Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 12:04 PM EST

PDB ID	:	8U7E
Title	:	Structure of Sts-1 HP domain with rebamipide derivative
Authors	:	Aziz, F.; Dey, R.; French, J.B.
Deposited on	:	2023-09-15
Resolution	:	2.63 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 (i) 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 (i)) were used in the production of this report:

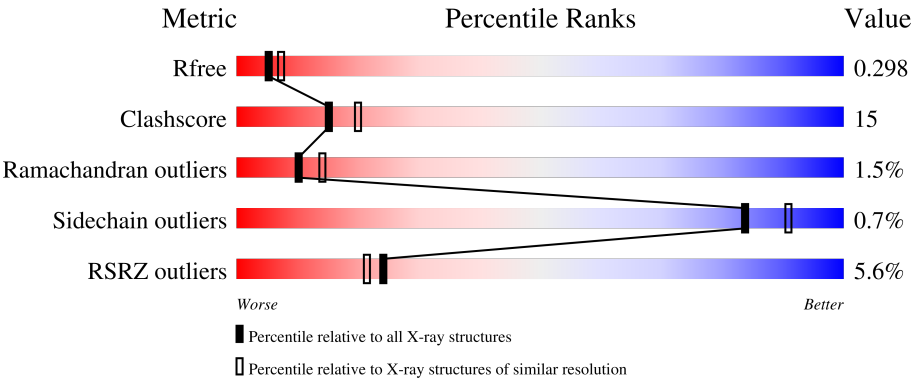
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	287	4% 64% 22% • 12%
1	B	287	2% 66% 21% • 10%
1	C	287	4% 63% 25% • 11%
1	D	287	7% 66% 22% 11%
1	E	287	7% 63% 23% • 12%

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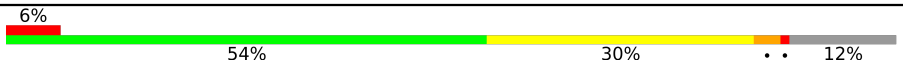
Mol	Chain	Length	Quality of chain
1	F	287	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21773 atoms, of which 10391 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 Ubiquitin-associated and SH3 domain-containing protein B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	253	Total	C	H	N	O	S	0	0	0
			3666	1212	1775	322	342	15			
1	B	257	Total	C	H	N	O	S	0	0	0
			3725	1226	1811	331	342	15			
1	C	256	Total	C	H	N	O	S	0	0	0
			3768	1231	1843	331	349	14			
1	D	255	Total	C	H	N	O	S	0	0	0
			3653	1204	1762	327	346	14			
1	E	253	Total	C	H	N	O	S	0	0	0
			3361	1134	1575	316	323	13			
1	F	253	Total	C	H	N	O	S	0	0	0
			3433	1155	1625	314	325	14			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	352	GLN	-	expression tag	UNP Q8TF42
A	353	GLY	-	expression tag	UNP Q8TF42
A	354	HIS	-	expression tag	UNP Q8TF42
A	355	MET	-	expression tag	UNP Q8TF42
A	356	ALA	-	expression tag	UNP Q8TF42
A	357	SER	-	expression tag	UNP Q8TF42
A	358	MET	-	expression tag	UNP Q8TF42
A	359	THR	-	expression tag	UNP Q8TF42
A	360	GLY	-	expression tag	UNP Q8TF42
A	361	GLY	-	expression tag	UNP Q8TF42
A	362	GLN	-	expression tag	UNP Q8TF42
A	363	GLN	-	expression tag	UNP Q8TF42
A	364	MET	-	expression tag	UNP Q8TF42
A	365	GLY	-	expression tag	UNP Q8TF42
A	366	ARG	-	expression tag	UNP Q8TF42
A	367	GLY	-	expression tag	UNP Q8TF42
A	368	SER	-	expression tag	UNP Q8TF42

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Chain	Residue	Modelled	Actual	Comment	Reference
B	352	GLN	-	expression tag	UNP Q8TF42
B	353	GLY	-	expression tag	UNP Q8TF42
B	354	HIS	-	expression tag	UNP Q8TF42
B	355	MET	-	expression tag	UNP Q8TF42
B	356	ALA	-	expression tag	UNP Q8TF42
B	357	SER	-	expression tag	UNP Q8TF42
B	358	MET	-	expression tag	UNP Q8TF42
B	359	THR	-	expression tag	UNP Q8TF42
B	360	GLY	-	expression tag	UNP Q8TF42
B	361	GLY	-	expression tag	UNP Q8TF42
B	362	GLN	-	expression tag	UNP Q8TF42
B	363	GLN	-	expression tag	UNP Q8TF42
B	364	MET	-	expression tag	UNP Q8TF42
B	365	GLY	-	expression tag	UNP Q8TF42
B	366	ARG	-	expression tag	UNP Q8TF42
B	367	GLY	-	expression tag	UNP Q8TF42
B	368	SER	-	expression tag	UNP Q8TF42
C	352	GLN	-	expression tag	UNP Q8TF42
C	353	GLY	-	expression tag	UNP Q8TF42
C	354	HIS	-	expression tag	UNP Q8TF42
C	355	MET	-	expression tag	UNP Q8TF42
C	356	ALA	-	expression tag	UNP Q8TF42
C	357	SER	-	expression tag	UNP Q8TF42
C	358	MET	-	expression tag	UNP Q8TF42
C	359	THR	-	expression tag	UNP Q8TF42
C	360	GLY	-	expression tag	UNP Q8TF42
C	361	GLY	-	expression tag	UNP Q8TF42
C	362	GLN	-	expression tag	UNP Q8TF42
C	363	GLN	-	expression tag	UNP Q8TF42
C	364	MET	-	expression tag	UNP Q8TF42
C	365	GLY	-	expression tag	UNP Q8TF42
C	366	ARG	-	expression tag	UNP Q8TF42
C	367	GLY	-	expression tag	UNP Q8TF42
C	368	SER	-	expression tag	UNP Q8TF42
D	352	GLN	-	expression tag	UNP Q8TF42
D	353	GLY	-	expression tag	UNP Q8TF42
D	354	HIS	-	expression tag	UNP Q8TF42
D	355	MET	-	expression tag	UNP Q8TF42
D	356	ALA	-	expression tag	UNP Q8TF42
D	357	SER	-	expression tag	UNP Q8TF42
D	358	MET	-	expression tag	UNP Q8TF42
D	359	THR	-	expression tag	UNP Q8TF42

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Chain	Residue	Modelled	Actual	Comment	Reference
D	360	GLY	-	expression tag	UNP Q8TF42
D	361	GLY	-	expression tag	UNP Q8TF42
D	362	GLN	-	expression tag	UNP Q8TF42
D	363	GLN	-	expression tag	UNP Q8TF42
D	364	MET	-	expression tag	UNP Q8TF42
D	365	GLY	-	expression tag	UNP Q8TF42
D	366	ARG	-	expression tag	UNP Q8TF42
D	367	GLY	-	expression tag	UNP Q8TF42
D	368	SER	-	expression tag	UNP Q8TF42
E	352	GLN	-	expression tag	UNP Q8TF42
E	353	GLY	-	expression tag	UNP Q8TF42
E	354	HIS	-	expression tag	UNP Q8TF42
E	355	MET	-	expression tag	UNP Q8TF42
E	356	ALA	-	expression tag	UNP Q8TF42
E	357	SER	-	expression tag	UNP Q8TF42
E	358	MET	-	expression tag	UNP Q8TF42
E	359	THR	-	expression tag	UNP Q8TF42
E	360	GLY	-	expression tag	UNP Q8TF42
E	361	GLY	-	expression tag	UNP Q8TF42
E	362	GLN	-	expression tag	UNP Q8TF42
E	363	GLN	-	expression tag	UNP Q8TF42
E	364	MET	-	expression tag	UNP Q8TF42
E	365	GLY	-	expression tag	UNP Q8TF42
E	366	ARG	-	expression tag	UNP Q8TF42
E	367	GLY	-	expression tag	UNP Q8TF42
E	368	SER	-	expression tag	UNP Q8TF42
F	352	GLN	-	expression tag	UNP Q8TF42
F	353	GLY	-	expression tag	UNP Q8TF42
F	354	HIS	-	expression tag	UNP Q8TF42
F	355	MET	-	expression tag	UNP Q8TF42
F	356	ALA	-	expression tag	UNP Q8TF42
F	357	SER	-	expression tag	UNP Q8TF42
F	358	MET	-	expression tag	UNP Q8TF42
F	359	THR	-	expression tag	UNP Q8TF42
F	360	GLY	-	expression tag	UNP Q8TF42
F	361	GLY	-	expression tag	UNP Q8TF42
F	362	GLN	-	expression tag	UNP Q8TF42
F	363	GLN	-	expression tag	UNP Q8TF42
F	364	MET	-	expression tag	UNP Q8TF42
F	365	GLY	-	expression tag	UNP Q8TF42
F	366	ARG	-	expression tag	UNP Q8TF42
F	367	GLY	-	expression tag	UNP Q8TF42

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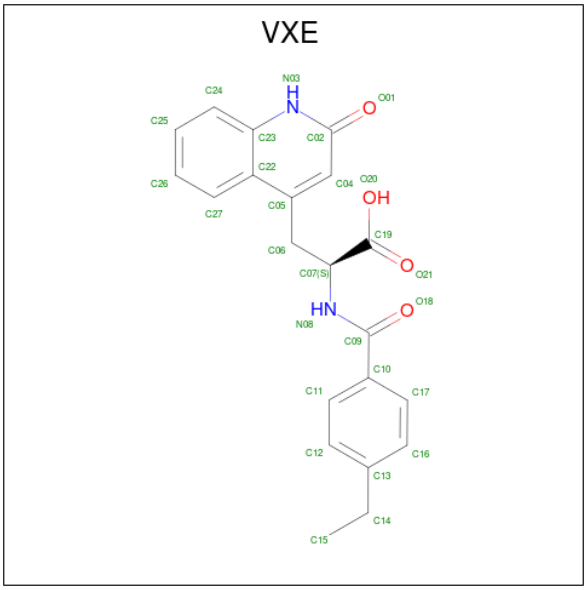
Chain	Residue	Modelled	Actual	Comment	Reference
F	368	SER	-	expression tag	UNP Q8TF42

- Molecule 2 is N-(4-ethylbenzoyl)-3-(2-oxo-1,2-dihydroquinolin-4-yl)-L-alanine (three-letter code: VXE) (formula: $C_{21}H_{20}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 27 21 2 4	0	0
2	C	1	Total C N O 27 21 2 4	0	0
2	D	1	Total C N O 27 21 2 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	26	Total O 26 26	0	0
3	B	18	Total O 18 18	0	0
3	C	25	Total O 25 25	0	0
3	D	4	Total O 4 4	0	0
3	E	1	Total O 1 1	0	0

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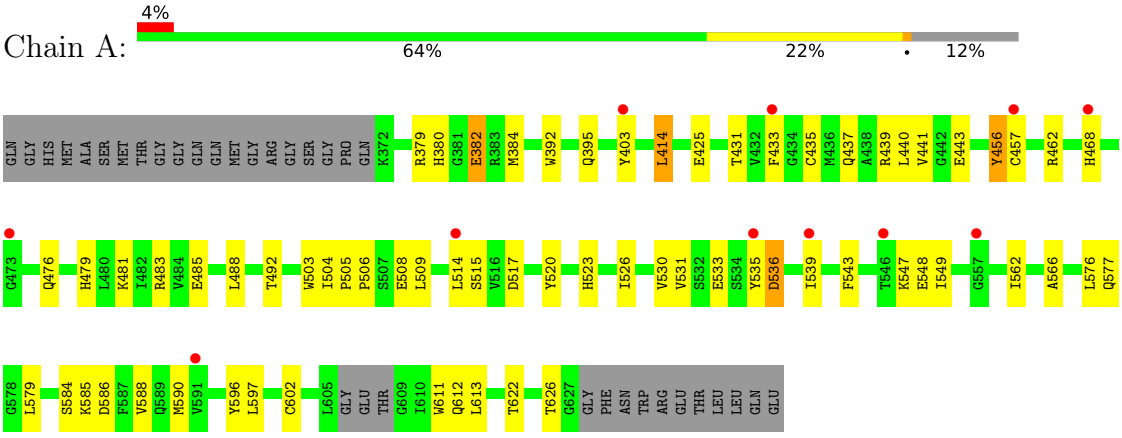
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	12	Total O 12 12	0	0

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.

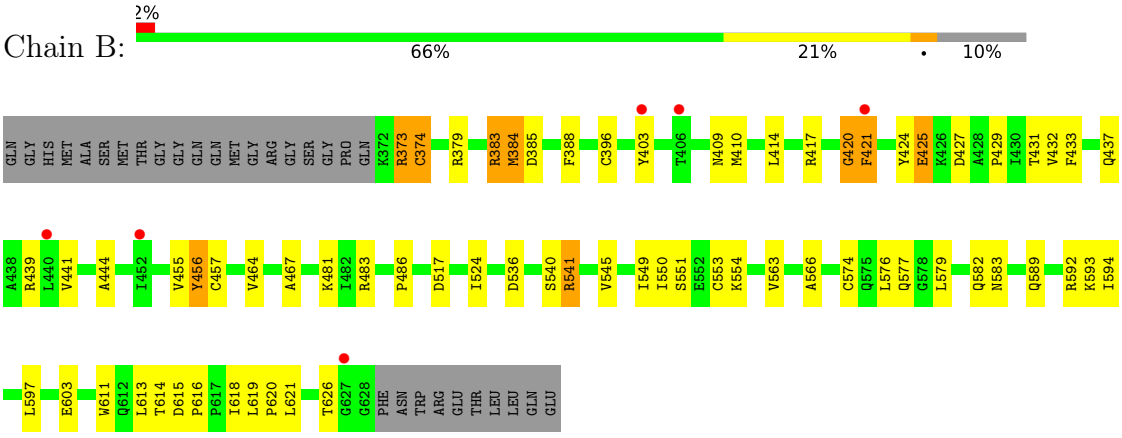
• Molecule 1: Ubiquitin-associated and SH3 domain-containing protein B

Chain A:



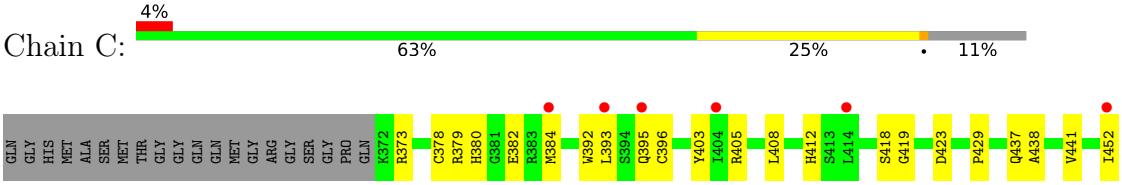
• Molecule 1: Ubiquitin-associated and SH3 domain-containing protein B

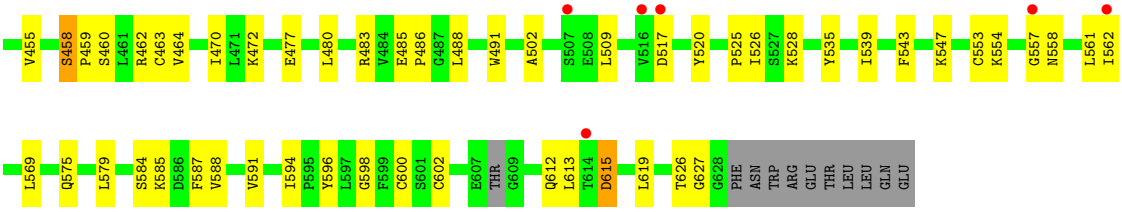
Chain B:



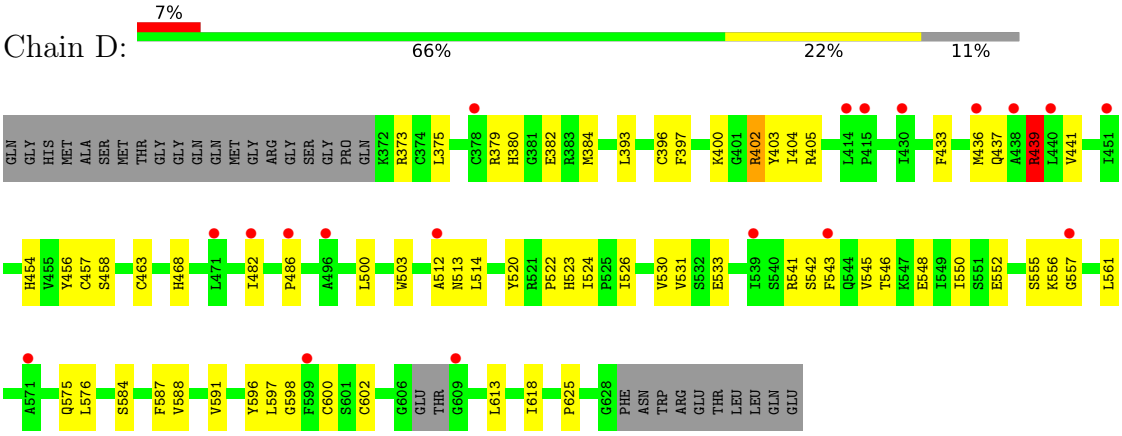
• Molecule 1: Ubiquitin-associated and SH3 domain-containing protein B

Chain C:

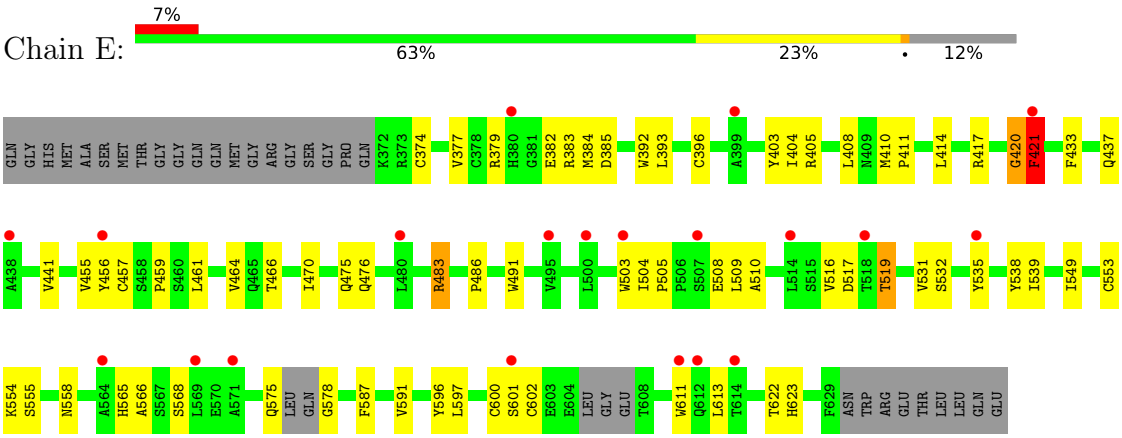




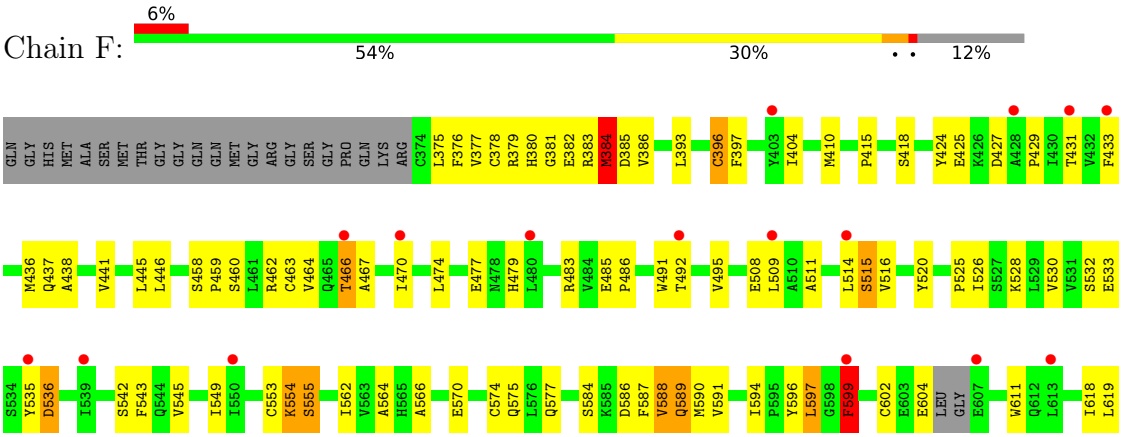
• Molecule 1: Ubiquitin-associated and SH3 domain-containing protein B

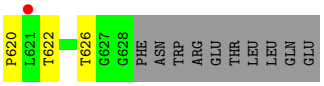


• Molecule 1: Ubiquitin-associated and SH3 domain-containing protein B



• Molecule 1: Ubiquitin-associated and SH3 domain-containing protein B




P620
L621
T622
T626
G627
G628
PHE
ASN
TRP
ARG
GLU
THR
LEU
LEU
GLN
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.78Å 122.70Å 99.94Å 90.00° 112.62° 90.00°	Depositor
Resolution (Å)	92.26 – 2.63 92.26 – 2.63	Depositor EDS
% Data completeness (in resolution range)	95.5 (92.26-2.63) 95.7 (92.26-2.63)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.62Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.215 , 0.298 0.220 , 0.298	Depositor DCC
R_{free} test set	2491 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	58.4	Xtriage
Anisotropy	0.883	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 76.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	21773	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: VXE

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	0.76	1/1939 (0.1%)	0.96	9/2650 (0.3%)
1	B	0.79	2/1963 (0.1%)	1.40	26/2681 (1.0%)
1	C	0.70	0/1973	0.89	3/2689 (0.1%)
1	D	0.65	1/1939 (0.1%)	0.87	7/2652 (0.3%)
1	E	0.56	0/1829	0.79	3/2507 (0.1%)
1	F	0.75	5/1854 (0.3%)	0.91	6/2545 (0.2%)
All	All	0.71	9/11497 (0.1%)	0.99	54/15724 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	2
1	F	0	1
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	425	GLU	CB-CG	13.07	1.76	1.52
1	F	485	GLU	CD-OE2	10.53	1.37	1.25
1	A	382	GLU	CB-CG	8.15	1.67	1.52
1	F	384	MET	CB-CG	6.86	1.73	1.51
1	B	374	CYS	CB-SG	-6.11	1.71	1.82
1	F	384	MET	SD-CE	5.66	2.09	1.77
1	F	485	GLU	CG-CD	5.62	1.60	1.51
1	D	384	MET	CG-SD	-5.62	1.66	1.81
1	F	396	CYS	CB-SG	-5.42	1.73	1.81

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	373	ARG	NE-CZ-NH2	-34.56	103.02	120.30
1	B	373	ARG	NE-CZ-NH1	18.32	129.46	120.30
1	B	425	GLU	CG-CD-OE1	15.46	149.23	118.30
1	F	384	MET	CG-SD-CE	-14.41	77.15	100.20
1	B	383	ARG	NE-CZ-NH2	-14.21	113.20	120.30
1	B	373	ARG	CG-CD-NE	-12.43	85.70	111.80
1	B	425	GLU	OE1-CD-OE2	-12.00	108.90	123.30
1	C	615	ASP	CB-CG-OD1	-11.27	108.16	118.30
1	A	382	GLU	CG-CD-OE1	10.50	139.29	118.30
1	A	382	GLU	CG-CD-OE2	-9.05	100.20	118.30
1	B	425	GLU	CG-CD-OE2	-8.78	100.74	118.30
1	E	483	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	B	373	ARG	CB-CG-CD	7.85	132.01	111.60
1	B	582	GLN	CA-CB-CG	7.75	130.45	113.40
1	D	439	ARG	CG-CD-NE	7.64	127.84	111.80
1	B	373	ARG	CD-NE-CZ	7.57	134.20	123.60
1	D	405	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	A	382	GLU	N-CA-CB	7.19	123.55	110.60
1	B	421	PHE	CB-CG-CD2	-7.18	115.77	120.80
1	B	373	ARG	CA-CB-CG	7.10	129.02	113.40
1	C	612	GLN	CA-CB-CG	7.07	128.94	113.40
1	F	599	PHE	CB-CA-C	6.96	124.33	110.40
1	F	436	MET	CB-CG-SD	-6.94	91.58	112.40
1	B	383	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	F	599	PHE	CB-CG-CD2	-6.74	116.08	120.80
1	A	382	GLU	CB-CG-CD	-6.53	96.56	114.20
1	B	373	ARG	NH1-CZ-NH2	6.28	126.31	119.40
1	B	427	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	D	436	MET	CB-CG-SD	-6.14	93.97	112.40
1	B	439	ARG	CB-CG-CD	-6.13	95.66	111.60
1	D	373	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	439	ARG	NE-CZ-NH1	-6.03	117.28	120.30
1	B	576	LEU	CA-CB-CG	5.95	128.99	115.30
1	C	579	LEU	CB-CG-CD2	-5.95	100.89	111.00
1	A	536	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	476	GLN	CA-CB-CG	-5.84	100.54	113.40
1	F	384	MET	CB-CG-SD	-5.81	94.97	112.40
1	D	402	ARG	CG-CD-NE	5.74	123.85	111.80
1	B	384	MET	CG-SD-CE	-5.68	91.11	100.20
1	A	536	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	421	PHE	N-CA-CB	-5.61	100.51	110.60
1	E	421	PHE	CB-CG-CD2	-5.58	116.90	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	582	GLN	N-CA-CB	5.46	120.43	110.60
1	B	536	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	B	421	PHE	CB-CA-C	5.39	121.18	110.40
1	D	384	MET	CA-CB-CG	5.34	122.38	113.30
1	B	425	GLU	CB-CG-CD	-5.27	99.96	114.20
1	A	382	GLU	CB-CA-C	-5.20	100.00	110.40
1	A	414	LEU	CA-CB-CG	5.16	127.16	115.30
1	D	561	LEU	CB-CG-CD1	-5.14	102.27	111.00
1	B	421	PHE	CB-CG-CD1	5.11	124.38	120.80
1	B	541	ARG	CG-CD-NE	5.09	122.48	111.80
1	F	410	MET	CG-SD-CE	5.03	108.25	100.20
1	E	483	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	420	GLY	Peptide
1	D	439	ARG	Sidechain
1	D	625	PRO	Peptide
1	F	384	MET	Mainchain

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	1891	1775	1776	52	0
1	B	1914	1811	1811	61	0
1	C	1925	1843	1846	47	0
1	D	1891	1762	1762	44	0
1	E	1786	1575	1575	54	0
1	F	1808	1625	1625	82	0
2	A	27	0	0	0	0
2	C	27	0	0	0	0
2	D	27	0	0	0	0
3	A	26	0	0	0	0
3	B	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	25	0	0	0	0
3	D	4	0	0	0	0
3	E	1	0	0	0	0
3	F	12	0	0	1	0
All	All	11382	10391	10395	325	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 15.

All (325) 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:425:GLU:CG	1:B:425:GLU:CB	1.77	1.62
1:F:384:MET:SD	1:F:384:MET:CE	2.09	1.40
1:F:384:MET:CE	1:F:384:MET:CG	2.43	0.97
1:F:378:CYS:HB2	1:F:599:PHE:HB2	1.48	0.95
1:F:384:MET:HG3	1:F:431:THR:HG22	1.55	0.87
1:B:379:ARG:NH1	1:B:594:ILE:O	2.09	0.86
1:B:541:ARG:O	1:B:545:VAL:HG23	1.76	0.85
1:B:383:ARG:HG3	1:B:385:ASP:OD1	1.77	0.85
1:B:589:GLN:O	1:B:593:LYS:HD3	1.77	0.84
1:F:378:CYS:CB	1:F:599:PHE:HB2	2.06	0.84
1:B:373:ARG:NH1	1:B:554:LYS:HA	1.98	0.78
1:A:456:TYR:CZ	1:A:549:ILE:HG23	2.18	0.78
1:B:425:GLU:CB	1:B:425:GLU:CD	2.54	0.77
1:B:425:GLU:CG	1:B:425:GLU:CA	2.63	0.76
1:D:526:ILE:H	1:D:526:ILE:HD12	1.51	0.75
1:E:393:LEU:HD23	1:E:421:PHE:CE1	2.23	0.74
1:F:379:ARG:NH1	1:F:594:ILE:O	2.21	0.73
1:E:510:ALA:HB2	1:E:516:VAL:HB	1.72	0.72
1:F:384:MET:CE	1:F:384:MET:HG2	2.19	0.72
1:F:466:THR:HG22	1:F:470:ILE:HD11	1.72	0.71
1:D:541:ARG:O	1:D:545:VAL:HG23	1.91	0.71
1:B:384:MET:HG2	1:B:431:THR:HG22	1.72	0.71
1:B:384:MET:HE1	1:B:410:MET:HG2	1.73	0.70
1:F:415:PRO:HD2	1:F:424:TYR:OH	1.91	0.70
1:C:472:LYS:HA	1:C:477:GLU:HG3	1.72	0.70
1:F:377:VAL:HG22	1:F:562:ILE:HB	1.74	0.70
1:C:584:SER:O	1:C:588:VAL:HG23	1.94	0.67
1:F:599:PHE:CE2	1:F:618:ILE:HD11	2.29	0.67
1:F:483:ARG:HG2	1:F:520:TYR:CD1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:526:ILE:HD12	1:F:526:ILE:H	1.60	0.66
1:F:379:ARG:HD2	1:F:566:ALA:HB2	1.78	0.65
1:E:466:THR:O	1:E:470:ILE:HG13	1.95	0.65
1:F:396:CYS:HB2	1:F:397:PHE:CD2	2.31	0.65
1:B:577:GLN:OE1	1:B:613:LEU:HG	1.96	0.65
1:A:492:THR:OG1	1:A:533:GLU:HG2	1.97	0.63
1:E:379:ARG:HD2	1:E:566:ALA:HB2	1.80	0.63
1:A:584:SER:O	1:A:588:VAL:HG23	1.97	0.63
1:F:437:GLN:O	1:F:441:VAL:HG23	1.99	0.63
1:D:546:THR:O	1:D:550:ILE:HG12	1.99	0.62
1:F:466:THR:HG22	1:F:470:ILE:CD1	2.28	0.62
1:F:542:SER:HA	1:F:545:VAL:HG12	1.81	0.62
1:D:533:GLU:OE2	1:D:541:ARG:NH1	2.33	0.62
1:C:526:ILE:HD12	1:C:526:ILE:H	1.64	0.62
1:A:503:TRP:HE3	1:A:526:ILE:HD13	1.65	0.61
1:B:384:MET:CE	1:B:410:MET:HG2	2.31	0.60
1:C:525:PRO:HD2	1:C:528:LYS:HG3	1.83	0.60
1:C:602:CYS:SG	1:C:613:LEU:HD23	2.42	0.60
1:E:417:ARG:HG2	1:E:504:ILE:HD11	1.84	0.60
1:D:584:SER:O	1:D:588:VAL:HG23	2.02	0.60
1:E:456:TYR:CZ	1:E:549:ILE:HG12	2.37	0.59
1:D:433:PHE:O	1:D:437:GLN:HG3	2.01	0.59
1:B:417:ARG:HB2	1:B:420:GLY:O	2.03	0.59
1:A:456:TYR:HB3	1:A:483:ARG:O	2.02	0.59
1:F:464:VAL:HG11	1:F:509:LEU:HD22	1.83	0.59
1:B:456:TYR:CZ	1:B:549:ILE:HG23	2.38	0.59
1:B:374:CYS:SG	1:B:603:GLU:HG2	2.42	0.58
1:C:405:ARG:NH1	1:C:412:HIS:NE2	2.50	0.58
1:F:530:VAL:HG23	1:F:533:GLU:HB3	1.85	0.58
1:A:602:CYS:SG	1:A:613:LEU:HD23	2.43	0.58
1:E:393:LEU:HD23	1:E:421:PHE:HE1	1.68	0.58
1:C:437:GLN:O	1:C:441:VAL:HG23	2.03	0.58
1:A:483:ARG:HG3	1:A:483:ARG:HH11	1.67	0.58
1:B:373:ARG:HH12	1:B:554:LYS:HA	1.66	0.58
1:A:504:ILE:HG23	1:A:508:GLU:HB3	1.86	0.58
1:D:520:TYR:OH	1:D:523:HIS:CD2	2.57	0.58
1:C:379:ARG:HG2	1:C:380:HIS:N	2.19	0.57
1:D:524:ILE:HD12	1:D:545:VAL:HG22	1.86	0.57
1:F:424:TYR:O	1:F:427:ASP:N	2.33	0.57
1:A:577:GLN:HE21	1:A:579:LEU:HD22	1.70	0.57
1:A:440:LEU:HD23	1:A:443:GLU:OE2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:619:LEU:N	1:C:619:LEU:HD12	2.21	0.56
1:F:380:HIS:CE1	1:F:462:ARG:HD2	2.41	0.56
1:A:586:ASP:O	1:A:590:MET:HG3	2.06	0.56
1:D:382:GLU:HA	1:D:596:TYR:CE2	2.41	0.56
1:B:379:ARG:HD2	1:B:566:ALA:HB2	1.87	0.56
1:F:433:PHE:O	1:F:437:GLN:HG3	2.06	0.56
1:B:456:TYR:HB3	1:B:483:ARG:O	2.06	0.56
1:A:505:PRO:HD2	1:A:508:GLU:HB2	1.88	0.55
1:F:384:MET:HB2	1:F:429:PRO:O	2.07	0.55
1:E:383:ARG:NH2	1:E:385:ASP:OD2	2.37	0.55
1:F:586:ASP:HA	1:F:589:GLN:CB	2.37	0.55
1:B:626:THR:HG23	1:E:623:HIS:CD2	2.42	0.55
1:A:456:TYR:CZ	1:A:483:ARG:HD3	2.42	0.55
1:F:545:VAL:O	1:F:549:ILE:HG13	2.06	0.55
1:A:626:THR:HG21	1:F:622:THR:HA	1.88	0.55
1:C:483:ARG:HD3	1:C:520:TYR:CD1	2.42	0.55
1:A:456:TYR:O	1:A:457:CYS:HB3	2.07	0.54
1:C:405:ARG:HH12	1:C:408:LEU:HD23	1.72	0.54
1:F:543:PHE:CD1	1:F:543:PHE:O	2.60	0.54
1:F:587:PHE:O	1:F:590:MET:N	2.40	0.54
1:D:375:LEU:HD22	1:D:550:ILE:HD11	1.89	0.54
1:A:392:TRP:O	1:A:395:GLN:N	2.36	0.54
1:F:588:VAL:HA	1:F:591:VAL:HG22	1.90	0.54
1:D:543:PHE:HE1	1:D:576:LEU:N	2.07	0.53
1:A:456:TYR:CE2	1:A:549:ILE:HG23	2.43	0.53
1:C:587:PHE:O	1:C:591:VAL:HG23	2.09	0.53
1:C:373:ARG:CG	1:C:558:ASN:HA	2.39	0.52
1:E:385:ASP:OD1	1:E:385:ASP:N	2.38	0.52
1:E:553:CYS:O	1:E:555:SER:N	2.42	0.52
1:F:379:ARG:O	1:F:597:LEU:HA	2.10	0.52
1:D:403:TYR:C	1:D:404:ILE:HG13	2.30	0.52
1:D:543:PHE:CD1	1:D:575:GLN:HB2	2.43	0.52
1:A:481:LYS:CB	1:A:517:ASP:HB2	2.39	0.52
1:D:393:LEU:HD23	1:D:397:PHE:HE1	1.75	0.52
1:D:400:LYS:HD2	1:D:402:ARG:HH21	1.75	0.52
1:F:467:ALA:HA	1:F:470:ILE:HD13	1.91	0.52
1:A:485:GLU:OE1	1:A:520:TYR:OH	2.25	0.52
1:A:523:HIS:HB3	1:A:548:GLU:OE2	2.09	0.52
1:F:375:LEU:HG	1:F:376:PHE:N	2.24	0.52
1:F:376:PHE:HB3	1:F:599:PHE:CE1	2.44	0.52
1:B:603:GLU:HG3	1:B:614:THR:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ARG:HD2	1:A:566:ALA:HB2	1.92	0.51
1:E:475:GLN:O	1:E:476:GLN:HG2	2.10	0.51
1:F:602:CYS:HB3	1:F:611:TRP:CE3	2.45	0.51
1:F:602:CYS:HB3	1:F:611:TRP:HE3	1.75	0.51
1:D:520:TYR:OH	1:D:523:HIS:HD2	1.93	0.51
1:E:392:TRP:CZ3	1:E:393:LEU:HD12	2.45	0.51
1:F:570:GLU:O	1:F:574:CYS:HB2	2.11	0.51
1:E:504:ILE:CG2	1:E:509:LEU:HD23	2.41	0.51
1:B:433:PHE:CE2	1:E:623:HIS:CD2	2.99	0.51
1:D:468:HIS:CG	1:D:514:LEU:HD23	2.46	0.51
1:F:384:MET:HB3	1:F:384:MET:HE2	1.92	0.51
1:D:523:HIS:ND1	1:D:548:GLU:HB3	2.26	0.51
1:B:583:ASN:C	1:B:583:ASN:OD1	2.49	0.51
1:E:441:VAL:HG21	1:E:597:LEU:HD12	1.91	0.51
1:C:626:THR:CG2	1:C:627:GLY:N	2.74	0.51
1:F:459:PRO:HD3	1:F:486:PRO:HA	1.93	0.51
1:C:392:TRP:O	1:C:395:GLN:N	2.41	0.50
1:F:577:GLN:CB	3:F:710:HOH:O	2.59	0.50
1:D:500:LEU:HD22	1:D:503:TRP:CH2	2.47	0.50
1:F:543:PHE:CD2	1:F:575:GLN:CB	2.95	0.50
1:E:374:CYS:HA	1:E:602:CYS:O	2.11	0.50
1:E:509:LEU:HB2	1:E:516:VAL:HG21	1.92	0.50
1:A:543:PHE:CZ	1:A:547:LYS:HE2	2.47	0.50
1:B:384:MET:CG	1:B:431:THR:HG22	2.40	0.50
1:B:456:TYR:CD1	1:B:456:TYR:N	2.79	0.50
1:B:417:ARG:HD2	1:B:424:TYR:CZ	2.47	0.50
1:B:433:PHE:O	1:B:437:GLN:HG3	2.12	0.49
1:C:379:ARG:NH1	1:C:594:ILE:O	2.45	0.49
1:D:441:VAL:HG13	1:D:618:ILE:CD1	2.43	0.49
1:D:602:CYS:SG	1:D:613:LEU:HD23	2.53	0.49
1:C:452:ILE:O	1:C:480:LEU:HD11	2.12	0.49
1:F:458:SER:OG	1:F:459:PRO:HD2	2.13	0.49
1:B:592:ARG:C	1:B:593:LYS:HD2	2.33	0.49
1:B:456:TYR:N	1:B:456:TYR:HD1	2.10	0.49
1:C:455:VAL:CG2	1:C:561:LEU:HD23	2.43	0.49
1:E:405:ARG:NH2	1:E:410:MET:O	2.46	0.49
1:F:380:HIS:HE1	1:F:383:ARG:HG3	1.77	0.49
1:D:454:HIS:NE2	1:D:556:LYS:O	2.46	0.48
1:F:438:ALA:HB1	1:F:470:ILE:CD1	2.43	0.48
1:A:433:PHE:O	1:A:437:GLN:HG3	2.14	0.48
1:B:457:CYS:SG	1:B:464:VAL:HG22	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:VAL:HG11	1:C:509:LEU:HD13	1.95	0.48
1:C:485:GLU:HB3	1:C:488:LEU:HD12	1.94	0.48
1:E:517:ASP:OD1	1:E:519:THR:HG23	2.13	0.48
1:E:392:TRP:CE3	1:E:393:LEU:HD12	2.48	0.48
1:E:517:ASP:OD1	1:E:519:THR:CG2	2.61	0.48
1:F:378:CYS:HB3	1:F:599:PHE:HB2	1.91	0.48
1:F:383:ARG:HB3	1:F:385:ASP:OD1	2.14	0.48
1:B:524:ILE:HD12	1:B:545:VAL:HG22	1.94	0.48
1:B:437:GLN:O	1:B:441:VAL:HG23	2.14	0.47
1:E:456:TYR:CE2	1:E:549:ILE:HG12	2.49	0.47
1:A:382:GLU:HG3	1:A:596:TYR:CE2	2.49	0.47
1:A:433:PHE:CD2	1:F:433:PHE:CD2	3.03	0.47
1:A:506:PRO:HA	1:A:509:LEU:HD12	1.94	0.47
1:F:393:LEU:HD23	1:F:397:PHE:CE2	2.49	0.47
1:A:530:VAL:HG12	1:A:531:VAL:N	2.28	0.47
1:B:409:ASN:ND2	1:E:622:THR:O	2.48	0.47
1:B:467:ALA:HA	1:B:563:VAL:HG21	1.96	0.47
1:F:514:LEU:O	1:F:516:VAL:N	2.47	0.47
1:B:384:MET:HE3	1:B:388:PHE:CD2	2.50	0.47
1:B:455:VAL:C	1:B:456:TYR:HD1	2.17	0.47
1:C:405:ARG:NH1	1:C:408:LEU:HD23	2.30	0.47
1:E:382:GLU:HA	1:E:596:TYR:CZ	2.50	0.47
1:C:491:TRP:CZ2	1:C:535:TYR:HB2	2.50	0.47
1:D:555:SER:O	1:D:557:GLY:N	2.39	0.47
1:A:514:LEU:O	1:A:515:SER:C	2.53	0.47
1:E:459:PRO:HD3	1:E:486:PRO:HA	1.97	0.47
1:E:601:SER:O	1:E:613:LEU:HD12	2.15	0.47
1:A:456:TYR:N	1:A:456:TYR:CD1	2.83	0.46
1:B:444:ALA:HB2	1:E:408:LEU:CD2	2.45	0.46
1:C:384:MET:HB2	1:C:429:PRO:O	2.15	0.46
1:A:380:HIS:CE1	1:A:462:ARG:HD2	2.51	0.46
1:B:620:PRO:O	1:E:408:LEU:HD12	2.16	0.46
1:D:454:HIS:CE1	1:D:556:LYS:O	2.68	0.46
1:E:384:MET:HE1	1:E:411:PRO:CD	2.45	0.46
1:A:504:ILE:CG2	1:A:508:GLU:HB3	2.45	0.46
1:A:622:THR:HG23	1:F:626:THR:HG21	1.98	0.46
1:C:543:PHE:HB2	1:C:575:GLN:OE1	2.16	0.46
1:E:531:VAL:HG12	1:E:532:SER:N	2.30	0.46
1:D:393:LEU:HD23	1:D:397:PHE:CE1	2.50	0.46
1:F:535:TYR:CE2	1:F:584:SER:HA	2.51	0.46
1:F:604:GLU:HB3	1:F:611:TRP:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:CYS:HB2	1:D:397:PHE:CD1	2.50	0.46
1:F:587:PHE:O	1:F:591:VAL:HG13	2.15	0.46
1:D:587:PHE:O	1:D:591:VAL:HG23	2.16	0.46
1:D:456:TYR:N	1:D:456:TYR:CD1	2.84	0.46
1:F:383:ARG:HB2	1:F:386:VAL:HG23	1.98	0.46
1:C:488:LEU:HD22	1:C:562:ILE:HG21	1.97	0.45
1:D:512:ALA:O	1:D:513:ASN:C	2.55	0.45
1:A:456:TYR:N	1:A:456:TYR:HD1	2.15	0.45
1:E:565:HIS:O	1:E:568:SER:HB3	2.16	0.45
1:F:577:GLN:HA	1:F:611:TRP:O	2.16	0.45
1:C:585:LYS:HD2	1:C:585:LYS:HA	1.75	0.45
1:B:444:ALA:HB1	1:B:618:ILE:HB	1.98	0.45
1:C:438:ALA:HB1	1:C:470:ILE:HG13	1.97	0.45
1:B:373:ARG:HH21	1:B:611:TRP:HZ2	1.64	0.45
1:B:615:ASP:HA	1:B:616:PRO:HD3	1.83	0.45
1:B:621:LEU:HD23	1:B:621:LEU:C	2.37	0.45
1:F:619:LEU:HB3	1:F:620:PRO:HD2	1.97	0.45
1:C:405:ARG:CZ	1:C:412:HIS:NE2	2.80	0.45
1:B:619:LEU:O	1:E:408:LEU:HD11	2.16	0.45
1:C:392:TRP:O	1:C:395:GLN:HB2	2.17	0.45
1:F:464:VAL:HG12	1:F:514:LEU:HD23	1.99	0.45
1:D:457:CYS:SG	1:D:482:ILE:HG21	2.57	0.45
1:F:466:THR:CG2	1:F:470:ILE:HD11	2.45	0.45
1:C:458:SER:HB3	1:C:463:CYS:SG	2.57	0.45
1:D:379:ARG:HG2	1:D:380:HIS:N	2.32	0.45
1:D:486:PRO:HD2	1:D:522:PRO:HB3	1.99	0.45
1:E:575:GLN:O	1:E:578:GLY:HA2	2.17	0.45
1:F:536:ASP:OD1	1:F:536:ASP:N	2.37	0.45
1:A:530:VAL:HG12	1:A:531:VAL:H	1.80	0.44
1:A:536:ASP:OD2	1:B:540:SER:HA	2.17	0.44
1:D:458:SER:HB3	1:D:463:CYS:SG	2.57	0.44
1:F:466:THR:O	1:F:470:ILE:HD12	2.18	0.44
1:A:483:ARG:HG2	1:A:520:TYR:CD1	2.53	0.44
1:D:523:HIS:NE2	1:D:552:GLU:OE2	2.50	0.44
1:C:396:CYS:HB2	1:C:403:TYR:CE1	2.53	0.44
1:E:491:TRP:HA	1:E:538:TYR:CD1	2.53	0.44
1:B:619:LEU:O	1:E:408:LEU:CD1	2.66	0.44
1:D:524:ILE:O	1:D:524:ILE:HG22	2.16	0.44
1:E:377:VAL:HB	1:E:600:CYS:SG	2.57	0.44
1:E:531:VAL:HG12	1:E:532:SER:H	1.82	0.44
1:A:576:LEU:HG	1:A:611:TRP:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:PRO:HD3	1:C:486:PRO:HA	2.00	0.44
1:A:384:MET:SD	1:A:431:THR:HG22	2.58	0.44
1:B:409:ASN:O	1:B:432:VAL:HG23	2.18	0.44
1:B:574:CYS:O	1:B:579:LEU:O	2.36	0.44
1:D:530:VAL:HG12	1:D:531:VAL:N	2.33	0.44
1:B:583:ASN:OD1	1:B:583:ASN:O	2.34	0.43
1:E:461:LEU:HD12	1:E:461:LEU:O	2.18	0.43
1:F:384:MET:HG2	1:F:384:MET:HE3	1.97	0.43
1:C:539:ILE:HD13	1:C:539:ILE:HA	1.84	0.43
1:C:569:LEU:HD23	1:C:600:CYS:HB3	2.00	0.43
1:E:433:PHE:O	1:E:437:GLN:HG3	2.18	0.43
1:A:468:HIS:CG	1:A:514:LEU:HD23	2.54	0.43
1:A:543:PHE:CE2	1:A:547:LYS:HE2	2.53	0.43
1:B:414:LEU:HD22	1:B:429:PRO:HG3	2.01	0.43
1:E:384:MET:HE1	1:E:411:PRO:HD3	2.00	0.43
1:E:392:TRP:CZ2	1:E:393:LEU:CD1	3.02	0.43
1:F:543:PHE:CG	1:F:575:GLN:CB	3.01	0.43
1:B:486:PRO:HD2	1:B:524:ILE:O	2.18	0.43
1:C:382:GLU:HA	1:C:596:TYR:CE1	2.54	0.43
1:B:373:ARG:NH2	1:B:550:ILE:HG23	2.34	0.43
1:C:396:CYS:HB2	1:C:403:TYR:HE1	1.83	0.43
1:C:455:VAL:HG23	1:C:561:LEU:HD23	2.00	0.43
1:D:500:LEU:HD22	1:D:503:TRP:HH2	1.83	0.43
1:C:526:ILE:HD12	1:C:526:ILE:N	2.33	0.43
1:F:542:SER:O	1:F:545:VAL:HG12	2.19	0.43
1:C:419:GLY:HA3	1:C:423:ASP:OD2	2.18	0.42
1:C:561:LEU:HG	1:C:562:ILE:N	2.34	0.42
1:F:438:ALA:HB1	1:F:470:ILE:HD12	2.00	0.42
1:F:508:GLU:O	1:F:511:ALA:HB3	2.19	0.42
1:A:433:PHE:CD2	1:F:433:PHE:HD2	2.37	0.42
1:A:602:CYS:HA	1:A:612:GLN:O	2.19	0.42
1:D:379:ARG:NH2	1:D:596:TYR:HE1	2.16	0.42
1:E:420:GLY:O	1:E:421:PHE:HB3	2.18	0.42
1:A:435:CYS:O	1:A:439:ARG:HG3	2.20	0.42
1:F:553:CYS:O	1:F:554:LYS:C	2.58	0.42
1:E:403:TYR:CE1	1:E:414:LEU:HG	2.55	0.42
1:A:488:LEU:HD22	1:A:562:ILE:HG21	2.02	0.42
1:B:577:GLN:HG2	1:B:611:TRP:O	2.19	0.42
1:F:396:CYS:O	1:F:404:ILE:N	2.48	0.42
1:A:425:GLU:O	1:A:425:GLU:HG2	2.19	0.42
1:A:479:HIS:O	1:A:479:HIS:ND1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:LYS:HD2	1:C:535:TYR:HE2	1.84	0.42
1:B:396:CYS:O	1:B:403:TYR:HA	2.19	0.42
1:F:445:LEU:HB2	1:F:474:LEU:HD21	2.01	0.42
1:F:554:LYS:O	1:F:555:SER:CB	2.67	0.42
1:F:604:GLU:O	1:F:604:GLU:HG3	2.19	0.42
1:B:592:ARG:HG3	1:B:593:LYS:NZ	2.34	0.42
1:B:611:TRP:CD1	1:B:611:TRP:N	2.88	0.42
1:F:460:SER:HB2	1:F:463:CYS:SG	2.60	0.42
1:A:492:THR:HG23	1:A:533:GLU:OE2	2.19	0.42
1:A:535:TYR:CE1	1:A:539:ILE:HD11	2.55	0.42
1:D:541:ARG:CG	1:D:542:SER:N	2.83	0.41
1:F:446:LEU:HD23	1:F:446:LEU:C	2.40	0.41
1:C:517:ASP:OD1	1:C:517:ASP:C	2.58	0.41
1:E:392:TRP:CH2	1:E:393:LEU:CD1	3.03	0.41
1:E:587:PHE:CE1	1:E:591:VAL:HG21	2.55	0.41
1:F:384:MET:CE	1:F:384:MET:CB	2.98	0.41
1:F:424:TYR:O	1:F:425:GLU:C	2.58	0.41
1:B:385:ASP:OD1	1:B:385:ASP:N	2.54	0.41
1:B:551:SER:C	1:B:553:CYS:H	2.22	0.41
1:D:530:VAL:HG12	1:D:531:VAL:O	2.20	0.41
1:E:457:CYS:SG	1:E:464:VAL:HG22	2.60	0.41
1:A:433:PHE:HD2	1:F:433:PHE:CD2	2.37	0.41
1:C:543:PHE:O	1:C:547:LYS:HG3	2.20	0.41
1:D:541:ARG:HG2	1:D:542:SER:N	2.35	0.41
1:F:382:GLU:HA	1:F:596:TYR:CZ	2.56	0.41
1:B:481:LYS:HB3	1:B:517:ASP:CA	2.51	0.41
1:E:455:VAL:O	1:E:483:ARG:HD2	2.21	0.41
1:E:396:CYS:HA	1:E:404:ILE:O	2.21	0.41
1:B:597:LEU:HD13	1:B:597:LEU:HA	1.96	0.41
1:E:505:PRO:O	1:E:508:GLU:N	2.52	0.41
1:F:441:VAL:HG21	1:F:597:LEU:HD12	2.03	0.41
1:F:492:THR:HA	1:F:495:VAL:HG23	2.03	0.41
1:C:553:CYS:O	1:C:554:LYS:C	2.59	0.41
1:D:441:VAL:HG13	1:D:618:ILE:HD11	2.03	0.41
1:F:477:GLU:O	1:F:515:SER:CB	2.69	0.41
1:D:597:LEU:O	1:D:598:GLY:C	2.58	0.41
1:E:519:THR:O	1:E:519:THR:OG1	2.39	0.41
1:E:535:TYR:O	1:E:539:ILE:HG12	2.21	0.41
1:C:392:TRP:CE3	1:C:393:LEU:HD23	2.55	0.40
1:F:483:ARG:HG2	1:F:520:TYR:CE1	2.57	0.40
1:B:444:ALA:HB2	1:E:408:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:TYR:CE2	1:B:549:ILE:HG12	2.57	0.40
1:C:380:HIS:CE1	1:C:462:ARG:HD2	2.56	0.40
1:C:378:CYS:HA	1:C:598:GLY:O	2.21	0.40
1:A:441:VAL:HG21	1:A:597:LEU:HD12	2.03	0.40
1:B:481:LYS:HB3	1:B:517:ASP:HB2	2.03	0.40
1:D:439:ARG:HH11	1:D:439:ARG:HG3	1.86	0.40
1:E:459:PRO:O	1:E:503:TRP:HB3	2.21	0.40
1:A:403:TYR:CE1	1:A:414:LEU:HG	2.57	0.40
1:F:525:PRO:HD2	1:F:528:LYS:CB	2.51	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	249/287 (87%)	226 (91%)	23 (9%)	0	100 100
1	B	255/287 (89%)	229 (90%)	26 (10%)	0	100 100
1	C	252/287 (88%)	224 (89%)	23 (9%)	5 (2%)	7 10
1	D	251/287 (88%)	219 (87%)	32 (13%)	0	100 100
1	E	247/287 (86%)	218 (88%)	24 (10%)	5 (2%)	7 10
1	F	249/287 (87%)	212 (85%)	24 (10%)	13 (5%)	2 2
All	All	1503/1722 (87%)	1328 (88%)	152 (10%)	23 (2%)	10 14

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	554	LYS
1	E	611	TRP
1	F	554	LYS

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Mol	Chain	Res	Type
1	E	519	THR
1	F	515	SER
1	F	532	SER
1	F	555	SER
1	C	418	SER
1	E	558	ASN
1	F	491	TRP
1	F	597	LEU
1	C	557	GLY
1	F	479	HIS
1	F	589	GLN
1	C	458	SER
1	C	502	ALA
1	F	466	THR
1	F	564	ALA
1	F	418	SER
1	E	420	GLY
1	F	588	VAL
1	C	615	ASP
1	F	381	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	190/249 (76%)	189 (100%)	1 (0%)	88 94
1	B	192/249 (77%)	190 (99%)	2 (1%)	76 86
1	C	200/249 (80%)	199 (100%)	1 (0%)	88 94
1	D	191/249 (77%)	190 (100%)	1 (0%)	88 94
1	E	162/249 (65%)	161 (99%)	1 (1%)	86 93
1	F	169/249 (68%)	167 (99%)	2 (1%)	71 83
All	All	1104/1494 (74%)	1096 (99%)	8 (1%)	84 91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	456	TYR
1	B	421	PHE
1	B	456	TYR
1	C	460	SER
1	D	600	CYS
1	E	421	PHE
1	F	536	ASP
1	F	599	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	412	HIS
1	B	565	HIS
1	D	395	GLN
1	D	523	HIS
1	F	380	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	VXE	D	701	-	29,29,29	3.02	8 (27%)	36,40,40	2.10	9 (25%)
2	VXE	A	701	-	29,29,29	2.83	8 (27%)	36,40,40	1.75	6 (16%)
2	VXE	C	701	-	29,29,29	3.16	12 (41%)	36,40,40	2.23	10 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VXE	D	701	-	-	2/18/18/18	0/3/3/3
2	VXE	A	701	-	-	1/18/18/18	0/3/3/3
2	VXE	C	701	-	-	2/18/18/18	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	VXE	C02-N03	8.32	1.48	1.37
2	C	701	VXE	C02-N03	8.25	1.47	1.37
2	D	701	VXE	C23-N03	8.10	1.53	1.39
2	A	701	VXE	C02-N03	7.97	1.47	1.37
2	C	701	VXE	C23-N03	7.80	1.53	1.39
2	A	701	VXE	C23-N03	7.77	1.53	1.39
2	D	701	VXE	C09-N08	6.92	1.49	1.34
2	C	701	VXE	C04-C05	6.36	1.48	1.35
2	A	701	VXE	C04-C05	5.54	1.46	1.35
2	D	701	VXE	C04-C05	5.47	1.46	1.35
2	A	701	VXE	C09-N08	5.30	1.45	1.34
2	C	701	VXE	C09-N08	5.21	1.45	1.34
2	C	701	VXE	C22-C05	5.18	1.57	1.46
2	D	701	VXE	C22-C05	4.15	1.55	1.46
2	A	701	VXE	C04-C02	3.85	1.50	1.42
2	A	701	VXE	C22-C05	3.53	1.53	1.46
2	C	701	VXE	O01-C02	-2.99	1.18	1.24
2	C	701	VXE	C04-C02	2.92	1.48	1.42
2	D	701	VXE	O01-C02	-2.70	1.19	1.24
2	C	701	VXE	O18-C09	-2.69	1.17	1.23
2	C	701	VXE	C06-C05	2.63	1.55	1.50
2	D	701	VXE	C10-C09	2.55	1.55	1.50
2	D	701	VXE	C04-C02	2.49	1.47	1.42
2	C	701	VXE	C22-C23	2.36	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	VXE	O21-C19	2.29	1.29	1.22
2	A	701	VXE	O18-C09	-2.29	1.18	1.23
2	C	701	VXE	C26-C25	2.07	1.43	1.38
2	C	701	VXE	O21-C19	2.03	1.28	1.22

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701	VXE	C04-C02-N03	6.30	120.99	115.81
2	A	701	VXE	C23-N03-C02	-5.55	119.00	124.54
2	D	701	VXE	O01-C02-C04	-5.52	117.72	125.47
2	D	701	VXE	C04-C02-N03	5.33	120.19	115.81
2	C	701	VXE	C06-C07-C19	4.96	120.42	110.83
2	A	701	VXE	C04-C02-N03	4.76	119.72	115.81
2	C	701	VXE	O01-C02-C04	-4.71	118.86	125.47
2	C	701	VXE	C23-N03-C02	-4.56	119.99	124.54
2	C	701	VXE	C07-C06-C05	-4.36	105.11	113.48
2	D	701	VXE	C06-C07-N08	-4.24	102.30	110.60
2	D	701	VXE	C23-N03-C02	-3.69	120.86	124.54
2	D	701	VXE	C07-C06-C05	-3.60	106.58	113.48
2	C	701	VXE	C06-C07-N08	-3.46	103.82	110.60
2	A	701	VXE	O01-C02-C04	-3.00	121.26	125.47
2	D	701	VXE	C19-C07-N08	2.89	117.38	110.55
2	A	701	VXE	C06-C07-N08	-2.70	105.31	110.60
2	C	701	VXE	O20-C19-C07	2.54	121.84	113.40
2	D	701	VXE	O20-C19-C07	2.53	121.80	113.40
2	C	701	VXE	O20-C19-O21	-2.50	118.42	124.09
2	A	701	VXE	O20-C19-C07	2.41	121.41	113.40
2	A	701	VXE	C22-C23-N03	2.31	121.31	119.49
2	D	701	VXE	C12-C13-C16	2.26	121.72	118.17
2	C	701	VXE	C10-C09-N08	2.17	121.22	117.06
2	D	701	VXE	C06-C07-C19	2.12	114.93	110.83
2	C	701	VXE	C12-C11-C10	-2.02	118.42	120.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	701	VXE	C05-C06-C07-C19
2	D	701	VXE	C05-C06-C07-N08
2	C	701	VXE	C05-C06-C07-C19
2	C	701	VXE	C05-C06-C07-N08

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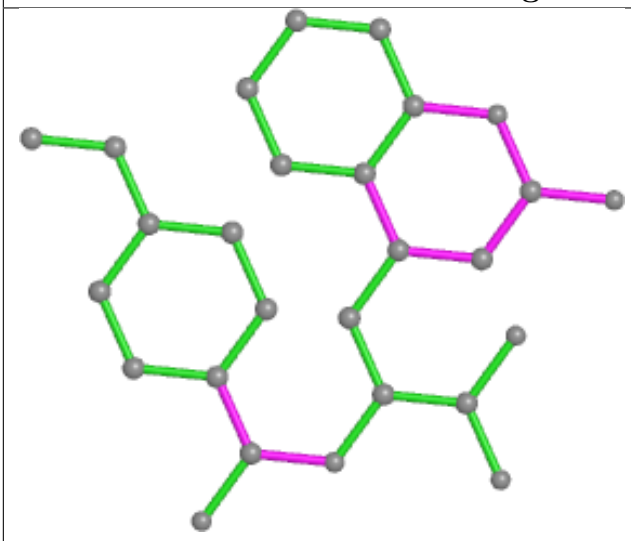
Mol	Chain	Res	Type	Atoms
2	A	701	VXE	C06-C07-C19-O20

There are no ring outliers.

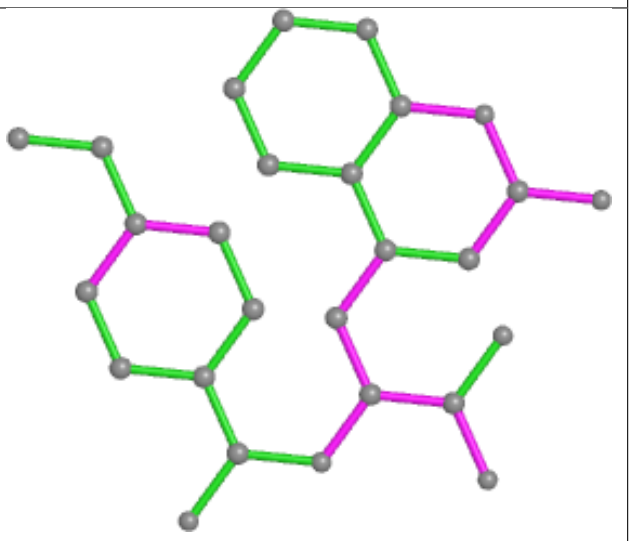
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

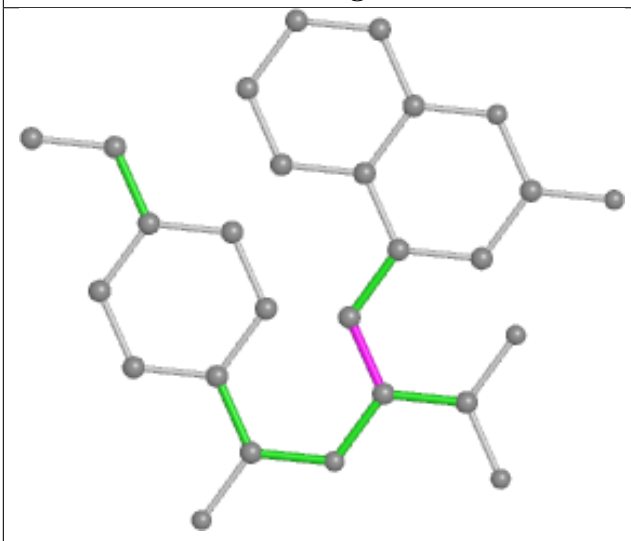
Ligand VXE D 701



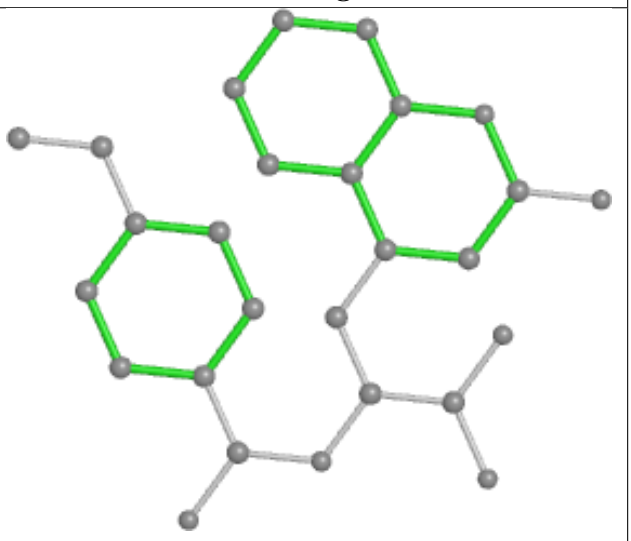
Bond lengths



Bond angles

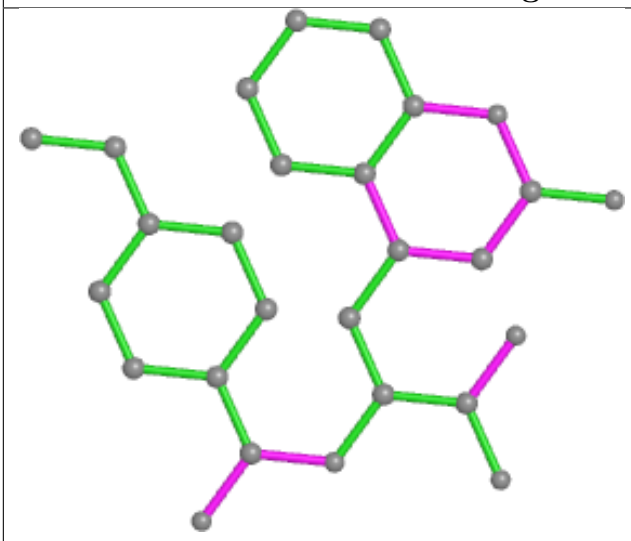


Torsions

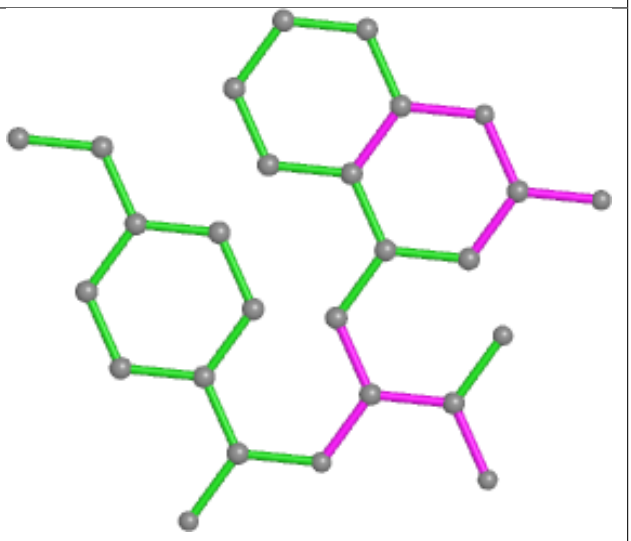


Rings

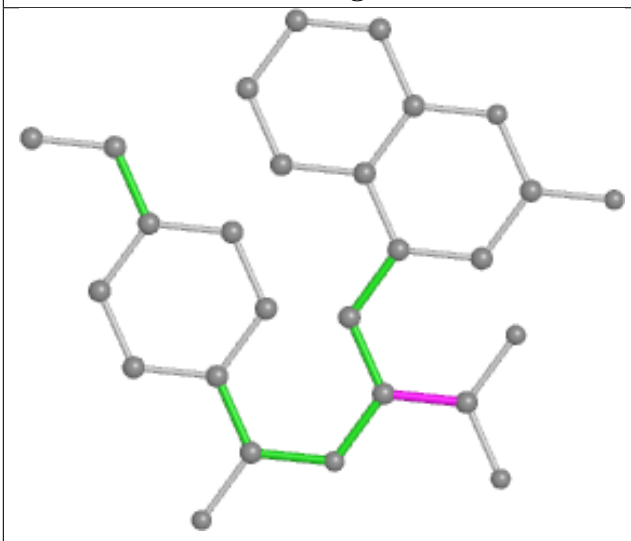
Ligand VXE A 701



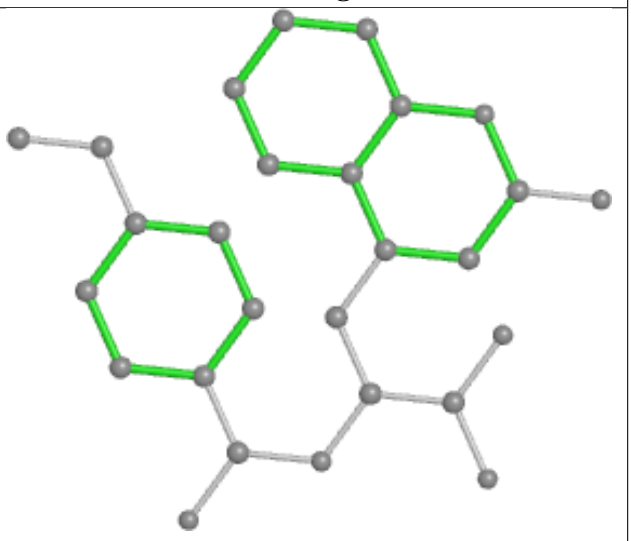
Bond lengths



Bond angles

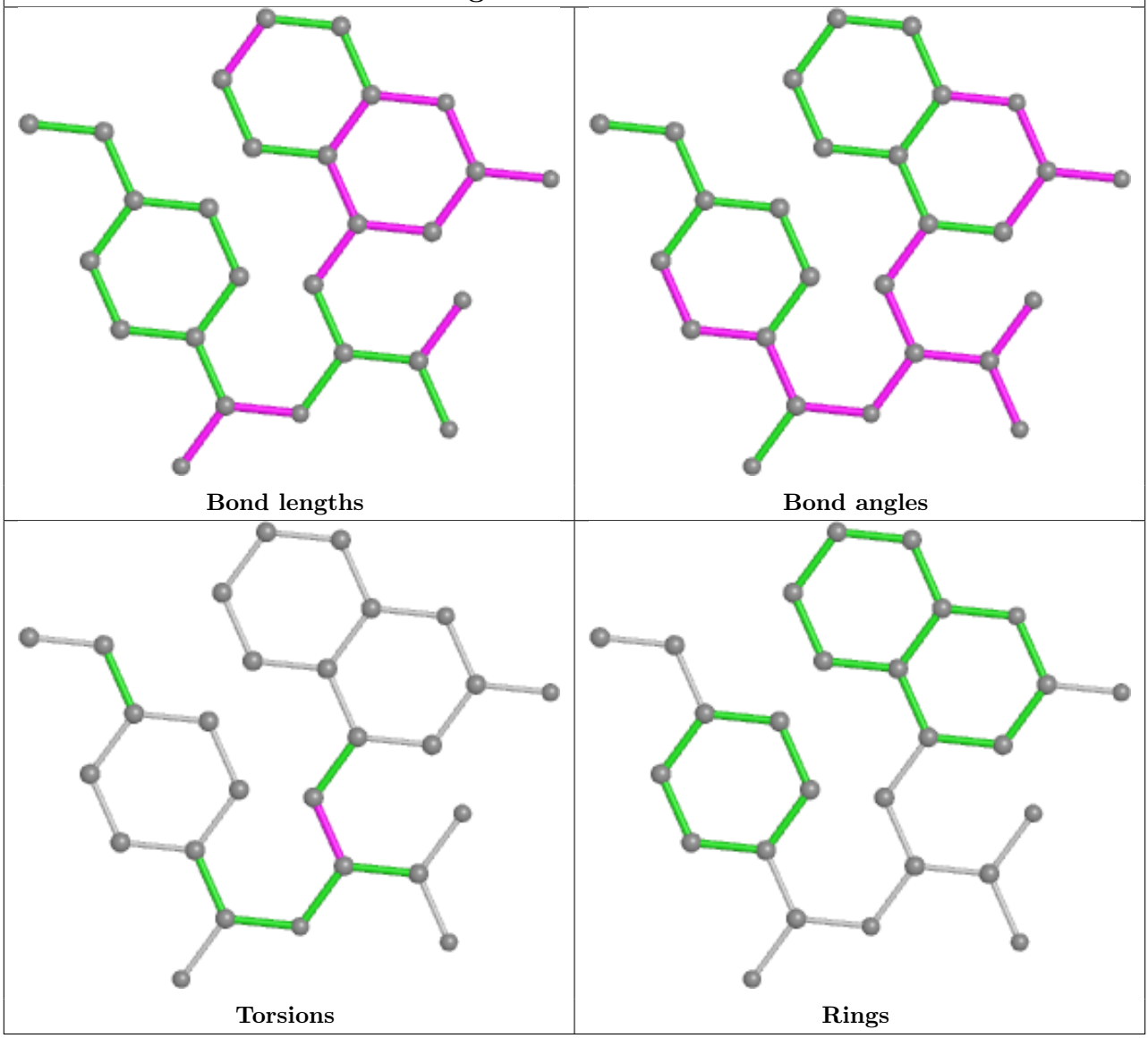


Torsions



Rings

Ligand VXE C 701



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, 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	253/287 (88%)	0.48	11 (4%)	35	31	38, 55, 74, 84	1 (0%)
1	B	257/287 (89%)	0.45	6 (2%)	60	57	40, 59, 80, 92	0
1	C	256/287 (89%)	0.62	12 (4%)	31	27	41, 59, 88, 110	0
1	D	255/287 (88%)	0.53	19 (7%)	14	11	44, 64, 88, 111	0
1	E	253/287 (88%)	0.58	20 (7%)	12	10	51, 87, 117, 142	0
1	F	253/287 (88%)	0.58	17 (6%)	17	15	42, 75, 102, 114	0
All	All	1527/1722 (88%)	0.54	85 (5%)	24	21	38, 63, 100, 142	1 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	557	GLY	7.0
1	D	571	ALA	4.2
1	A	539	ILE	3.9
1	D	557	GLY	3.8
1	E	601	SER	3.7
1	D	512	ALA	3.7
1	B	440	LEU	3.6
1	D	414	LEU	3.6
1	F	433	PHE	3.4
1	E	456	TYR	3.3
1	F	466	THR	3.3
1	A	433	PHE	3.2
1	B	406	THR	3.2
1	A	535	TYR	3.1
1	F	509	LEU	3.1
1	E	611	TRP	3.0
1	E	503	TRP	3.0
1	D	438	ALA	3.0
1	F	550	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	539	ILE	2.9
1	C	507	SER	2.9
1	E	421	PHE	2.9
1	A	546	THR	2.9
1	E	495	VAL	2.9
1	C	517	ASP	2.8
1	A	473	GLY	2.8
1	D	430	ILE	2.8
1	F	607	GLU	2.7
1	F	428	ALA	2.7
1	D	496	ALA	2.7
1	D	471	LEU	2.7
1	A	514	LEU	2.7
1	B	421	PHE	2.7
1	C	452	ILE	2.7
1	E	614	THR	2.6
1	E	399	ALA	2.6
1	F	599	PHE	2.6
1	F	480	LEU	2.6
1	E	438	ALA	2.6
1	D	451	ILE	2.5
1	C	404	ILE	2.5
1	E	612	GLN	2.5
1	E	380	HIS	2.5
1	D	486	PRO	2.5
1	E	514	LEU	2.5
1	E	569	LEU	2.5
1	B	627	GLY	2.4
1	D	482	ILE	2.4
1	A	557	GLY	2.4
1	C	384	MET	2.4
1	E	564	ALA	2.4
1	F	470	ILE	2.4
1	B	403	TYR	2.3
1	A	468	HIS	2.3
1	F	403	TYR	2.3
1	E	480	LEU	2.3
1	F	514	LEU	2.3
1	D	543	PHE	2.3
1	C	614	THR	2.3
1	A	591	VAL	2.3
1	F	492	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	415	PRO	2.2
1	D	440	LEU	2.2
1	A	457	CYS	2.2
1	C	414	LEU	2.2
1	E	535	TYR	2.2
1	D	436	MET	2.2
1	C	562	ILE	2.2
1	E	507	SER	2.2
1	D	378	CYS	2.2
1	F	431	THR	2.2
1	C	395	GLN	2.1
1	C	516	VAL	2.1
1	F	535	TYR	2.1
1	E	518	THR	2.1
1	E	571	ALA	2.1
1	F	613	LEU	2.1
1	B	452	ILE	2.1
1	E	500	LEU	2.1
1	A	403	TYR	2.1
1	D	539	ILE	2.0
1	D	609	GLY	2.0
1	F	621	LEU	2.0
1	D	599	PHE	2.0
1	C	393	LEU	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)

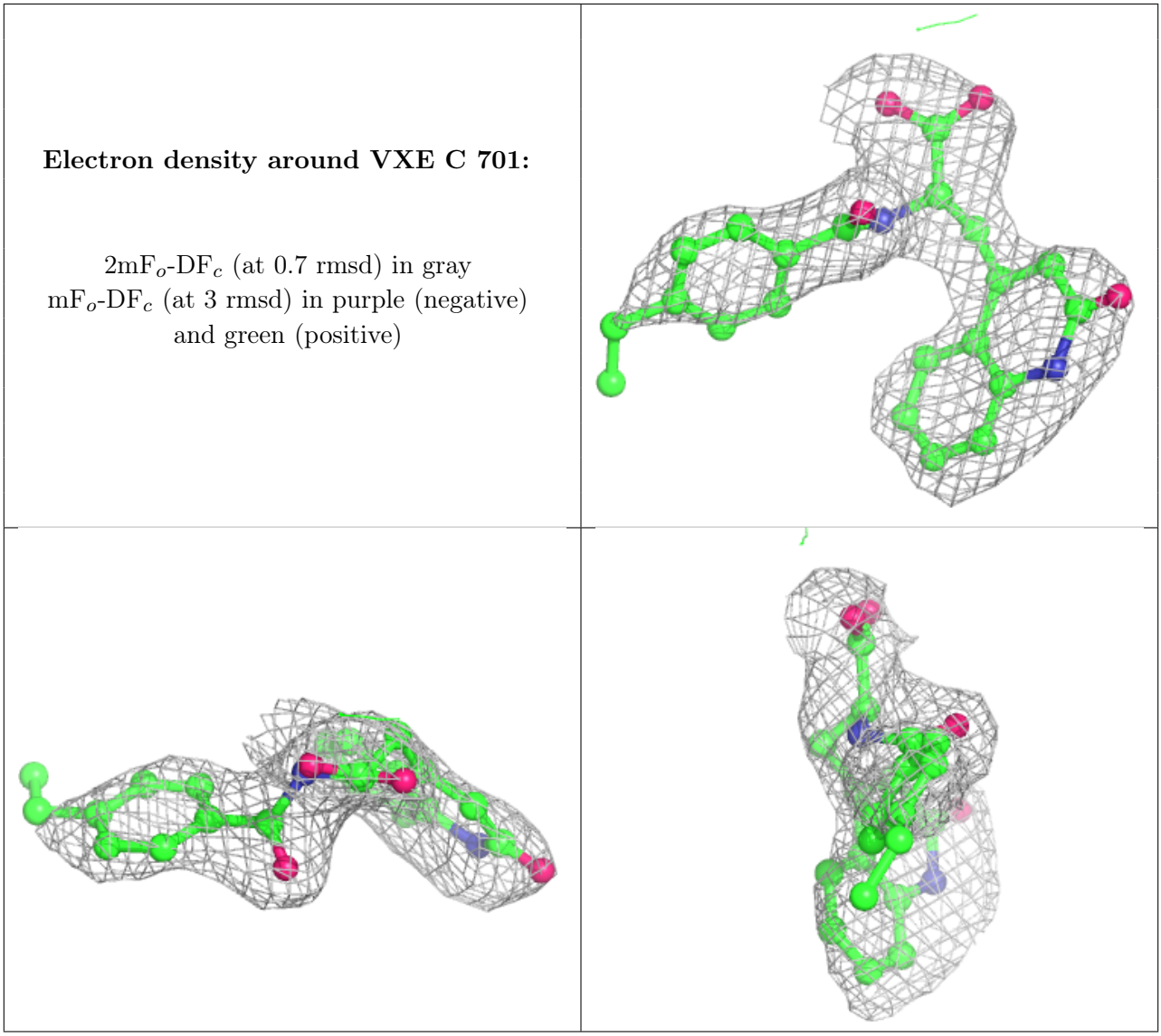
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	VXE	C	701	27/27	0.83	0.36	48,60,73,78	0
2	VXE	A	701	27/27	0.86	0.26	48,59,65,67	0
2	VXE	D	701	27/27	0.86	0.24	60,68,74,81	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

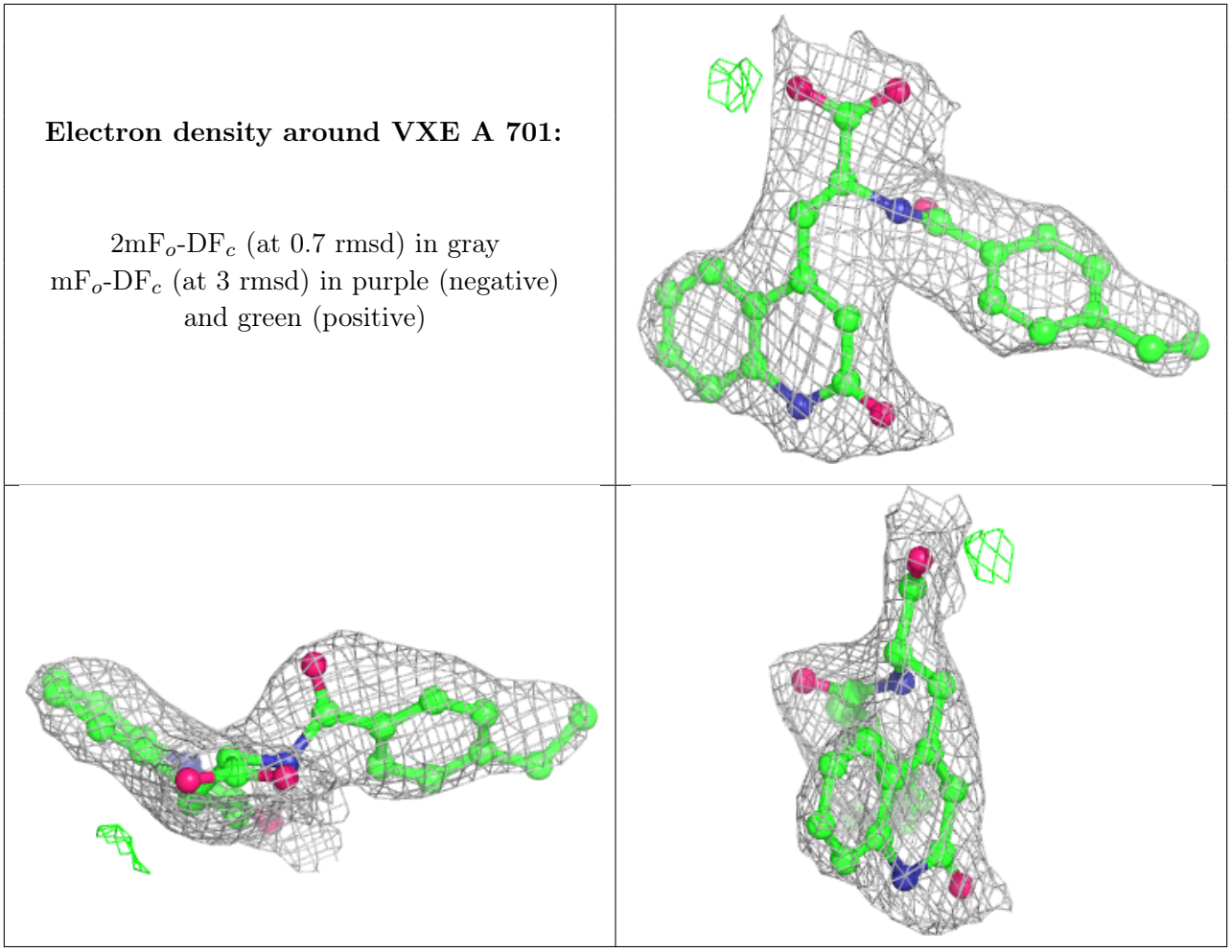
Electron density around VXE C 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



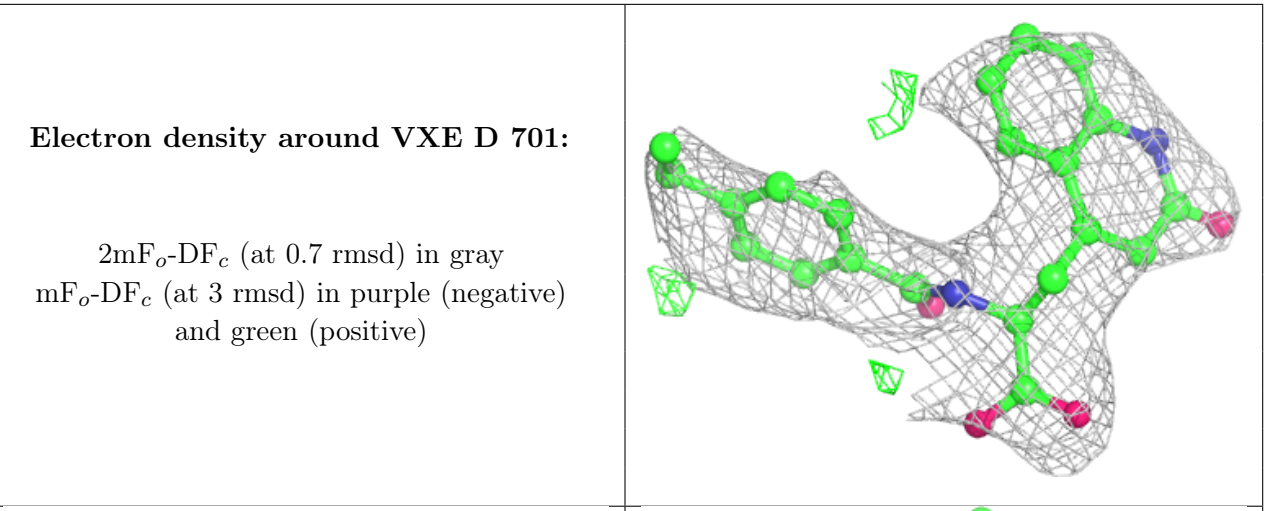
Electron density around VXE A 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around VXE D 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.