



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2023 – 01:17 pm BST

PDB ID : 7Z1X
Title : Crystal structure of human Gasdermin D complexed with nanobodies VHH-2 and VHH-6
Authors : Kopp, A.; Hagelueken, G.; Geyer, M.
Deposited on : 2022-02-25
Resolution : 1.86 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

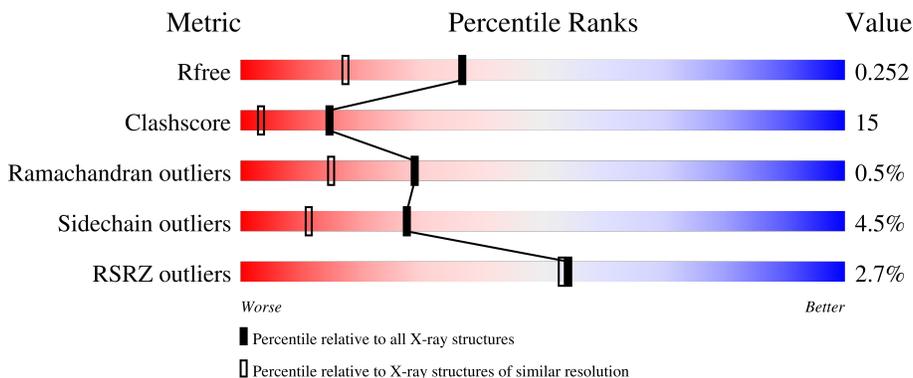
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	447	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 62% 22% 14%</p>
1	D	447	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">4% 63% 22% 13%</p>
2	B	132	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 53%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 53% 33% 13%</p>
2	E	132	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 63% 23% 12%</p>
3	C	141	<div style="display: flex; align-items: center;"> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">71% 15% 13%</p>

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Mol	Chain	Length	Quality of chain
3	F	141	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into three segments: a green segment on the left labeled '69%', a yellow segment in the middle labeled '15%', and a grey segment on the right labeled '13%'. A small red square is positioned at the beginning of the bar, and a small black dot is at the end of the grey segment. A '%' symbol is located above the bar.</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19822 atoms, of which 9559 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 Gasdermin-D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	386	6002	1913	2994	503	580	12	0	1	0
1	D	391	6097	1939	3039	512	593	14	42	6	0

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	deletion	UNP P57764
A	?	-	SER	deletion	UNP P57764
A	?	-	LEU	deletion	UNP P57764
A	?	-	PRO	deletion	UNP P57764
A	?	-	GLY	deletion	UNP P57764
A	?	-	ALA	deletion	UNP P57764
A	?	-	THR	deletion	UNP P57764
A	?	-	CYS	deletion	UNP P57764
A	?	-	LEU	deletion	UNP P57764
A	?	-	GLN	deletion	UNP P57764
A	?	-	GLY	deletion	UNP P57764
A	?	-	HIS	deletion	UNP P57764
A	?	-	LYS	deletion	UNP P57764
A	?	-	ARG	deletion	UNP P57764
A	?	-	SER	deletion	UNP P57764
A	?	-	THR	deletion	UNP P57764
A	?	-	SER	deletion	UNP P57764
A	?	-	GLU	deletion	UNP P57764
A	?	-	GLY	deletion	UNP P57764
A	?	-	ALA	deletion	UNP P57764
A	?	-	TRP	deletion	UNP P57764
A	?	-	PRO	deletion	UNP P57764
A	?	-	GLN	deletion	UNP P57764
A	?	-	LEU	deletion	UNP P57764
A	?	-	PRO	deletion	UNP P57764

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P57764
A	?	-	GLY	deletion	UNP P57764
A	?	-	LEU	deletion	UNP P57764
A	?	-	SER	deletion	UNP P57764
A	?	-	MET	deletion	UNP P57764
A	?	-	MET	deletion	UNP P57764
A	?	-	ARG	deletion	UNP P57764
A	?	-	CYS	deletion	UNP P57764
A	?	-	LEU	deletion	UNP P57764
A	?	-	HIS	deletion	UNP P57764
A	?	-	ASN	deletion	UNP P57764
A	?	-	PHE	deletion	UNP P57764
D	?	-	PHE	deletion	UNP P57764
D	?	-	SER	deletion	UNP P57764
D	?	-	LEU	deletion	UNP P57764
D	?	-	PRO	deletion	UNP P57764
D	?	-	GLY	deletion	UNP P57764
D	?	-	ALA	deletion	UNP P57764
D	?	-	THR	deletion	UNP P57764
D	?	-	CYS	deletion	UNP P57764
D	?	-	LEU	deletion	UNP P57764
D	?	-	GLN	deletion	UNP P57764
D	?	-	GLY	deletion	UNP P57764
D	?	-	HIS	deletion	UNP P57764
D	?	-	LYS	deletion	UNP P57764
D	?	-	ARG	deletion	UNP P57764
D	?	-	SER	deletion	UNP P57764
D	?	-	THR	deletion	UNP P57764
D	?	-	SER	deletion	UNP P57764
D	?	-	GLU	deletion	UNP P57764
D	?	-	GLY	deletion	UNP P57764
D	?	-	ALA	deletion	UNP P57764
D	?	-	TRP	deletion	UNP P57764
D	?	-	PRO	deletion	UNP P57764
D	?	-	GLN	deletion	UNP P57764
D	?	-	LEU	deletion	UNP P57764
D	?	-	PRO	deletion	UNP P57764
D	?	-	SER	deletion	UNP P57764
D	?	-	GLY	deletion	UNP P57764
D	?	-	LEU	deletion	UNP P57764
D	?	-	SER	deletion	UNP P57764
D	?	-	MET	deletion	UNP P57764

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	MET	deletion	UNP P57764
D	?	-	ARG	deletion	UNP P57764
D	?	-	CYS	deletion	UNP P57764
D	?	-	LEU	deletion	UNP P57764
D	?	-	HIS	deletion	UNP P57764
D	?	-	ASN	deletion	UNP P57764
D	?	-	PHE	deletion	UNP P57764

- Molecule 2 is a protein called VHH-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	115	Total	C	H	N	O	S	0	0	0
			1751	555	861	158	174	3			
2	E	116	Total	C	H	N	O	S	0	0	0
			1762	558	866	159	176	3			

- Molecule 3 is a protein called VHH-6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	122	Total	C	H	N	O	S	0	0	0
			1821	574	894	167	180	6			
3	F	122	Total	C	H	N	O	S	0	0	0
			1832	574	905	167	180	6			

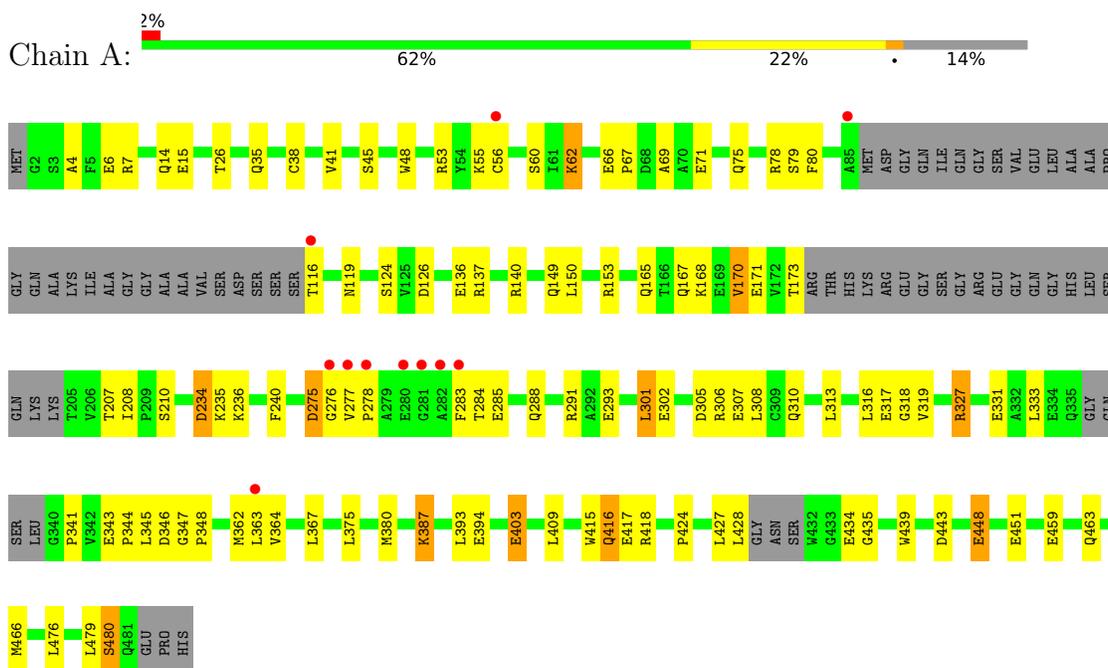
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	162	Total	O	0	0
			162	162		
4	B	43	Total	O	0	0
			43	43		
4	C	70	Total	O	0	0
			70	70		
4	D	153	Total	O	0	0
			153	153		
4	E	47	Total	O	0	0
			47	47		
4	F	82	Total	O	0	0
			82	82		

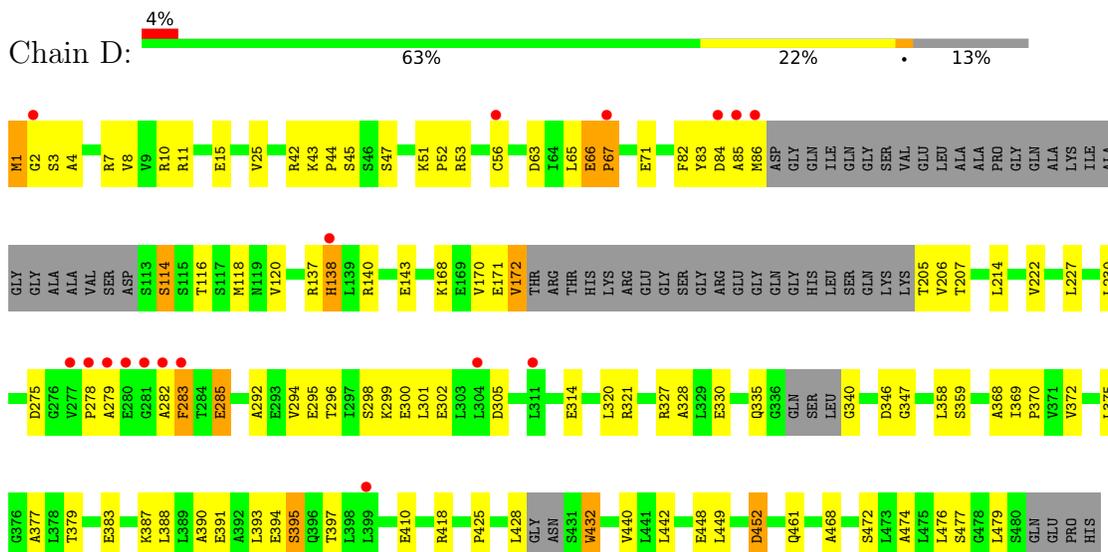
3 Residue-property plots [i](#)

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.

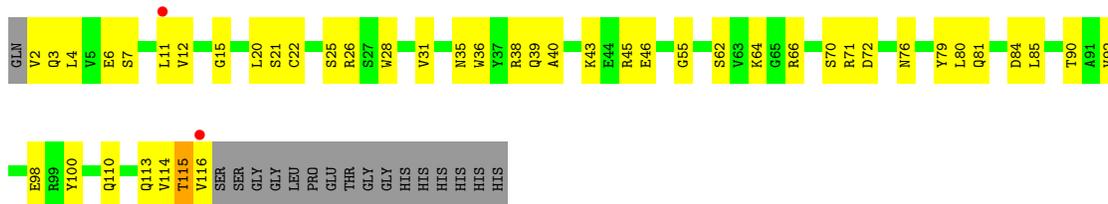
• Molecule 1: Gasdermin-D



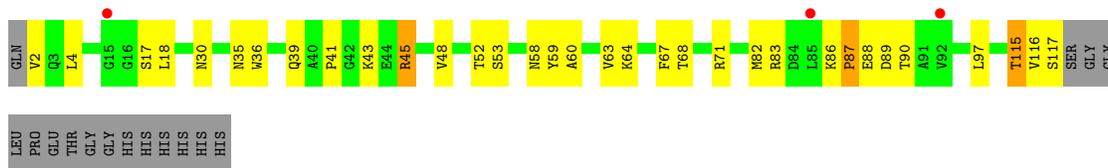
• Molecule 1: Gasdermin-D



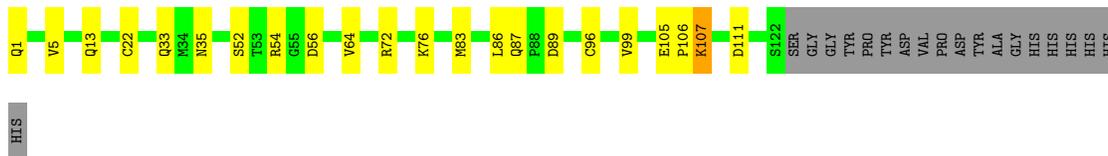
• Molecule 2: VHH-2



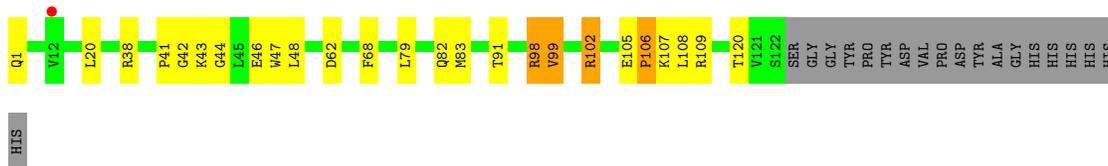
• Molecule 2: VHH-2



• Molecule 3: VHH-6



• Molecule 3: VHH-6



4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	108.35Å 108.35Å 124.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	93.84 – 1.86 93.84 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.0 (93.84-1.86) 89.8 (93.84-1.86)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.27 (at 1.86Å)	Xtrriage
Refinement program	PHENIX (1.20_4444: ???)	Depositor
R, R_{free}	0.212 , 0.249 0.217 , 0.252	Depositor DCC
R_{free} test set	2003 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtrriage
Anisotropy	0.266	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.013 for -h,-k,l 0.488 for h,-h-k,-l 0.014 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19822	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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](#)

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	0.41	0/3068	0.56	0/4176
1	D	0.42	0/3132	0.57	0/4261
2	B	0.41	0/908	0.58	0/1234
2	E	0.41	0/914	0.58	0/1242
3	C	0.50	0/944	0.64	1/1279 (0.1%)
3	F	0.45	0/944	0.62	0/1279
All	All	0.43	0/9910	0.58	1/13471 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	54	ARG	NE-CZ-NH1	-5.48	117.56	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3008	2994	2992	99	0
1	D	3058	3039	3021	98	1
2	B	890	861	861	42	0
2	E	896	866	866	25	1
3	C	927	894	905	23	0
3	F	927	905	905	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	162	0	0	36	2
4	B	43	0	0	13	0
4	C	70	0	0	11	1
4	D	153	0	0	25	0
4	E	47	0	0	13	0
4	F	82	0	0	9	0
All	All	10263	9559	9550	295	3

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.

The worst 5 of 295 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:38:CYS:SG	4:A:590:HOH:O	2.14	1.04
1:D:168:LYS:NZ	4:D:501:HOH:O	1.91	1.04
1:A:116:THR:N	4:A:503:HOH:O	1.90	1.03
3:C:22:CYS:SG	4:C:263:HOH:O	2.15	1.02
2:B:12:VAL:HG23	2:B:116:VAL:HG13	1.41	1.01

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:623:HOH:O	4:C:243:HOH:O[2_655]	1.86	0.34
4:A:569:HOH:O	4:A:620:HOH:O[2_655]	1.90	0.30
1:D:394:GLU:OE2	2:E:83:ARG:NH2[2_655]	1.95	0.25

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	377/447 (84%)	364 (97%)	13 (3%)	0	100	100
1	D	387/447 (87%)	366 (95%)	17 (4%)	4 (1%)	15	5
2	B	113/132 (86%)	109 (96%)	4 (4%)	0	100	100
2	E	114/132 (86%)	111 (97%)	2 (2%)	1 (1%)	17	6
3	C	120/141 (85%)	114 (95%)	5 (4%)	1 (1%)	19	7
3	F	120/141 (85%)	116 (97%)	2 (2%)	2 (2%)	9	2
All	All	1231/1440 (86%)	1180 (96%)	43 (4%)	8 (1%)	29	12

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	106	PRO
3	C	99	VAL
1	D	66[A]	GLU
1	D	66[B]	GLU
3	F	99	VAL

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	334/377 (89%)	315 (94%)	19 (6%)	20	6
1	D	342/377 (91%)	328 (96%)	14 (4%)	30	13
2	B	95/108 (88%)	91 (96%)	4 (4%)	30	13
2	E	96/108 (89%)	90 (94%)	6 (6%)	18	4
3	C	101/116 (87%)	99 (98%)	2 (2%)	55	40
3	F	101/116 (87%)	97 (96%)	4 (4%)	31	14
All	All	1069/1202 (89%)	1020 (95%)	49 (5%)	27	11

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	120	VAL

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Mol	Chain	Res	Type
1	D	395	SER
1	D	138[A]	HIS
1	D	283	PHE
1	D	452	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	463	GLN
1	D	396	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	386/447 (86%)	0.32	11 (2%) 53 52	35, 48, 68, 93	0
1	D	391/447 (87%)	0.32	17 (4%) 35 33	33, 49, 70, 95	0
2	B	115/132 (87%)	0.17	2 (1%) 70 70	39, 51, 67, 70	0
2	E	116/132 (87%)	0.21	3 (2%) 56 54	36, 51, 77, 83	0
3	C	122/141 (86%)	0.11	0 100 100	34, 42, 57, 77	0
3	F	122/141 (86%)	0.08	1 (0%) 86 86	33, 41, 54, 83	0
All	All	1252/1440 (86%)	0.25	34 (2%) 54 53	33, 48, 69, 95	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	GLY	7.5
1	D	278	PRO	7.4
1	D	282	ALA	6.8
1	A	282	ALA	5.3
1	A	277	VAL	5.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.