



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 03:33 PM UTC

PDB ID : 3UDB / pdb_00003udb
Title : Crystal structure of SnRK2.6
Authors : Xie, T.; Ren, R.; Pang, Y.; Yan, C.
Deposited on : 2011-10-27
Resolution : 2.57 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

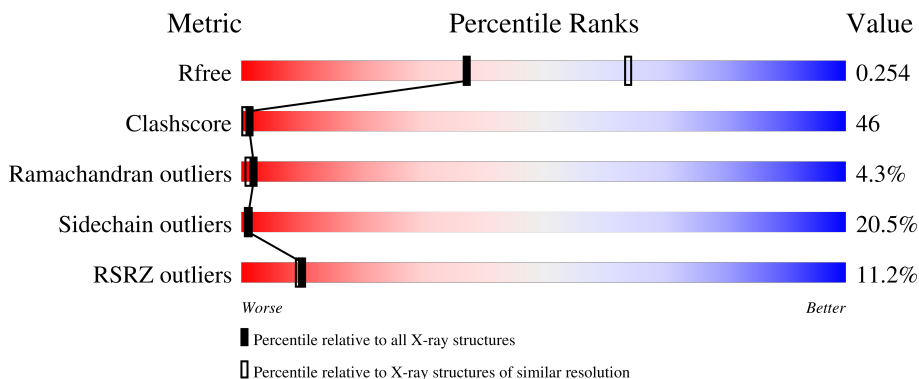
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



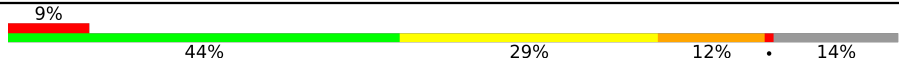
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	317	
1	B	317	
1	C	317	
1	D	317	
1	E	317	

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Mol	Chain	Length	Quality of chain
1	F	317	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into five segments: a red segment (9%), a green segment (44%), a yellow segment (29%), an orange segment (12%), and a grey segment (14%).</p>

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 13176 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 Serine/threonine-protein kinase SRK2E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	Total 2214	C 1418	N 386	O 401	S 9	0	0	0
1	B	278	Total 2245	C 1437	N 394	O 405	S 9	0	1	0
1	C	261	Total 2109	C 1351	N 367	O 381	S 10	0	0	0
1	D	279	Total 2235	C 1428	N 390	O 408	S 9	0	0	0
1	E	255	Total 2036	C 1304	N 360	O 363	S 9	0	0	0
1	F	273	Total 2202	C 1411	N 385	O 397	S 9	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	SER	engineered mutation	UNP Q940H6
A	29	ALA	SER	engineered mutation	UNP Q940H6
A	43	ALA	SER	engineered mutation	UNP Q940H6
A	131	ALA	CYS	engineered mutation	UNP Q940H6
A	137	ALA	CYS	engineered mutation	UNP Q940H6
A	159	ALA	CYS	engineered mutation	UNP Q940H6
A	166	ALA	SER	engineered mutation	UNP Q940H6
A	176	ALA	THR	engineered mutation	UNP Q940H6
B	7	ALA	SER	engineered mutation	UNP Q940H6
B	29	ALA	SER	engineered mutation	UNP Q940H6
B	43	ALA	SER	engineered mutation	UNP Q940H6
B	131	ALA	CYS	engineered mutation	UNP Q940H6
B	137	ALA	CYS	engineered mutation	UNP Q940H6
B	159	ALA	CYS	engineered mutation	UNP Q940H6
B	166	ALA	SER	engineered mutation	UNP Q940H6
B	176	ALA	THR	engineered mutation	UNP Q940H6
C	7	ALA	SER	engineered mutation	UNP Q940H6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	29	ALA	SER	engineered mutation	UNP Q940H6
C	43	ALA	SER	engineered mutation	UNP Q940H6
C	131	ALA	CYS	engineered mutation	UNP Q940H6
C	137	ALA	CYS	engineered mutation	UNP Q940H6
C	159	ALA	CYS	engineered mutation	UNP Q940H6
C	166	ALA	SER	engineered mutation	UNP Q940H6
C	176	ALA	THR	engineered mutation	UNP Q940H6
D	7	ALA	SER	engineered mutation	UNP Q940H6
D	29	ALA	SER	engineered mutation	UNP Q940H6
D	43	ALA	SER	engineered mutation	UNP Q940H6
D	131	ALA	CYS	engineered mutation	UNP Q940H6
D	137	ALA	CYS	engineered mutation	UNP Q940H6
D	159	ALA	CYS	engineered mutation	UNP Q940H6
D	166	ALA	SER	engineered mutation	UNP Q940H6
D	176	ALA	THR	engineered mutation	UNP Q940H6
E	7	ALA	SER	engineered mutation	UNP Q940H6
E	29	ALA	SER	engineered mutation	UNP Q940H6
E	43	ALA	SER	engineered mutation	UNP Q940H6
E	131	ALA	CYS	engineered mutation	UNP Q940H6
E	137	ALA	CYS	engineered mutation	UNP Q940H6
E	159	ALA	CYS	engineered mutation	UNP Q940H6
E	166	ALA	SER	engineered mutation	UNP Q940H6
E	176	ALA	THR	engineered mutation	UNP Q940H6
F	7	ALA	SER	engineered mutation	UNP Q940H6
F	29	ALA	SER	engineered mutation	UNP Q940H6
F	43	ALA	SER	engineered mutation	UNP Q940H6
F	131	ALA	CYS	engineered mutation	UNP Q940H6
F	137	ALA	CYS	engineered mutation	UNP Q940H6
F	159	ALA	CYS	engineered mutation	UNP Q940H6
F	166	ALA	SER	engineered mutation	UNP Q940H6
F	176	ALA	THR	engineered mutation	UNP Q940H6

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total 1	Cl 1	0	0
2	F	1	Total 1	Cl 1	0	0

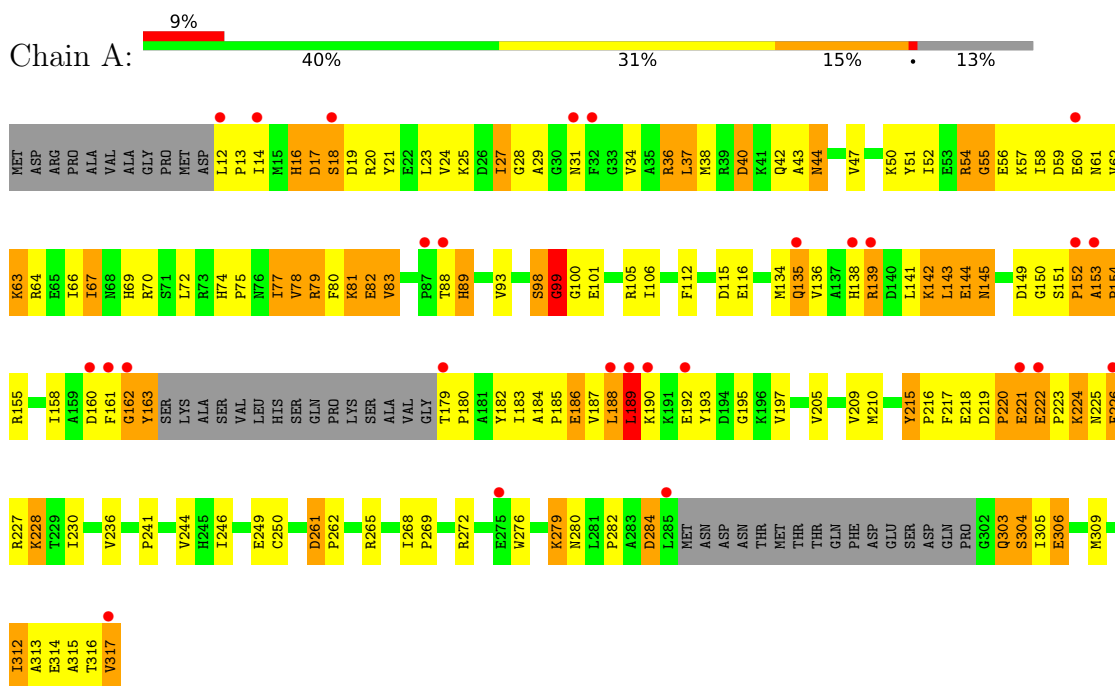
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total 14	O 14	0	0
3	B	32	Total 32	O 32	0	0
3	C	32	Total 32	O 32	0	0
3	D	20	Total 20	O 20	0	0
3	E	13	Total 13	O 13	0	0
3	F	18	Total 18	O 18	0	0

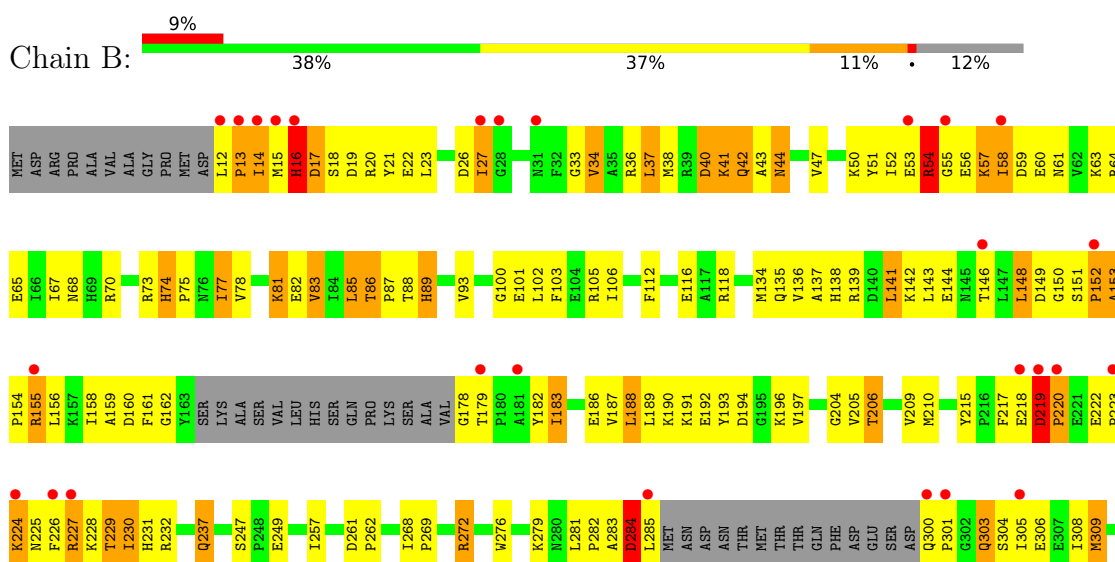
3 Residue-property plots [i](#)

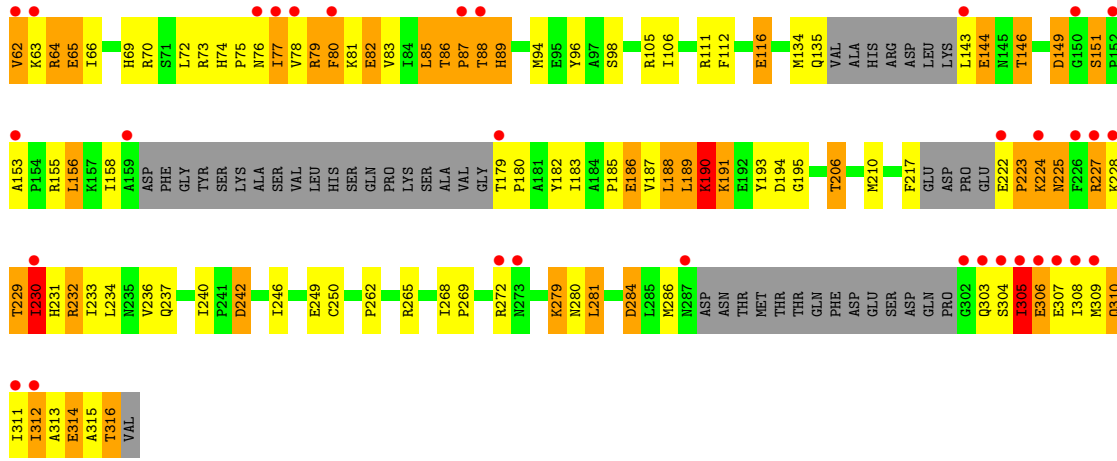
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Serine/threonine-protein kinase SRK2E

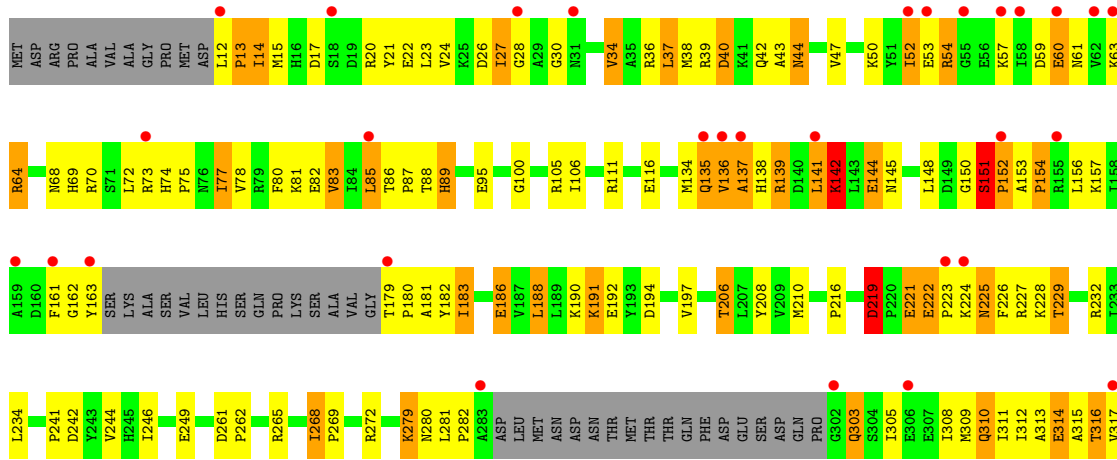


- Molecule 1: Serine/threonine-protein kinase SRK2E





● Molecule 1: Serine/threonine-protein kinase SRK2E



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	228.09Å 98.79Å 113.10Å 90.00° 98.48° 90.00°	Depositor
Resolution (Å)	37.08 – 2.57 37.08 – 2.57	Depositor EDS
% Data completeness (in resolution range)	98.4 (37.08-2.57) 98.2 (37.08-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.58Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.236 , 0.259 0.230 , 0.254	Depositor DCC
R_{free} test set	3933 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtrriage
Anisotropy	0.371	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13176	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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

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	0.61	0/2263	1.00	11/3062 (0.4%)
1	B	0.60	0/2295	0.94	10/3104 (0.3%)
1	C	0.69	0/2150	0.97	7/2901 (0.2%)
1	D	0.71	2/2285 (0.1%)	1.06	13/3093 (0.4%)
1	E	0.58	0/2077	1.07	10/2805 (0.4%)
1	F	0.65	2/2251 (0.1%)	0.99	6/3044 (0.2%)
All	All	0.64	4/13321 (0.0%)	1.01	57/18009 (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	D	0	1
1	E	0	4
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	282	PRO	CA-C	7.73	1.63	1.52
1	D	218	GLU	CA-C	-5.66	1.45	1.52
1	F	145	ASN	CA-C	-5.54	1.47	1.53
1	F	145	ASN	CA-CB	-5.04	1.49	1.53

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	219	ASP	N-CA-CB	-14.10	89.42	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	219	ASP	N-CA-C	-13.88	87.95	109.04
1	E	53	GLU	CB-CA-C	-13.70	87.65	109.70
1	D	39	ARG	NE-CZ-NH2	12.73	130.65	119.20
1	E	53	GLU	N-CA-C	12.44	127.78	110.24

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	281	LEU	Mainchain
1	E	57	LYS	Peptide
1	E	59	ASP	Peptide,Mainchain
1	E	87	PRO	Peptide

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	2214	0	2210	210	0
1	B	2245	0	2243	211	0
1	C	2109	0	2128	202	0
1	D	2235	0	2212	227	0
1	E	2036	0	2035	222	1
1	F	2202	0	2206	157	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	14	0	0	1	0
3	B	32	0	0	5	1
3	C	32	0	0	3	0
3	D	20	0	0	4	0
3	E	13	0	0	2	0
3	F	18	0	0	5	0
All	All	13176	0	13034	1203	1

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 46.

The worst 5 of 1203 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:E:88:THR:CG2	1:E:89:HIS:HD2	1.03	1.62
1:C:126:SER:CB	1:C:286:MET:CE	1.74	1.60
1:E:88:THR:HG23	1:E:89:HIS:CD2	1.05	1.54
1:C:126:SER:HB2	1:C:286:MET:CE	0.98	1.43
1:A:88:THR:HG23	1:A:89:HIS:CD2	1.55	1.41

All (1) 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)
1:E:111:ARG:NH2	3:B:324:HOH:O[2_556]	2.16	0.04

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	269/317 (85%)	232 (86%)	24 (9%)	13 (5%)	2	1
1	B	273/317 (86%)	229 (84%)	31 (11%)	13 (5%)	2	1
1	C	249/317 (78%)	220 (88%)	22 (9%)	7 (3%)	4	3
1	D	273/317 (86%)	233 (85%)	28 (10%)	12 (4%)	2	1
1	E	243/317 (77%)	203 (84%)	26 (11%)	14 (6%)	1	0
1	F	267/317 (84%)	229 (86%)	29 (11%)	9 (3%)	3	2
All	All	1574/1902 (83%)	1346 (86%)	160 (10%)	68 (4%)	2	1

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	GLY
1	A	221	GLU
1	B	13	PRO
1	B	42	GLN
1	B	152	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	237/274 (86%)	187 (79%)	50 (21%)	1	1
1	B	240/274 (88%)	192 (80%)	48 (20%)	1	1
1	C	229/274 (84%)	186 (81%)	43 (19%)	1	1
1	D	238/274 (87%)	191 (80%)	47 (20%)	1	1
1	E	216/274 (79%)	164 (76%)	52 (24%)	1	0
1	F	236/274 (86%)	189 (80%)	47 (20%)	1	1
All	All	1396/1644 (85%)	1109 (79%)	287 (21%)	1	1

5 of 287 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	232	ARG
1	F	316	THR
1	E	305	ILE
1	F	89	HIS
1	B	309	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	237	GLN
1	F	303	GLN
1	E	303	GLN
1	F	225	ASN

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Mol	Chain	Res	Type
1	B	235	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	275/317 (86%)	0.56	27 (9%) 13 13	30, 53, 102, 178	0
1	B	278/317 (87%)	0.53	27 (9%) 13 13	27, 53, 103, 134	1 (0%)
1	C	261/317 (82%)	0.50	24 (9%) 14 14	26, 50, 100, 121	0
1	D	279/317 (88%)	0.72	29 (10%) 11 12	31, 58, 105, 158	0
1	E	255/317 (80%)	1.00	45 (17%) 4 3	32, 63, 118, 161	0
1	F	273/317 (86%)	0.58	30 (10%) 10 10	31, 55, 106, 128	0
All	All	1621/1902 (85%)	0.64	182 (11%) 10 9	26, 55, 106, 178	1 (0%)

The worst 5 of 182 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	143	LEU	8.8
1	D	283	ALA	6.5
1	A	161	PHE	5.6
1	A	189	LEU	5.5
1	D	161	PHE	4.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	F	318	1/1	0.80	0.25	88,88,88,88	0
2	CL	E	318	1/1	0.87	0.19	86,86,86,86	0
2	CL	D	318	1/1	0.87	0.24	91,91,91,91	0
2	CL	A	318	1/1	0.88	0.15	83,83,83,83	0
2	CL	C	318	1/1	0.89	0.23	86,86,86,86	0
2	CL	B	318	1/1	0.91	0.15	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.