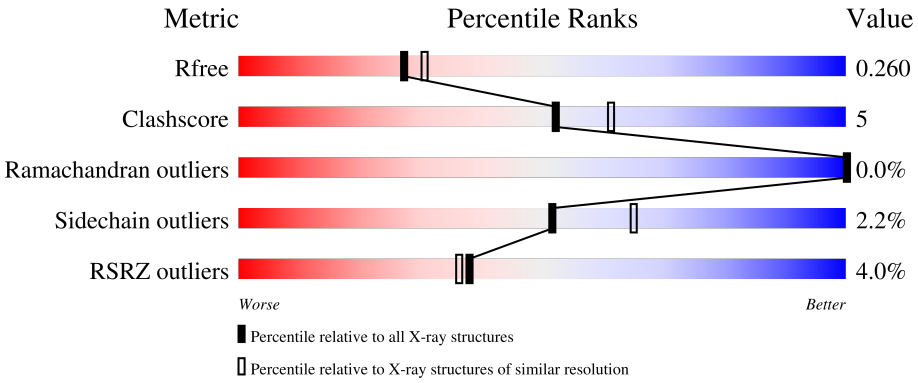
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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	5% 83% 13%
1	B	480	2% 83% 14%
1	C	480	84% 13%
1	D	480	2% 85% 14%
1	E	480	4% 86% 11%

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Mol	Chain	Length	Quality of chain
1	F	480	5% 81% 14%
2	a	68	7% 90% 7%
2	b	68	4% 93%
2	c	68	% 97%
2	d	68	6% 96%
2	e	68	10% 91% 6%
2	f	68	24% 82% 15%

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 (i)

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 (three-letter code: RB) (formula: Rb).

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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
4	a	1	Total Zn 1 1	0	0

- Molecule 5 is water.

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

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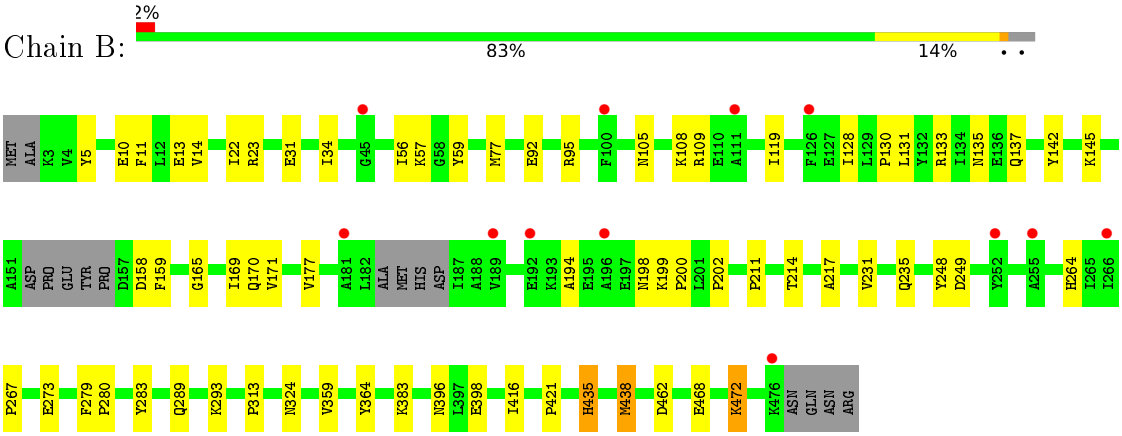
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	b	15	Total O 15 15	0	0
5	c	7	Total O 7 7	0	0
5	d	6	Total O 6 6	0	0
5	e	9	Total O 9 9	0	0
5	f	3	Total O 3 3	0	0
5	a	14	Total O 14 14	0	0

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.

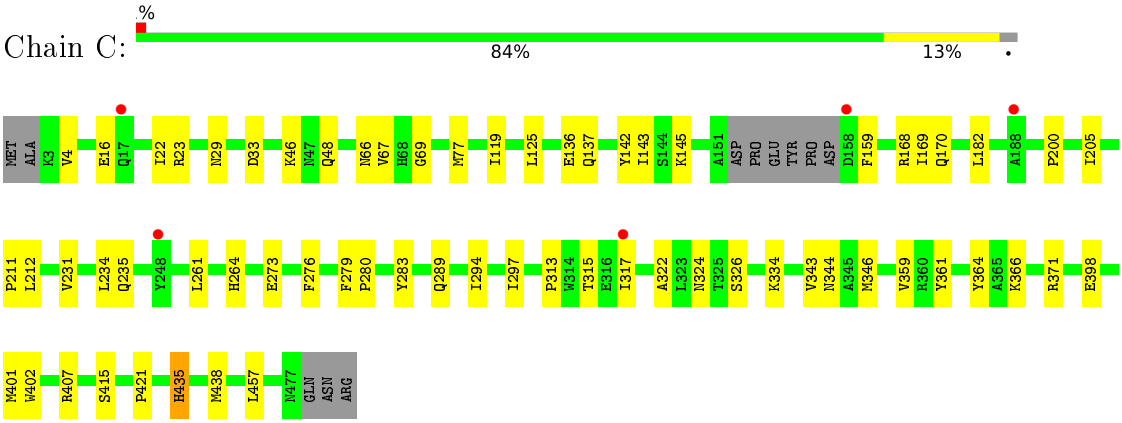
- Molecule 1: Phenolic acid decarboxylase

Chain B:



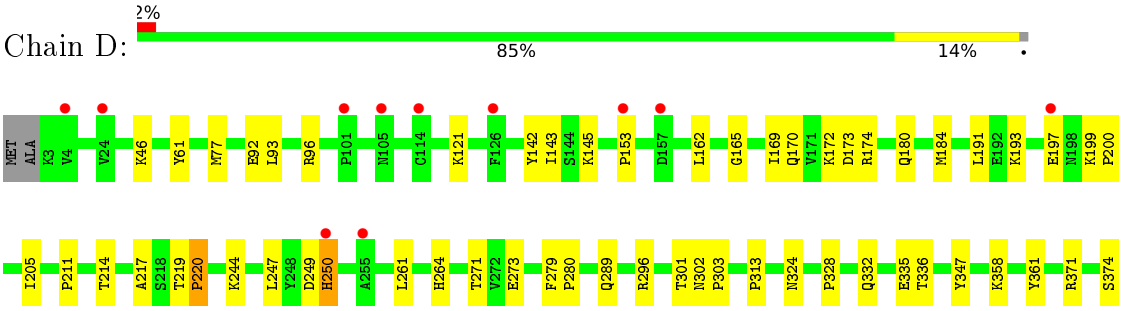
- Molecule 1: Phenolic acid decarboxylase

Chain C:

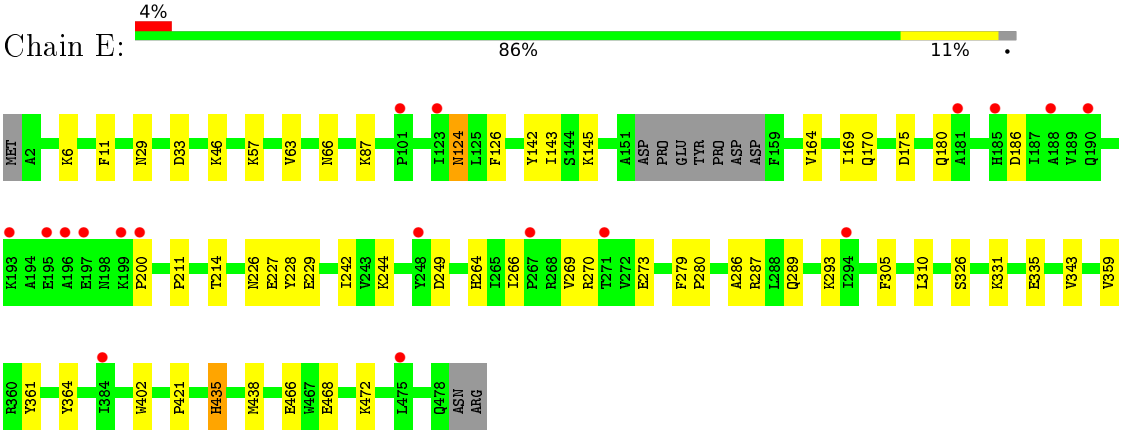


- Molecule 1: Phenolic acid decarboxylase

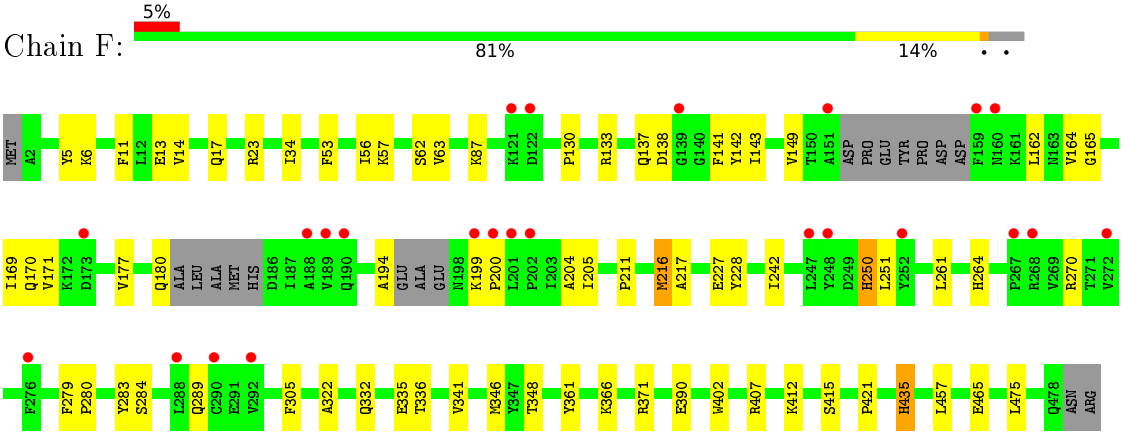
Chain D:



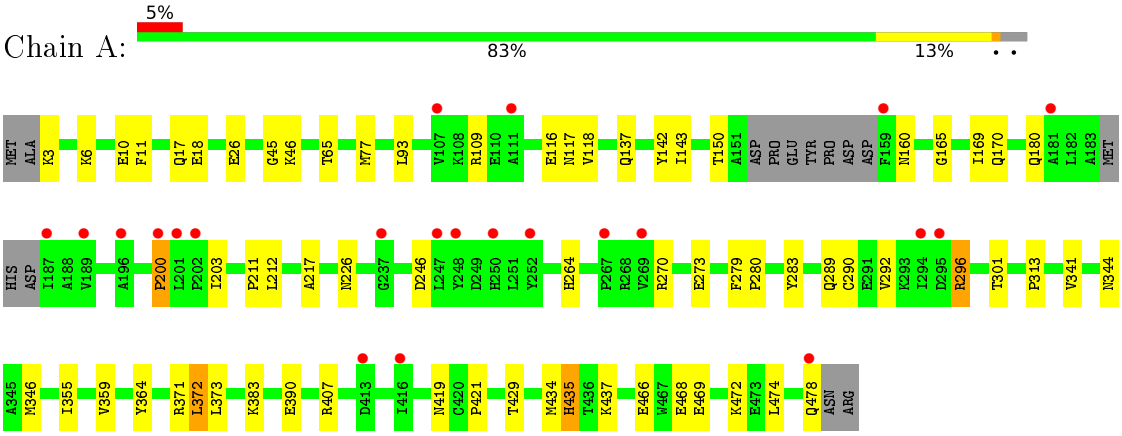
• Molecule 1: Phenolic acid decarboxylase



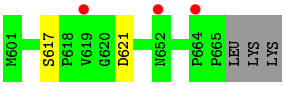
• Molecule 1: Phenolic acid decarboxylase



• Molecule 1: Phenolic acid decarboxylase

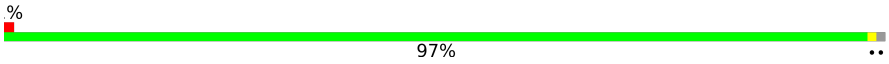


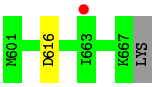
• Molecule 2: Protein ShdD



• Molecule 2: Protein ShdD

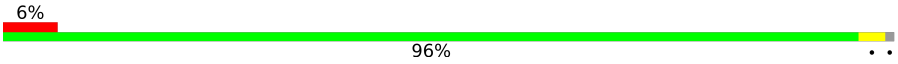
Chain c:

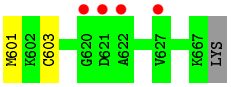




• Molecule 2: Protein ShdD

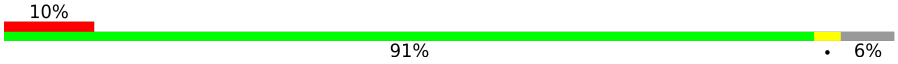
Chain d:

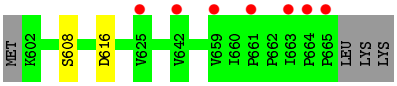




• Molecule 2: Protein ShdD

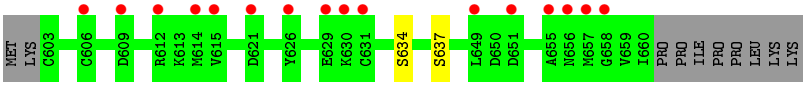
Chain e:





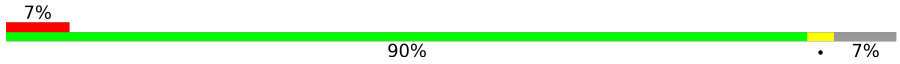
• Molecule 2: Protein ShdD

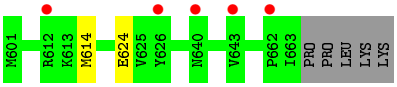
Chain f:



• Molecule 2: Protein ShdD

Chain a:





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.57 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.223 , 0.263 0.222 , 0.260	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)	0.32 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.25	0/3673	0.49	0/5016
1	B	0.25	0/3694	0.49	0/5040
1	C	0.27	0/3745	0.49	0/5109
1	D	0.27	0/3779	0.51	0/5157
1	E	0.26	0/3715	0.49	0/5070
1	F	0.26	0/3615	0.48	0/4936
2	a	0.26	0/469	0.54	0/637
2	b	0.26	0/510	0.54	0/692
2	c	0.24	0/533	0.48	0/722
2	d	0.25	0/529	0.51	0/718
2	e	0.26	0/473	0.50	0/647
2	f	0.24	0/384	0.50	0/526
All	All	0.26	0/25119	0.49	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

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	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3606	0	3515	39	0
1	C	3655	0	3583	39	0
1	D	3688	0	3630	40	0
1	E	3625	0	3517	30	0
1	F	3528	0	3379	44	0
2	a	458	0	400	0	0
2	b	497	0	464	0	0
2	c	520	0	499	0	0
2	d	516	0	483	0	0
2	e	460	0	395	0	0
2	f	377	0	298	0	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	4	0
5	D	132	0	0	2	0
5	E	136	0	0	1	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	0	0
5	e	9	0	0	0	0
5	f	3	0	0	0	0
All	All	25337	0	23657	225	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 5.

All (225) 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
1:C:22:ILE:HD11	1:D:475:LEU:HG	1.68	0.76
1:F:407:ARG:HH22	1:F:457:LEU:HD21	1.54	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:D:374:SER:HA	1:D:379:MET:HE2	1.78	0.66
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: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: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:143:ILE:HB	1:E:169:ILE:HB	1.85	0.58
1:A:137:GLN:HB2	1:A:283:TYR:CZ	2.39	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
1:D:358:LYS:NZ	5:D:608:HOH:O	2.36	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
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:B:273:GLU:HB3	1:B:289:GLN:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:MET:HG3	1:A:211:PRO:HB2	1.89	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: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:F:180:GLN:HG3	1:F:289:GLN:NE2	2.25	0.52
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
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:A:466:GLU:H	1:A:466:GLU:CD	2.13	0.51
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:B:313:PRO:HG2	1:F:402:TRP:CD1	2.49	0.48
1:C:16:GLU:OE1	1:C:23:ARG:HD2	2.14	0.48
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:A:45:GLY:C	1:A:46:LYS:HD2	2.35	0.47
1:D:180:GLN:O	1:D:184:MET:HG3	2.14	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: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
1:D:145:LYS:HE2	1:D:214:THR:HG21	1.97	0.46
1:D:412:LYS:NZ	5:D:612:HOH:O	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:202:PRO:HB3	1:B:248:TYR:CD1	2.51	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: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: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:D:324:ASN:OD1	1:D:324:ASN:N	2.44	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: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:E:124:ASN:HD22	1:E:124:ASN:C	2.20	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:E:286:ALA:C	1:E:287:ARG:HD3	2.38	0.44
1:F:216:MET:SD	1:F:227:GLU:HB3	2.58	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
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:A:429:THR:HG22	1:A:435:HIS:HD2	1.84	0.43
1:E:29:ASN:O	1:E:33:ASP:HB2	2.19	0.43
1:A:165:GLY:HA2	1:A:217:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:199:LYS:C	1:B:267:PRO:HG3	2.40	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: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
1:C:334:LYS:NZ	5:C:605:HOH:O	2.53	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:212:LEU:HD23	1:A:212:LEU:HA	1.92	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: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: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: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 (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	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%)	47	55
1	E	466/480 (97%)	454 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (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	378/419 (90%)	371 (98%)	7 (2%)	57	71
1	B	384/419 (92%)	377 (98%)	7 (2%)	59	72
1	C	394/419 (94%)	389 (99%)	5 (1%)	69	81
1	D	394/419 (94%)	385 (98%)	9 (2%)	50	63
1	E	383/419 (91%)	374 (98%)	9 (2%)	50	63
1	F	368/419 (88%)	357 (97%)	11 (3%)	41	53
2	a	45/63 (71%)	43 (96%)	2 (4%)	28	35
2	b	55/63 (87%)	53 (96%)	2 (4%)	35	45
2	c	59/63 (94%)	58 (98%)	1 (2%)	60	74
2	d	58/63 (92%)	56 (97%)	2 (3%)	37	47
2	e	44/63 (70%)	42 (96%)	2 (4%)	27	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	f	30/63 (48%)	28 (93%)	2 (7%)	16 18
All	All	2592/2892 (90%)	2533 (98%)	59 (2%)	52 63

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	105	ASN
1	B	249	ASP
1	B	293	LYS
1	B	435	HIS
1	B	438	MET
1	B	462	ASP
1	B	472	LYS
1	C	46	LYS
1	C	159	PHE
1	C	361	TYR
1	C	435	HIS
1	C	438	MET
1	D	46	LYS
1	D	121	LYS
1	D	162	LEU
1	D	191	LEU
1	D	250	HIS
1	D	361	TYR
1	D	407[A]	ARG
1	D	407[B]	ARG
1	D	438	MET
1	E	6	LYS
1	E	46	LYS
1	E	57	LYS
1	E	124	ASN
1	E	186	ASP
1	E	310	LEU
1	E	361	TYR
1	E	435	HIS
1	E	438	MET
1	F	23	ARG
1	F	57	LYS
1	F	216	MET
1	F	250	HIS
1	F	270	ARG
1	F	284	SER

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Mol	Chain	Res	Type
1	F	348	THR
1	F	361	TYR
1	F	412	LYS
1	F	435	HIS
1	F	465	GLU
1	A	3	LYS
1	A	93	LEU
1	A	200	PRO
1	A	296	ARG
1	A	372	LEU
1	A	407	ARG
1	A	435	HIS
2	b	617	SER
2	b	621	ASP
2	c	616	ASP
2	d	601	MET
2	d	603	CYS
2	e	608	SER
2	e	616	ASP
2	f	634	SER
2	f	637	SER
2	a	614	MET
2	a	624	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	419	ASN
1	C	399	GLN
1	C	477	ASN
1	D	180	GLN
1	D	302	ASN
1	D	377	HIS
1	E	124	ASN
1	E	180	GLN
1	E	235	GLN
1	E	478	GLN
1	F	29	ASN
1	F	124	ASN
1	F	180	GLN
1	F	226	ASN
1	F	289	GLN

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Mol	Chain	Res	Type
1	A	17	GLN
1	A	83	ASN
1	A	117	ASN
1	A	180	GLN
1	A	226	ASN
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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

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^{th} 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%)	0.47	22 (4%)	31	30	28, 54, 93, 124	0
1	B	465/480 (96%)	0.30	12 (2%)	56	53	30, 52, 87, 125	0
1	C	469/480 (97%)	0.25	5 (1%)	80	79	27, 45, 74, 110	0
1	D	476/480 (99%)	0.38	12 (2%)	57	55	27, 53, 94, 129	0
1	E	470/480 (97%)	0.50	18 (3%)	40	38	29, 50, 89, 143	0
1	F	462/480 (96%)	0.51	24 (5%)	27	26	28, 55, 93, 130	0
2	a	63/68 (92%)	0.66	5 (7%)	12	11	50, 69, 99, 114	0
2	b	65/68 (95%)	0.65	3 (4%)	32	31	49, 70, 97, 114	0
2	c	67/68 (98%)	0.33	1 (1%)	73	72	41, 57, 82, 117	0
2	d	67/68 (98%)	0.55	4 (5%)	21	20	39, 64, 92, 122	0
2	e	64/68 (94%)	0.94	7 (10%)	5	5	58, 81, 115, 126	0
2	f	58/68 (85%)	1.43	16 (27%)	0	0	70, 96, 111, 117	0
All	All	3192/3288 (97%)	0.44	129 (4%)	38	36	27, 53, 96, 143	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	196	ALA	6.1
2	a	626	TYR	4.9
1	F	267	PRO	4.8
2	d	622	ALA	4.4
2	f	655	ALA	4.3
1	D	153	PRO	4.2
1	E	267	PRO	4.1
1	A	252	TYR	4.0
2	f	630	LYS	3.9
2	f	649	LEU	3.8
1	A	196	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	200	PRO	3.6
1	E	195	GLU	3.6
1	A	200	PRO	3.5
1	E	193	LYS	3.5
1	B	196	ALA	3.4
1	F	159	PHE	3.4
1	B	111	ALA	3.4
1	F	160	ASN	3.3
1	F	201	LEU	3.3
2	e	664	PRO	3.3
2	f	651	ASP	3.2
2	e	659	VAL	3.2
2	f	606	CYS	3.2
2	f	609	ASP	3.1
1	B	476	LYS	3.1
2	b	619	VAL	3.1
2	e	665	PRO	3.0
1	E	188	ALA	3.0
1	F	199	LYS	3.0
1	F	202	PRO	3.0
2	e	661	PRO	3.0
1	A	294	ILE	3.0
2	f	656	ASN	3.0
2	a	640	ASN	2.9
1	F	189	VAL	2.9
1	E	200	PRO	2.9
1	F	122	ASP	2.9
1	A	187	ILE	2.8
1	A	413	ASP	2.8
2	d	620	GLY	2.8
1	D	24	VAL	2.8
2	d	627	VAL	2.8
2	f	612	ARG	2.7
1	E	190	GLN	2.7
1	E	181	ALA	2.7
1	F	252	TYR	2.7
1	D	105	ASN	2.7
1	A	107	VAL	2.6
1	A	111	ALA	2.6
1	A	250	HIS	2.6
1	F	188	ALA	2.6
1	A	237	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	100	PHE	2.6
1	E	475	LEU	2.6
1	D	101	PRO	2.5
2	f	614	MET	2.5
2	b	664	PRO	2.5
1	A	201	LEU	2.5
1	F	121	LYS	2.5
1	F	272	VAL	2.5
1	A	269	VAL	2.5
1	E	101	PRO	2.5
2	e	663	ILE	2.5
2	f	629	GLU	2.5
2	e	642	VAL	2.5
1	F	173	ASP	2.5
1	A	248	TYR	2.5
1	A	181	ALA	2.5
1	A	247	LEU	2.4
1	E	197	GLU	2.4
2	a	662	PRO	2.4
1	A	189	VAL	2.4
1	B	252	TYR	2.4
1	D	250	HIS	2.4
1	F	276	PHE	2.4
1	F	292	VAL	2.4
1	B	255	ALA	2.4
1	D	126	PHE	2.4
1	A	159	PHE	2.4
1	B	192	GLU	2.4
2	f	657	MET	2.3
1	E	123	ILE	2.3
1	C	317	ILE	2.3
1	F	247	LEU	2.3
1	B	189	VAL	2.3
2	f	615	VAL	2.3
2	a	643	VAL	2.3
1	F	151	ALA	2.3
1	F	268	ARG	2.3
1	C	188	ALA	2.3
1	D	255	ALA	2.3
2	e	625	VAL	2.3
1	E	199	LYS	2.3
1	D	157	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	185	HIS	2.3
1	F	190	GLN	2.3
1	F	248	TYR	2.2
1	D	114	CYS	2.2
2	f	658	GLY	2.2
1	B	126	PHE	2.2
1	E	248	TYR	2.2
1	D	4	VAL	2.2
1	D	197	GLU	2.2
1	A	267	PRO	2.2
1	A	295	ASP	2.2
1	A	478	GLN	2.1
2	f	621	ASP	2.1
1	C	248	TYR	2.1
2	d	621	ASP	2.1
1	F	288	LEU	2.1
1	B	181	ALA	2.1
2	a	612	ARG	2.1
1	B	266	ILE	2.1
1	F	139	GLY	2.1
1	E	384	ILE	2.1
1	A	416	ILE	2.1
1	E	271	THR	2.1
2	f	626	TYR	2.1
2	f	631	CYS	2.1
1	D	413	ASP	2.0
2	b	652	ASN	2.0
2	c	663	ILE	2.0
1	C	17	GLN	2.0
1	C	158	ASP	2.0
1	E	294	ILE	2.0
1	A	202	PRO	2.0
1	F	290	CYS	2.0
1	B	45	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 monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
3	RB	D	502	1/1	-0.30	0.71	367,367,367,367	0
3	RB	C	502	1/1	0.87	0.14	60,60,60,60	0
3	RB	A	501	1/1	0.91	0.16	67,67,67,67	0
3	RB	B	502	1/1	0.92	0.15	75,75,75,75	0
3	RB	F	502	1/1	0.94	0.12	75,75,75,75	0
3	RB	F	501	1/1	0.96	0.11	63,63,63,63	0
3	RB	A	502	1/1	0.96	0.09	64,64,64,64	0
3	RB	B	501	1/1	0.97	0.06	45,45,45,45	0
4	ZN	a	701	1/1	0.97	0.09	55,55,55,55	0
3	RB	E	501	1/1	0.98	0.08	47,47,47,47	0
3	RB	E	502	1/1	0.99	0.08	47,47,47,47	0
3	RB	C	501	1/1	0.99	0.07	44,44,44,44	0
4	ZN	e	701	1/1	0.99	0.04	68,68,68,68	0
4	ZN	f	701	1/1	0.99	0.04	87,87,87,87	0
3	RB	D	501	1/1	0.99	0.07	48,48,48,48	0
4	ZN	b	701	1/1	1.00	0.09	51,51,51,51	0
4	ZN	c	701	1/1	1.00	0.10	40,40,40,40	0
4	ZN	d	701	1/1	1.00	0.10	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.