



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:54 AM GMT

PDB ID : 3UDB
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 full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

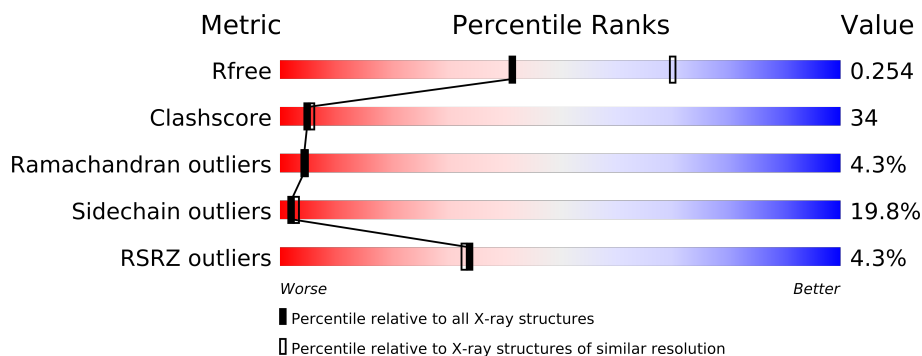
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2347 (2.60-2.52)
Clashscore	79885	2876 (2.60-2.52)
Ramachandran outliers	78287	2826 (2.60-2.52)
Sidechain outliers	78261	2826 (2.60-2.52)
RSRZ outliers	66119	2347 (2.60-2.52)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	317	
1	B	317	
1	C	317	
1	D	317	
1	E	317	
1	F	317	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CL	C	318	-	X
2	CL	F	318	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13176 atoms, of which 0 are hydrogen and 0 are deuterium.

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-proteinkinase SRK2E.

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

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 (three-letter code: CL) (formula: Cl).

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

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

- Molecule 3 is water.

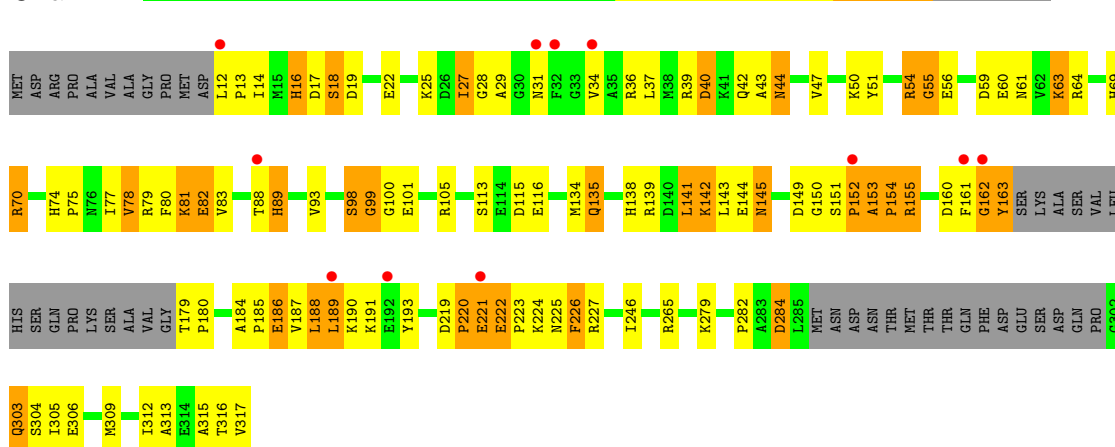
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total 14	O 14	0	0
3	B	32	Total 32	O 32	0	0
3	C	32	Total 32	O 32	0	0
3	D	20	Total 20	O 20	0	0
3	E	13	Total 13	O 13	0	0
3	F	18	Total 18	O 18	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

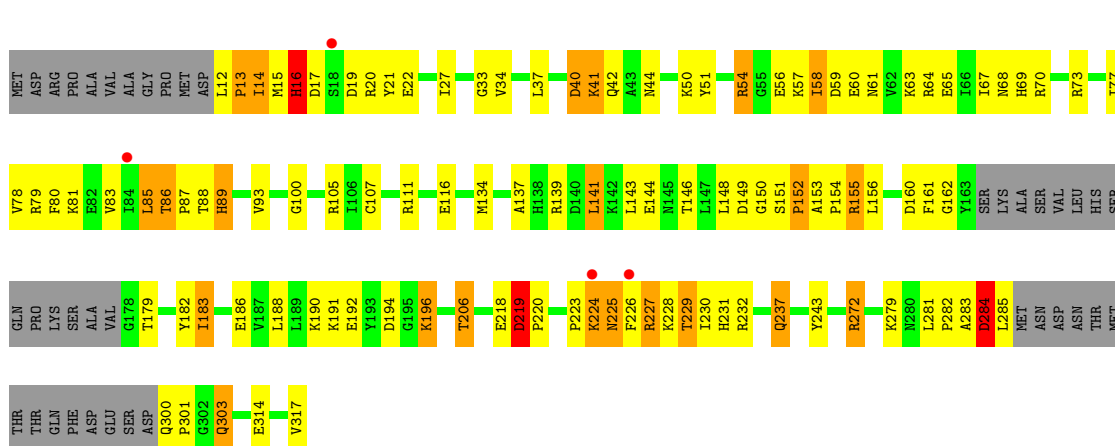
• Molecule 1: Serine/threonine-proteinkinase SRK2E

Chain A:



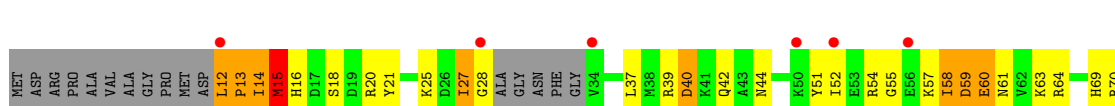
• Molecule 1: Serine/threonine-proteinkinase SRK2E

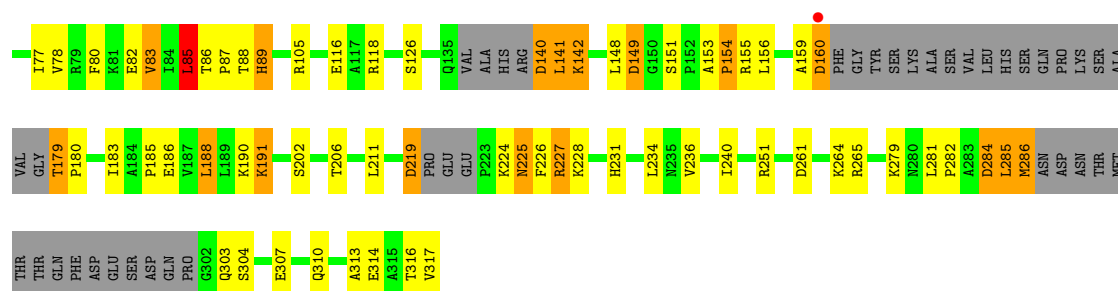
Chain B:



• Molecule 1: Serine/threonine-proteinkinase SRK2E

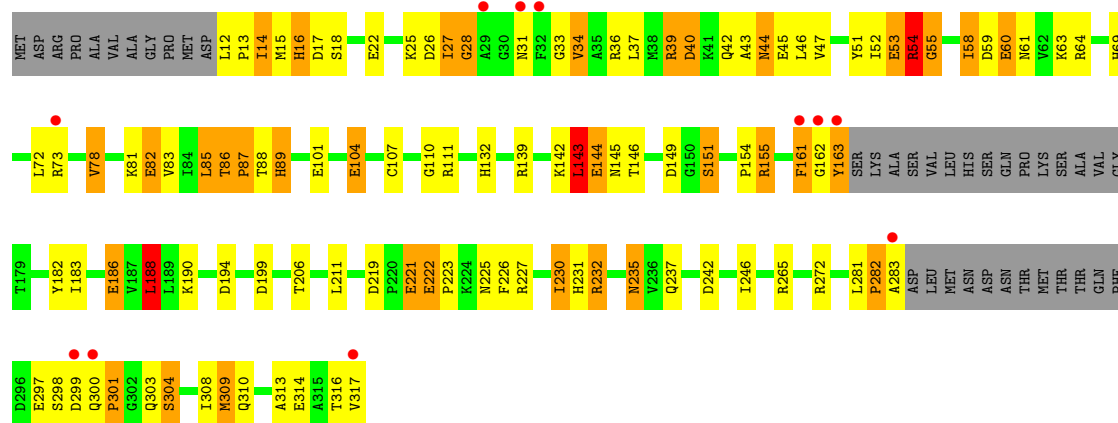
Chain C:





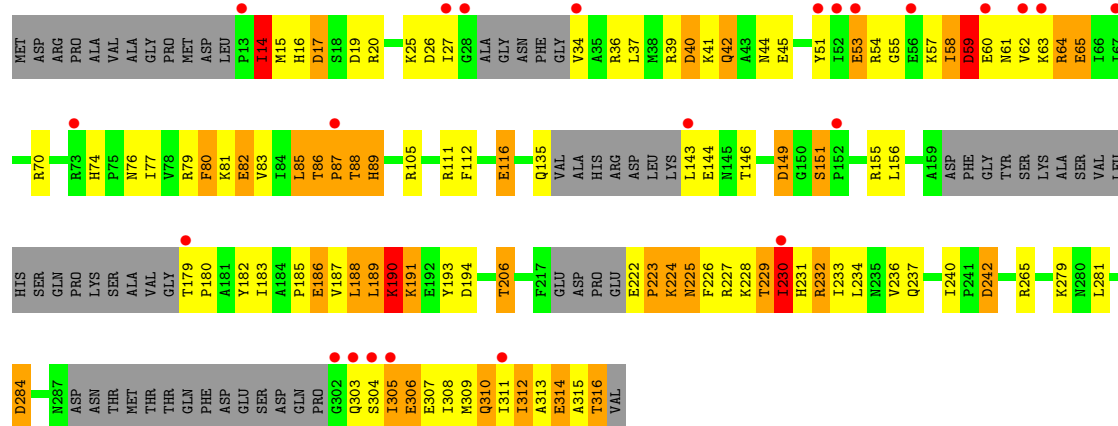
• Molecule 1: Serine/threonine-proteinkinase SRK2E

Chain D:



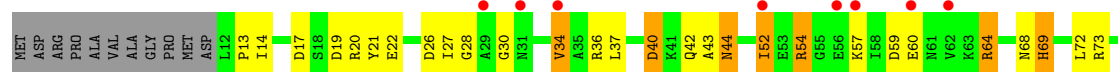
• Molecule 1: Serine/threonine-proteinkinase SRK2E

Chain E:



• Molecule 1: Serine/threonine-proteinkinase SRK2E

Chain F:





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) 98.3 (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)	Xtriage
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	3923 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 31.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 78264 reflections	Xtriage
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

Xtriage'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.

5 Model quality

5.1 Standard geometry

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	0.47	0/2263	0.67	6/3062 (0.2%)
1	B	0.48	1/2295 (0.0%)	0.61	5/3104 (0.2%)
1	C	0.56	0/2150	0.69	6/2901 (0.2%)
1	D	0.56	2/2285 (0.1%)	0.89	8/3093 (0.3%)
1	E	0.46	0/2077	0.73	7/2805 (0.2%)
1	F	0.51	0/2251	0.69	5/3044 (0.2%)
All	All	0.51	3/13321 (0.0%)	0.72	37/18009 (0.2%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	107	CYS	CB-SG	-5.66	1.72	1.81
1	D	282	PRO	CA-C	5.27	1.63	1.52
1	B	107	CYS	CB-SG	-5.12	1.73	1.81

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	39	ARG	NE-CZ-NH1	-21.76	109.42	120.30
1	D	39	ARG	NE-CZ-NH2	20.71	130.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	219	ASP	N-CA-CB	-11.77	89.42	110.60
1	E	53	GLU	CB-CA-C	-11.38	87.65	110.40
1	D	39	ARG	CD-NE-CZ	10.36	138.11	123.60
1	E	59	ASP	CB-CA-C	-9.35	91.70	110.40
1	A	18	SER	CB-CA-C	9.34	127.85	110.10
1	C	59	ASP	CB-CA-C	-9.11	92.17	110.40
1	A	16	HIS	CB-CA-C	-8.95	92.50	110.40
1	F	219	ASP	N-CA-C	-8.54	87.95	111.00
1	E	87	PRO	CB-CA-C	8.36	132.91	112.00
1	C	285	LEU	CB-CA-C	-7.73	95.51	110.20
1	C	85	LEU	CA-CB-CG	7.26	132.00	115.30
1	F	85	LEU	CA-CB-CG	7.03	131.46	115.30
1	D	85	LEU	CA-CB-CG	6.94	131.26	115.30
1	B	17	ASP	CB-CA-C	-6.91	96.58	110.40
1	D	16	HIS	CB-CA-C	-6.71	96.98	110.40
1	E	85	LEU	CA-CB-CG	6.62	130.52	115.30
1	B	16	HIS	CB-CA-C	-6.54	97.31	110.40
1	E	53	GLU	N-CA-C	6.21	127.78	111.00
1	D	188	LEU	CA-CB-CG	6.15	129.44	115.30
1	F	135	GLN	CB-CA-C	5.96	122.32	110.40
1	D	282	PRO	CA-C-N	5.92	130.21	117.20
1	C	151	SER	CB-CA-C	5.73	120.98	110.10
1	C	39	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	39	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	E	59	ASP	C-N-CA	5.57	135.62	121.70
1	A	282	PRO	CB-CA-C	-5.56	98.09	112.00
1	A	99	GLY	N-CA-C	5.52	126.90	113.10
1	F	30	GLY	N-CA-C	-5.46	99.46	113.10
1	A	141	LEU	CB-CA-C	5.40	120.46	110.20
1	A	150	GLY	N-CA-C	5.30	126.35	113.10
1	B	137	ALA	N-CA-C	-5.15	97.10	111.00
1	E	86	THR	CB-CA-C	5.11	125.41	111.60
1	D	282	PRO	C-N-CA	5.10	134.46	121.70
1	B	150	GLY	N-CA-C	5.10	125.85	113.10
1	B	284	ASP	N-CA-C	5.07	124.68	111.00

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

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Mol	Chain	Res	Type	Group
1	E	59	ASP	Mainchain,Peptide
1	E	87	PRO	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2214	0	0	78	0
1	B	2245	0	0	76	0
1	C	2109	0	0	72	0
1	D	2235	0	0	81	0
1	E	2036	0	14	97	1
1	F	2202	0	2	50	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	3	0
3	B	32	0	0	7	1
3	C	32	0	0	3	0
3	D	20	0	0	5	0
3	E	13	0	0	3	0
3	F	18	0	0	3	0
All	All	13176	0	16	447	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 34.

All (447) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:126:SER:CB	1:C:286:MET:CE	1.74	1.60
1:E:88:THR:CG2	1:E:89:HIS:CD2	1.86	1.56
1:B:61:ASN:OD1	1:B:64:ARG:NH2	1.59	1.35

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:14:ILE:O	1:E:36:ARG:NH2	1.73	1.22
1:F:68:ASN:OD1	1:F:139:ARG:NH1	1.79	1.15
1:A:88:THR:CG2	1:A:89:HIS:CD2	2.30	1.15
1:C:284:ASP:OD2	3:C:326:HOH:O	1.61	1.14
1:B:88:THR:CG2	1:B:89:HIS:CD2	2.30	1.14
1:B:146:THR:CG2	1:B:156:LEU:CD1	2.27	1.10
1:A:101:GLU:OE2	1:A:145:ASN:ND2	1.86	1.08
1:E:16:HIS:NE2	1:E:51:TYR:OH	1.88	1.07
1:E:82:GLU:CG	1:E:303:GLN:NE2	2.16	1.06
1:E:310:GLN:O	1:E:314:GLU:CB	2.02	1.06
1:F:313:ALA:O	1:F:316:THR:OG1	1.72	1.05
1:A:88:THR:C	1:A:89:HIS:CD2	2.30	1.05
1:D:88:THR:CG2	1:D:89:HIS:CD2	2.40	1.05
1:A:225:ASN:OD1	1:A:226:PHE:N	1.89	1.05
1:C:126:SER:CA	1:C:286:MET:CE	2.36	1.03
1:D:231:HIS:O	1:D:235:ASN:OD1	1.76	1.02
1:F:310:GLN:NE2	1:F:314:GLU:OE2	1.93	1.01
1:A:40:ASP:OD2	1:A:42:GLN:O	1.78	1.01
1:C:88:THR:CG2	1:C:89:HIS:NE2	2.24	1.01
1:B:152:PRO:O	1:B:154:PRO:CD	2.09	1.00
1:C:140:ASP:C	1:C:141:LEU:CD1	2.30	1.00
1:A:70:ARG:NH2	1:A:303:GLN:O	1.96	0.99
1:A:60:GLU:OE2	1:A:63:LYS:NZ	1.97	0.97
1:D:300:GLN:CB	1:D:301:PRO:CA	2.44	0.95
1:B:300:GLN:N	1:B:301:PRO:CD	2.30	0.95
1:F:141:LEU:N	1:F:141:LEU:CD1	2.30	0.95
1:C:142:LYS:CE	1:C:159:ALA:O	2.15	0.94
1:A:188:LEU:N	1:A:188:LEU:CD1	2.30	0.94
1:D:88:THR:CG2	1:D:89:HIS:NE2	2.30	0.93
1:C:142:LYS:N	1:C:142:LYS:CD	2.30	0.93
1:E:191:LYS:NZ	1:E:191:LYS:CB	2.30	0.92
1:B:20:ARG:O	1:B:41:LYS:CG	2.18	0.92
1:E:14:ILE:CG2	1:E:15:MET:N	2.30	0.92
1:A:16:HIS:NE2	1:A:51:TYR:OH	2.03	0.92
1:A:12:LEU:CD2	1:A:13:PRO:CD	2.48	0.92
1:E:82:GLU:CG	1:E:303:GLN:HE22	1.82	0.91
1:E:82:GLU:CB	1:E:303:GLN:NE2	2.34	0.90
1:C:16:HIS:CE1	1:C:51:TYR:OH	2.24	0.90
1:D:219:ASP:OD2	1:D:221:GLU:CG	2.19	0.89
1:C:88:THR:CG2	1:C:89:HIS:CD2	2.55	0.89
1:D:82:GLU:CB	1:D:303:GLN:NE2	2.37	0.88
1:E:54:ARG:NH2	1:E:86:THR:O	2.07	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:12:LEU:N	1:D:13:PRO:CD	2.37	0.87
1:B:314:GLU:OE1	3:B:347:HOH:O	1.93	0.86
1:B:225:ASN:ND2	1:B:226:PHE:N	2.22	0.86
1:C:83:VAL:N	1:C:303:GLN:NE2	2.24	0.85
1:B:219:ASP:OD2	1:B:232:ARG:NE	2.10	0.85
1:D:72:LEU:O	3:D:325:HOH:O	1.94	0.85
1:A:60:GLU:CD	1:A:63:LYS:NZ	2.30	0.85
1:E:80:PHE:O	1:E:80:PHE:CD2	2.30	0.85
1:E:70:ARG:CG	1:E:80:PHE:CE2	2.59	0.85
1:A:88:THR:CB	1:A:89:HIS:CD2	2.59	0.85
1:F:88:THR:C	1:F:89:HIS:CD2	2.51	0.84
1:F:100:GLY:N	3:F:319:HOH:O	2.09	0.84
1:C:211:LEU:O	3:C:323:HOH:O	1.96	0.83
1:C:13:PRO:CG	1:C:89:HIS:NE2	2.41	0.83
1:D:52:ILE:O	1:D:89:HIS:CB	2.26	0.83
1:A:187:VAL:O	1:C:227:ARG:NE	2.11	0.83
1:D:282:PRO:CB	1:D:283:ALA:CB	2.57	0.82
1:A:219:ASP:OD1	1:A:220:PRO:CD	2.28	0.82
1:D:162:GLY:O	1:D:163:TYR:O	1.98	0.81
1:E:227:ARG:NH1	3:E:319:HOH:O	2.11	0.81
1:C:27:ILE:CB	1:C:28:GLY:CA	2.59	0.81
1:E:59:ASP:C	1:E:59:ASP:OD2	2.19	0.81
1:B:85:LEU:CD1	1:B:85:LEU:C	2.50	0.80
1:E:61:ASN:O	1:E:64:ARG:CD	2.30	0.80
1:D:303:GLN:O	1:D:304:SER:O	2.00	0.80
1:D:78:VAL:CG1	1:D:78:VAL:O	2.30	0.80
1:E:58:ILE:CG2	1:E:58:ILE:O	2.30	0.80
1:D:89:HIS:CD2	1:D:89:HIS:N	2.49	0.80
1:D:27:ILE:CG2	1:D:28:GLY:N	2.45	0.79
1:A:88:THR:OG1	1:A:89:HIS:CD2	2.36	0.79
1:E:313:ALA:CA	1:E:316:THR:OG1	2.30	0.79
1:F:317:VAL:O	1:F:317:VAL:CG1	2.30	0.79
1:B:139:ARG:NH1	1:B:160:ASP:OD2	2.16	0.78
1:C:140:ASP:O	1:C:141:LEU:CD1	2.30	0.78
1:B:58:ILE:CG2	1:B:58:ILE:O	2.30	0.78
1:F:221:GLU:CA	1:F:221:GLU:OE1	2.30	0.78
1:D:63:LYS:CD	1:D:309:MET:CE	2.61	0.78
1:A:88:THR:O	1:A:89:HIS:CD2	2.37	0.78
1:F:310:GLN:OE1	1:F:310:GLN:CA	2.31	0.78
1:F:135:GLN:CA	1:F:135:GLN:OE1	2.30	0.77
1:B:88:THR:OG1	1:B:89:HIS:CD2	2.38	0.77
1:C:227:ARG:O	1:C:231:HIS:CD2	2.37	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:144:GLU:CB	1:D:182:TYR:CE1	2.67	0.77
1:D:88:THR:CB	1:D:89:HIS:CD2	2.68	0.76
1:B:219:ASP:CB	1:B:232:ARG:CZ	2.63	0.76
1:F:89:HIS:CD2	1:F:89:HIS:N	2.51	0.76
1:B:183:ILE:CD1	1:B:183:ILE:N	2.49	0.76
1:E:58:ILE:CG2	1:E:316:THR:CG2	2.65	0.75
1:C:58:ILE:CG2	1:C:58:ILE:O	2.35	0.74
1:D:46:LEU:O	3:D:324:HOH:O	2.04	0.74
1:D:63:LYS:CG	1:D:309:MET:CE	2.66	0.73
1:A:116:GLU:OE1	3:A:319:HOH:O	2.05	0.73
1:B:85:LEU:CD1	1:B:86:THR:N	2.51	0.73
1:D:183:ILE:CG2	1:D:188:LEU:CD1	2.65	0.73
1:A:27:ILE:CG1	1:A:28:GLY:N	2.51	0.73
1:B:139:ARG:NH2	3:B:322:HOH:O	2.22	0.73
1:C:314:GLU:O	1:C:317:VAL:CG2	2.37	0.73
1:C:236:VAL:CG1	1:C:236:VAL:O	2.36	0.72
1:F:181:ALA:O	3:F:320:HOH:O	2.06	0.72
1:C:61:ASN:OD1	1:C:64:ARG:NH2	2.22	0.72
1:D:142:LYS:C	1:D:144:GLU:OE2	2.28	0.72
1:F:134:MET:O	1:F:135:GLN:CG	2.38	0.72
1:E:105:ARG:NH2	3:E:330:HOH:O	2.23	0.72
1:E:61:ASN:O	1:E:65:GLU:CG	2.38	0.71
1:D:110:GLY:O	3:D:327:HOH:O	2.06	0.71
1:D:183:ILE:CD1	1:F:226:PHE:CZ	2.74	0.71
1:E:189:LEU:CD2	1:E:189:LEU:N	2.54	0.71
1:E:309:MET:O	1:E:311:ILE:N	2.24	0.71
1:C:89:HIS:CD2	1:C:89:HIS:N	2.58	0.71
1:A:188:LEU:O	1:C:231:HIS:CE1	2.43	0.71
1:C:27:ILE:CG1	1:C:28:GLY:CA	2.69	0.70
1:B:88:THR:CB	1:B:89:HIS:CD2	2.73	0.70
1:C:141:LEU:CD1	1:C:141:LEU:N	2.49	0.70
1:A:40:ASP:C	1:A:40:ASP:OD2	2.30	0.70
1:A:27:ILE:CD1	1:A:29:ALA:O	2.40	0.70
1:C:88:THR:CB	1:C:89:HIS:CD2	2.74	0.70
1:E:180:PRO:O	1:E:233:ILE:CD1	2.39	0.70
1:C:219:ASP:OD1	1:C:219:ASP:C	2.30	0.70
1:E:304:SER:O	1:E:306:GLU:N	2.26	0.69
1:C:70:ARG:NH2	1:C:303:GLN:O	2.25	0.69
1:F:151:SER:O	1:F:152:PRO:C	2.30	0.69
1:B:192:GLU:CG	1:B:192:GLU:O	2.40	0.69
1:A:141:LEU:CD1	1:A:160:ASP:OD2	2.41	0.68
1:E:112:PHE:CD2	1:E:116:GLU:CG	2.76	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:45:GLU:OE1	1:E:81:LYS:NZ	2.26	0.68
1:D:16:HIS:CE1	1:D:51:TYR:OH	2.47	0.68
1:F:313:ALA:O	1:F:316:THR:N	2.28	0.67
1:C:126:SER:OG	1:C:286:MET:CE	2.42	0.67
1:E:310:GLN:O	1:E:314:GLU:N	2.28	0.67
1:D:142:LYS:O	1:D:144:GLU:N	2.27	0.67
1:A:220:PRO:O	1:A:223:PRO:CD	2.43	0.67
1:F:21:TYR:CE1	1:F:40:ASP:CB	2.77	0.67
1:C:69:HIS:NE2	1:C:78:VAL:O	2.28	0.66
1:A:63:LYS:CD	1:A:309:MET:CE	2.73	0.66
1:A:70:ARG:CD	1:A:70:ARG:O	2.44	0.66
1:B:223:PRO:O	1:B:225:ASN:N	2.29	0.65
1:B:225:ASN:O	1:B:229:THR:CG2	2.45	0.65
1:C:86:THR:O	1:C:88:THR:N	2.30	0.65
1:C:160:ASP:N	1:C:160:ASP:OD2	2.30	0.65
1:A:88:THR:OG1	1:A:89:HIS:NE2	2.30	0.65
1:E:61:ASN:OD1	1:E:64:ARG:NH1	2.30	0.65
1:F:151:SER:O	1:F:153:ALA:N	2.30	0.65
1:A:220:PRO:O	1:A:222:GLU:N	2.30	0.65
1:B:89:HIS:N	1:B:89:HIS:CD2	2.64	0.65
1:E:307:GLU:O	1:E:309:MET:N	2.30	0.65
1:F:72:LEU:O	3:F:322:HOH:O	2.15	0.65
1:D:143:LEU:O	1:D:145:ASN:N	2.30	0.64
1:B:21:TYR:CE1	1:B:40:ASP:CB	2.80	0.64
1:A:284:ASP:N	1:A:284:ASP:OD1	2.30	0.64
1:E:313:ALA:O	1:E:315:ALA:N	2.30	0.64
1:D:149:ASP:OD1	1:D:155:ARG:N	2.30	0.64
1:D:186:GLU:OE2	1:D:265:ARG:NH2	2.31	0.64
1:B:88:THR:OG1	1:B:89:HIS:NE2	2.30	0.64
1:D:303:GLN:O	1:D:304:SER:C	2.36	0.64
1:B:284:ASP:OD1	1:B:284:ASP:N	2.30	0.64
1:D:86:THR:O	1:D:88:THR:N	2.30	0.64
1:D:82:GLU:CA	1:D:303:GLN:NE2	2.60	0.64
1:B:86:THR:O	1:B:88:THR:N	2.30	0.64
1:C:52:ILE:O	1:C:89:HIS:CB	2.45	0.64
1:B:70:ARG:CD	1:B:70:ARG:O	2.46	0.64
1:D:226:PHE:CZ	1:D:230:ILE:CD1	2.82	0.63
1:C:59:ASP:OD2	1:C:59:ASP:O	2.17	0.63
1:A:54:ARG:O	1:A:315:ALA:O	2.16	0.63
1:A:151:SER:CB	1:A:152:PRO:CD	2.77	0.63
1:D:58:ILE:CD1	1:D:316:THR:CG2	2.77	0.63
1:C:105:ARG:NH1	1:C:116:GLU:OE2	2.32	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:80:PHE:N	3:C:319:HOH:O	2.31	0.62
1:B:149:ASP:C	1:B:149:ASP:OD1	2.37	0.62
1:C:60:GLU:O	1:C:63:LYS:N	2.33	0.62
1:A:162:GLY:O	1:A:163:TYR:C	2.37	0.62
1:A:220:PRO:O	1:A:221:GLU:C	2.37	0.62
1:A:141:LEU:O	1:A:142:LYS:CG	2.48	0.61
1:D:299:ASP:O	1:D:299:ASP:CG	2.38	0.61
1:D:142:LYS:O	1:D:143:LEU:C	2.38	0.61
1:A:138:HIS:O	1:A:138:HIS:CG	2.52	0.61
1:B:317:VAL:C	3:B:323:HOH:O	2.39	0.61
1:B:65:GLU:CD	1:B:162:GLY:O	2.39	0.61
1:F:28:GLY:O	1:F:34:VAL:CA	2.49	0.61
1:A:190:LYS:O	1:C:227:ARG:NH2	2.33	0.61
1:F:105:ARG:NH1	1:F:116:GLU:OE2	2.34	0.60
1:B:272:ARG:NH1	1:B:272:ARG:CG	2.63	0.60
1:D:86:THR:O	1:D:87:PRO:C	2.39	0.60
1:E:185:PRO:O	1:E:189:LEU:CD2	2.49	0.60
1:D:58:ILE:CD1	1:D:316:THR:N	2.65	0.60
1:B:105:ARG:NH1	1:B:116:GLU:OE2	2.35	0.60
1:E:16:HIS:NE2	1:E:51:TYR:CZ	2.70	0.59
1:E:224:LYS:O	1:E:225:ASN:C	2.39	0.59
1:A:313:ALA:O	1:A:316:THR:OG1	2.19	0.59
1:E:242:ASP:N	1:E:242:ASP:OD2	2.36	0.58
1:E:20:ARG:NH2	1:E:82:GLU:OE2	2.36	0.58
1:E:82:GLU:CG	1:E:303:GLN:HE21	2.12	0.58
1:F:219:ASP:OD1	1:F:221:GLU:CB	2.52	0.57
1:A:184:ALA:O	1:A:188:LEU:CD1	2.52	0.57
1:D:272:ARG:NH1	3:D:336:HOH:O	2.36	0.57
1:B:151:SER:O	1:B:152:PRO:C	2.42	0.57
1:A:89:HIS:CD2	1:A:89:HIS:N	2.72	0.57
1:A:61:ASN:OD1	1:A:64:ARG:NH2	2.37	0.57
1:D:226:PHE:CE2	1:D:230:ILE:CD1	2.88	0.57
1:B:73:ARG:CG	1:B:73:ARG:O	2.53	0.57
1:B:70:ARG:NH2	1:B:303:GLN:O	2.38	0.57
1:D:143:LEU:O	1:D:146:THR:CG2	2.53	0.57
1:E:16:HIS:ND1	1:E:17:ASP:OD2	2.38	0.56
1:D:149:ASP:OD1	1:D:154:PRO:CA	2.53	0.56
1:D:69:HIS:NE2	1:D:78:VAL:O	2.38	0.56
1:F:54:ARG:NH1	1:F:314:GLU:O	2.38	0.56
1:D:55:GLY:O	1:D:58:ILE:CG2	2.53	0.56
1:D:162:GLY:O	1:D:163:TYR:C	2.44	0.56
1:C:82:GLU:CA	1:C:303:GLN:NE2	2.69	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:186:GLU:OE2	1:F:265:ARG:NH2	2.39	0.56
1:E:304:SER:O	1:E:305:ILE:C	2.43	0.56
1:F:95:GLU:OE1	1:F:157:LYS:NZ	2.39	0.56
1:A:60:GLU:OE1	1:A:63:LYS:NZ	2.38	0.56
1:E:284:ASP:OD2	1:E:284:ASP:N	2.38	0.56
1:E:232:ARG:NH1	1:E:237:GLN:NE2	2.54	0.55
1:E:61:ASN:CA	1:E:64:ARG:CD	2.84	0.55
1:D:142:LYS:O	1:D:144:GLU:OE2	2.25	0.55
1:A:113:SER:N	3:A:319:HOH:O	2.38	0.55
1:B:65:GLU:OE2	1:B:162:GLY:O	2.24	0.55
1:B:60:GLU:OE1	1:B:63:LYS:NZ	2.40	0.54
1:A:193:TYR:CD1	1:A:193:TYR:O	2.60	0.54
1:D:144:GLU:CB	1:D:182:TYR:CD1	2.90	0.54
1:E:307:GLU:C	1:E:309:MET:N	2.61	0.54
1:E:149:ASP:C	1:E:149:ASP:OD1	2.46	0.54
1:D:26:ASP:OD2	1:D:36:ARG:NH1	2.41	0.54
1:A:223:PRO:O	1:A:225:ASN:N	2.39	0.54
1:D:222:GLU:N	1:D:223:PRO:CD	2.71	0.54
1:E:309:MET:O	1:E:310:GLN:C	2.46	0.53
1:E:59:ASP:O	1:E:59:ASP:OD2	2.26	0.53
1:C:54:ARG:NH2	1:C:85:LEU:CD2	2.71	0.53
1:A:98:SER:O	1:A:100:GLY:N	2.42	0.53
1:C:179:THR:CB	1:C:180:PRO:CD	2.87	0.53
1:F:86:THR:O	1:F:88:THR:N	2.42	0.53
1:C:86:THR:C	1:C:88:THR:N	2.61	0.53
1:B:161:PHE:O	1:B:161:PHE:CD2	2.61	0.53
1:E:186:GLU:OE2	1:E:265:ARG:NH1	2.42	0.53
1:A:309:MET:CE	1:B:68:ASN:OD1	2.58	0.52
1:B:232:ARG:CZ	1:B:237:GLN:NE2	2.72	0.52
1:E:183:ILE:CG2	1:E:188:LEU:CD2	2.86	0.52
1:E:88:THR:CG2	1:E:89:HIS:N	2.71	0.52
1:C:183:ILE:CG2	1:C:188:LEU:CD1	2.87	0.52
1:A:186:GLU:OE2	1:A:265:ARG:NH1	2.42	0.52
1:F:69:HIS:CE1	1:F:78:VAL:O	2.63	0.52
1:A:81:LYS:CB	1:A:93:VAL:O	2.57	0.52
1:D:144:GLU:N	1:D:144:GLU:OE2	2.43	0.52
1:B:88:THR:C	1:B:89:HIS:CD2	2.83	0.52
1:A:219:ASP:OD1	1:A:220:PRO:N	2.42	0.51
1:B:218:GLU:O	1:B:219:ASP:C	2.48	0.51
1:A:193:TYR:CD1	1:A:193:TYR:C	2.83	0.51
1:D:58:ILE:CD1	1:D:316:THR:CA	2.88	0.51
1:C:186:GLU:O	1:C:190:LYS:N	2.43	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:136:VAL:C	1:F:137:ALA:O	2.49	0.51
1:E:229:THR:O	1:E:230:ILE:C	2.48	0.51
1:E:229:THR:CG2	1:E:230:ILE:N	2.72	0.51
1:E:74:HIS:CE1	1:E:76:ASN:CB	2.94	0.51
1:E:313:ALA:O	1:E:316:THR:N	2.44	0.51
1:B:86:THR:C	1:B:88:THR:N	2.64	0.51
1:D:143:LEU:C	1:D:145:ASN:N	2.64	0.51
1:A:151:SER:O	1:A:152:PRO:C	2.48	0.51
1:E:229:THR:O	1:E:232:ARG:N	2.44	0.51
1:D:58:ILE:O	1:D:58:ILE:CG1	2.58	0.51
1:C:313:ALA:O	1:C:316:THR:OG1	2.28	0.51
1:E:135:GLN:NE2	1:E:135:GLN:CA	2.74	0.50
1:F:136:VAL:O	1:F:137:ALA:O	2.30	0.50
1:D:40:ASP:OD2	1:D:42:GLN:O	2.29	0.50
1:C:88:THR:CG2	1:C:89:HIS:CE1	2.92	0.50
1:A:80:PHE:CD1	1:A:81:LYS:N	2.78	0.50
1:E:189:LEU:O	1:E:190:LYS:CB	2.60	0.50
1:D:299:ASP:O	1:D:299:ASP:OD1	2.30	0.50
1:F:310:GLN:OE1	1:F:310:GLN:O	2.30	0.50
1:B:12:LEU:O	1:B:13:PRO:O	2.30	0.50
1:E:16:HIS:NE2	1:E:51:TYR:CE1	2.79	0.50
1:C:12:LEU:O	1:C:13:PRO:O	2.30	0.50
1:B:218:GLU:O	1:B:219:ASP:O	2.30	0.49
1:E:149:ASP:OD2	1:E:151:SER:OG	2.30	0.49
1:C:14:ILE:O	1:C:15:MET:O	2.30	0.49
1:B:223:PRO:C	1:B:225:ASN:N	2.65	0.49
1:C:185:PRO:O	1:C:186:GLU:C	2.50	0.49
1:C:59:ASP:C	1:C:59:ASP:OD2	2.50	0.49
1:D:317:VAL:O	1:D:317:VAL:CG1	2.59	0.49
1:B:232:ARG:NH2	1:B:237:GLN:NE2	2.61	0.49
1:C:27:ILE:CG1	1:C:28:GLY:N	2.72	0.49
1:D:149:ASP:OD2	1:D:151:SER:OG	2.30	0.49
1:E:312:ILE:O	1:E:316:THR:OG1	2.30	0.49
1:D:297:GLU:O	1:D:299:ASP:N	2.45	0.49
1:E:40:ASP:OD1	1:E:42:GLN:CB	2.60	0.49
1:A:88:THR:CA	1:A:89:HIS:CD2	2.96	0.49
1:D:313:ALA:O	1:D:316:THR:OG1	2.30	0.49
1:C:14:ILE:O	1:C:15:MET:C	2.51	0.49
1:F:26:ASP:OD2	1:F:36:ARG:NH1	2.45	0.49
1:A:113:SER:OG	3:A:320:HOH:O	2.20	0.49
1:A:54:ARG:O	1:A:55:GLY:O	2.31	0.49
1:E:149:ASP:OD1	1:E:151:SER:OG	2.30	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:21:TYR:CE1	1:C:40:ASP:CB	2.96	0.49
1:E:309:MET:C	1:E:311:ILE:N	2.62	0.49
1:B:14:ILE:O	1:B:16:HIS:ND1	2.46	0.49
1:C:179:THR:OG1	1:C:180:PRO:CD	2.60	0.49
1:F:222:GLU:OE2	1:F:228:LYS:NZ	2.46	0.48
1:C:191:LYS:CD	1:C:191:LYS:O	2.61	0.48
1:F:134:MET:O	1:F:135:GLN:CB	2.61	0.48
1:B:155[B]:ARG:NH1	1:B:155[B]:ARG:CG	2.76	0.48
1:A:40:ASP:O	1:A:40:ASP:OD2	2.31	0.48
1:E:236:VAL:O	1:E:236:VAL:CG1	2.61	0.48
1:E:310:GLN:O	1:E:314:GLU:CA	2.60	0.48
1:B:218:GLU:O	1:B:223:PRO:CB	2.61	0.48
1:A:54:ARG:NH1	1:A:54:ARG:CG	2.77	0.48
1:F:59:ASP:N	1:F:59:ASP:OD2	2.46	0.48
1:E:313:ALA:C	1:E:315:ALA:N	2.65	0.48
1:A:161:PHE:CD1	1:A:161:PHE:N	2.80	0.48
1:D:53:GLU:CA	1:D:89:HIS:CB	2.92	0.48
1:C:40:ASP:OD2	1:C:42:GLN:O	2.31	0.48
1:E:26:ASP:OD2	1:E:36:ARG:CG	2.62	0.48
1:B:194:ASP:C	1:B:194:ASP:OD2	2.52	0.47
1:C:54:ARG:NH1	1:C:317:VAL:O	2.47	0.47
1:F:40:ASP:OD2	1:F:42:GLN:O	2.33	0.47
1:E:182:TYR:CE2	1:E:206:THR:CG2	2.97	0.47
1:B:194:ASP:OD2	1:B:196:LYS:N	2.47	0.47
1:B:56:GLU:O	1:B:56:GLU:CG	2.62	0.47
1:E:61:ASN:OD1	1:E:64:ARG:CD	2.63	0.47
1:E:179:THR:CB	1:E:180:PRO:CD	2.93	0.47
1:C:224:LYS:O	1:C:226:PHE:N	2.48	0.47
1:E:313:ALA:O	1:E:316:THR:OG1	2.33	0.47
1:B:41:LYS:NZ	3:B:345:HOH:O	2.47	0.47
1:D:297:GLU:C	1:D:299:ASP:N	2.67	0.47
1:A:179:THR:CB	1:A:180:PRO:CD	2.92	0.47
1:A:74:HIS:ND1	1:A:75:PRO:CD	2.78	0.47
1:D:27:ILE:N	1:D:27:ILE:CD1	2.78	0.46
1:F:224:LYS:O	1:F:225:ASN:C	2.54	0.46
1:D:54:ARG:CG	1:D:54:ARG:NH1	2.78	0.46
1:F:161:PHE:N	1:F:161:PHE:CD1	2.83	0.46
1:C:227:ARG:NE	1:C:231:HIS:NE2	2.63	0.46
1:F:226:PHE:CA	1:F:229:THR:CG2	2.93	0.46
1:F:316:THR:O	1:F:317:VAL:C	2.53	0.46
1:E:149:ASP:CG	1:E:151:SER:OG	2.54	0.46
1:D:25:LYS:CE	1:D:27:ILE:CD1	2.93	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:15:MET:CE	1:B:21:TYR:O	2.64	0.46
1:E:58:ILE:O	1:E:59:ASP:O	2.34	0.46
1:A:223:PRO:C	1:A:225:ASN:N	2.68	0.46
1:D:303:GLN:O	1:D:308:ILE:CD1	2.64	0.46
1:D:139:ARG:CB	1:D:139:ARG:NH1	2.78	0.46
1:F:64:ARG:NH1	1:F:64:ARG:CB	2.79	0.46
1:E:313:ALA:O	1:E:314:GLU:C	2.53	0.46
1:E:189:LEU:O	1:E:190:LYS:CD	2.63	0.46
1:B:69:HIS:NE2	1:B:78:VAL:O	2.49	0.46
1:C:281:LEU:O	1:C:282:PRO:C	2.52	0.46
1:E:80:PHE:CD2	1:E:80:PHE:C	2.90	0.45
1:E:64:ARG:CG	1:E:65:GLU:N	2.79	0.45
1:F:138:HIS:O	1:F:138:HIS:ND1	2.49	0.45
1:E:304:SER:C	1:E:306:GLU:N	2.69	0.45
1:E:19:ASP:OD2	1:E:19:ASP:C	2.53	0.45
1:A:187:VAL:O	1:C:227:ARG:CZ	2.64	0.45
1:B:186:GLU:OE1	1:B:186:GLU:N	2.49	0.45
1:A:69:HIS:NE2	1:A:78:VAL:O	2.49	0.45
1:E:39:ARG:NH1	1:E:44:ASN:OD1	2.50	0.45
1:D:211:LEU:O	3:D:319:HOH:O	2.20	0.45
1:E:225:ASN:ND2	3:E:322:HOH:O	2.50	0.45
1:E:61:ASN:OD1	1:E:64:ARG:CZ	2.64	0.45
1:D:142:LYS:O	1:D:145:ASN:N	2.49	0.45
1:C:149:ASP:C	1:C:149:ASP:OD1	2.53	0.45
1:C:148:LEU:C	1:C:149:ASP:O	2.53	0.45
1:B:50:LYS:NZ	3:B:327:HOH:O	2.50	0.45
1:E:187:VAL:O	1:E:187:VAL:CG1	2.65	0.45
1:B:22:GLU:OE1	3:B:324:HOH:O	2.21	0.45
1:B:237:GLN:O	1:B:237:GLN:CG	2.64	0.45
1:A:105:ARG:NH1	1:A:116:GLU:OE2	2.50	0.45
1:C:55:GLY:C	1:C:57:LYS:N	2.69	0.45
1:C:60:GLU:O	1:C:64:ARG:N	2.50	0.45
1:A:153:ALA:O	1:A:154:PRO:C	2.55	0.45
1:A:149:ASP:OD1	1:A:155:ARG:N	2.50	0.45
1:A:88:THR:C	1:A:89:HIS:CG	2.89	0.44
1:F:52:ILE:O	1:F:89:HIS:CB	2.65	0.44
1:F:86:THR:C	1:F:88:THR:N	2.70	0.44
1:C:153:ALA:O	1:C:154:PRO:C	2.55	0.44
1:E:222:GLU:CB	1:E:223:PRO:CD	2.95	0.44
1:D:59:ASP:OD2	1:D:60:GLU:N	2.50	0.44
1:A:60:GLU:O	1:A:64:ARG:N	2.50	0.44
1:E:149:ASP:OD1	1:E:149:ASP:O	2.36	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:227:ARG:O	1:B:231:HIS:CD2	2.69	0.44
1:B:282:PRO:C	1:B:284:ASP:N	2.72	0.43
1:B:80:PHE:N	3:B:350:HOH:O	2.49	0.43
1:B:81:LYS:CB	1:B:93:VAL:O	2.66	0.43
1:E:70:ARG:CG	1:E:80:PHE:CZ	2.99	0.43
1:F:310:GLN:O	1:F:314:GLU:CG	2.67	0.43
1:B:230:ILE:CD1	1:E:188:LEU:CD1	2.96	0.43
1:B:225:ASN:ND2	1:B:225:ASN:C	2.68	0.43
1:B:219:ASP:OD2	1:B:232:ARG:CZ	2.67	0.43
1:E:310:GLN:O	1:E:314:GLU:CG	2.65	0.43
1:C:27:ILE:CD1	1:C:28:GLY:CA	2.97	0.43
1:D:33:GLY:O	1:D:34:VAL:C	2.57	0.43
1:D:88:THR:C	1:D:89:HIS:CD2	2.92	0.43
1:C:227:ARG:CZ	1:C:231:HIS:NE2	2.82	0.43
1:F:186:GLU:OE2	1:F:265:ARG:NH1	2.52	0.43
1:A:80:PHE:CD1	1:A:80:PHE:C	2.92	0.43
1:A:43:ALA:O	1:A:44:ASN:C	2.57	0.43
1:F:150:GLY:O	1:F:151:SER:CB	2.66	0.43
1:E:232:ARG:CG	1:E:237:GLN:O	2.67	0.42
1:B:182:TYR:CE2	1:B:206:THR:CG2	3.02	0.42
1:A:17:ASP:C	1:A:19:ASP:N	2.72	0.42
1:B:218:GLU:O	1:B:223:PRO:CA	2.67	0.42
1:D:223:PRO:C	1:D:225:ASN:N	2.71	0.42
1:E:311:ILE:O	1:E:313:ALA:N	2.52	0.42
1:A:69:HIS:CD2	1:A:69:HIS:O	2.72	0.42
1:C:153:ALA:O	1:C:154:PRO:O	2.37	0.42
1:F:43:ALA:O	1:F:44:ASN:C	2.57	0.42
1:E:16:HIS:C	1:E:17:ASP:OD2	2.56	0.42
1:E:80:PHE:CG	1:E:80:PHE:O	2.71	0.42
1:D:43:ALA:O	1:D:44:ASN:C	2.57	0.42
1:B:281:LEU:O	1:B:282:PRO:C	2.57	0.42
1:F:141:LEU:C	1:F:142:LYS:CG	2.87	0.42
1:E:230:ILE:CG2	1:E:231:HIS:N	2.82	0.42
1:E:70:ARG:NH2	1:E:303:GLN:O	2.53	0.42
1:A:22:GLU:OE2	1:A:39:ARG:NH2	2.53	0.42
1:A:141:LEU:C	1:A:142:LYS:CG	2.88	0.42
1:A:101:GLU:CD	1:A:145:ASN:ND2	2.66	0.42
1:B:152:PRO:O	1:B:154:PRO:N	2.51	0.42
1:C:261:ASP:O	1:C:264:LYS:N	2.53	0.41
1:E:311:ILE:C	1:E:313:ALA:N	2.72	0.41
1:A:219:ASP:C	1:A:219:ASP:OD1	2.57	0.41
1:A:185:PRO:O	1:A:189:LEU:CB	2.67	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:61:ASN:C	1:E:64:ARG:CD	2.88	0.41
1:B:70:ARG:CD	1:B:70:ARG:C	2.89	0.41
1:D:54:ARG:O	1:D:55:GLY:O	2.38	0.41
1:D:132:HIS:NE2	1:D:199:ASP:OD1	2.53	0.41
1:D:101:GLU:O	1:D:104:GLU:N	2.52	0.41
1:F:224:LYS:O	1:F:226:PHE:N	2.53	0.41
1:A:59:ASP:OD2	1:A:59:ASP:C	2.59	0.41
1:A:135:GLN:CG	1:A:138:HIS:CA	2.98	0.41
1:D:232:ARG:NH1	1:D:232:ARG:CG	2.83	0.41
1:D:161:PHE:N	1:D:161:PHE:CD1	2.89	0.41
1:C:304:SER:N	1:C:307:GLU:OE1	2.54	0.41
1:D:26:ASP:OD2	1:D:36:ARG:CG	2.69	0.41
1:B:141:LEU:CD1	1:B:141:LEU:N	2.84	0.41
1:C:285:LEU:C	1:C:286:MET:CG	2.89	0.41
1:E:189:LEU:O	1:E:190:LYS:CE	2.70	0.41
1:C:186:GLU:OE1	1:C:265:ARG:NH2	2.54	0.41
1:D:61:ASN:OD1	1:D:64:ARG:NH2	2.54	0.40
1:E:311:ILE:O	1:E:312:ILE:C	2.59	0.40
1:B:219:ASP:CB	1:B:232:ARG:NH1	2.84	0.40
1:B:13:PRO:CG	1:B:51:TYR:CE1	3.04	0.40
1:D:14:ILE:CG2	1:D:15:MET:N	2.83	0.40
1:B:14:ILE:O	1:B:15:MET:C	2.60	0.40
1:F:123:GLN:OE1	1:F:156:LEU:N	2.55	0.40
1:E:193:TYR:CD1	1:E:193:TYR:C	2.94	0.40

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

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	4	3
1	B	273/317 (86%)	229 (84%)	31 (11%)	13 (5%)	4	3
1	C	249/317 (78%)	220 (88%)	22 (9%)	7 (3%)	8	11
1	D	273/317 (86%)	233 (85%)	28 (10%)	12 (4%)	4	4
1	E	243/317 (77%)	203 (84%)	26 (11%)	14 (6%)	3	2
1	F	267/317 (84%)	229 (86%)	29 (11%)	9 (3%)	6	8
All	All	1574/1902 (83%)	1346 (86%)	160 (10%)	68 (4%)	4	4

All (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
1	B	153	ALA
1	B	220	PRO
1	C	13	PRO
1	C	15	MET
1	C	225	ASN
1	D	87	PRO
1	D	143	LEU
1	D	304	SER
1	E	194	ASP
1	E	229	THR
1	E	305	ILE
1	E	310	GLN
1	F	137	ALA
1	F	152	PRO
1	A	55	GLY
1	A	162	GLY
1	A	224	LYS
1	B	100	GLY
1	B	224	LYS
1	D	34	VAL
1	D	55	GLY
1	D	144	GLU
1	D	298	SER
1	E	190	LYS
1	E	223	PRO

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Mol	Chain	Res	Type
1	E	308	ILE
1	E	314	GLU
1	F	225	ASN
1	A	220	PRO
1	B	44	ASN
1	B	87	PRO
1	C	87	PRO
1	C	149	ASP
1	C	154	PRO
1	D	54	ARG
1	E	225	ASN
1	E	306	GLU
1	F	13	PRO
1	F	154	PRO
1	A	44	ASN
1	A	139	ARG
1	A	152	PRO
1	A	154	PRO
1	B	54	ARG
1	B	283	ALA
1	D	301	PRO
1	E	14	ILE
1	E	230	ILE
1	A	82	GLU
1	B	219	ASP
1	C	44	ASN
1	D	44	ASN
1	F	44	ASN
1	F	142	LYS
1	F	151	SER
1	A	153	ALA
1	D	28	GLY
1	E	55	GLY
1	B	33	GLY
1	F	87	PRO
1	D	78	VAL
1	E	312	ILE
1	A	78	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/274 (86%)	190 (80%)	47 (20%)	2	3
1	B	240/274 (88%)	193 (80%)	47 (20%)	2	3
1	C	229/274 (84%)	191 (83%)	38 (17%)	3	5
1	D	238/274 (87%)	192 (81%)	46 (19%)	2	3
1	E	216/274 (79%)	166 (77%)	50 (23%)	1	2
1	F	236/274 (86%)	187 (79%)	49 (21%)	2	2
All	All	1396/1644 (85%)	1119 (80%)	277 (20%)	2	3

All (277) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	18	SER
1	A	25	LYS
1	A	27	ILE
1	A	31	ASN
1	A	34	VAL
1	A	36	ARG
1	A	37	LEU
1	A	40	ASP
1	A	47	VAL
1	A	50	LYS
1	A	54	ARG
1	A	56	GLU
1	A	63	LYS
1	A	70	ARG
1	A	77	ILE
1	A	79	ARG
1	A	81	LYS
1	A	82	GLU
1	A	83	VAL
1	A	89	HIS
1	A	98	SER
1	A	115	ASP

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Mol	Chain	Res	Type
1	A	134	MET
1	A	135	GLN
1	A	142	LYS
1	A	143	LEU
1	A	144	GLU
1	A	145	ASN
1	A	155	ARG
1	A	163	TYR
1	A	186	GLU
1	A	188	LEU
1	A	189	LEU
1	A	191	LYS
1	A	222	GLU
1	A	226	PHE
1	A	227	ARG
1	A	246	ILE
1	A	279	LYS
1	A	284	ASP
1	A	303	GLN
1	A	304	SER
1	A	305	ILE
1	A	306	GLU
1	A	312	ILE
1	A	317	VAL
1	B	14	ILE
1	B	16	HIS
1	B	19	ASP
1	B	27	ILE
1	B	34	VAL
1	B	37	LEU
1	B	40	ASP
1	B	41	LYS
1	B	54	ARG
1	B	57	LYS
1	B	58	ILE
1	B	59	ASP
1	B	67	ILE
1	B	77	ILE
1	B	79	ARG
1	B	83	VAL
1	B	85	LEU
1	B	86	THR

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Mol	Chain	Res	Type
1	B	89	HIS
1	B	111	ARG
1	B	134	MET
1	B	141	LEU
1	B	143	LEU
1	B	144	GLU
1	B	148	LEU
1	B	155[A]	ARG
1	B	155[B]	ARG
1	B	179	THR
1	B	183	ILE
1	B	188	LEU
1	B	190	LYS
1	B	191	LYS
1	B	196	LYS
1	B	206	THR
1	B	219	ASP
1	B	224	LYS
1	B	225	ASN
1	B	227	ARG
1	B	228	LYS
1	B	229	THR
1	B	237	GLN
1	B	243	TYR
1	B	272	ARG
1	B	279	LYS
1	B	284	ASP
1	B	285	LEU
1	B	303	GLN
1	C	12	LEU
1	C	14	ILE
1	C	15	MET
1	C	18	SER
1	C	20	ARG
1	C	25	LYS
1	C	27	ILE
1	C	37	LEU
1	C	40	ASP
1	C	58	ILE
1	C	60	GLU
1	C	77	ILE
1	C	83	VAL

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Mol	Chain	Res	Type
1	C	85	LEU
1	C	89	HIS
1	C	118	ARG
1	C	140	ASP
1	C	141	LEU
1	C	142	LYS
1	C	155	ARG
1	C	156	LEU
1	C	160	ASP
1	C	179	THR
1	C	188	LEU
1	C	191	LYS
1	C	202	SER
1	C	206	THR
1	C	219	ASP
1	C	225	ASN
1	C	227	ARG
1	C	228	LYS
1	C	234	LEU
1	C	240	ILE
1	C	251	ARG
1	C	279	LYS
1	C	284	ASP
1	C	286	MET
1	C	310	GLN
1	D	14	ILE
1	D	17	ASP
1	D	18	SER
1	D	22	GLU
1	D	27	ILE
1	D	31	ASN
1	D	37	LEU
1	D	39	ARG
1	D	40	ASP
1	D	45	GLU
1	D	47	VAL
1	D	53	GLU
1	D	54	ARG
1	D	58	ILE
1	D	60	GLU
1	D	73	ARG
1	D	81	LYS

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Mol	Chain	Res	Type
1	D	82	GLU
1	D	83	VAL
1	D	85	LEU
1	D	86	THR
1	D	89	HIS
1	D	104	GLU
1	D	111	ARG
1	D	143	LEU
1	D	151	SER
1	D	155	ARG
1	D	161	PHE
1	D	163	TYR
1	D	186	GLU
1	D	188	LEU
1	D	190	LYS
1	D	194	ASP
1	D	206	THR
1	D	221	GLU
1	D	222	GLU
1	D	227	ARG
1	D	230	ILE
1	D	232	ARG
1	D	235	ASN
1	D	237	GLN
1	D	242	ASP
1	D	246	ILE
1	D	309	MET
1	D	310	GLN
1	D	314	GLU
1	E	14	ILE
1	E	17	ASP
1	E	25	LYS
1	E	27	ILE
1	E	34	VAL
1	E	37	LEU
1	E	40	ASP
1	E	41	LYS
1	E	42	GLN
1	E	53	GLU
1	E	58	ILE
1	E	60	GLU
1	E	62	VAL

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Mol	Chain	Res	Type
1	E	63	LYS
1	E	64	ARG
1	E	65	GLU
1	E	77	ILE
1	E	79	ARG
1	E	80	PHE
1	E	82	GLU
1	E	83	VAL
1	E	85	LEU
1	E	88	THR
1	E	89	HIS
1	E	116	GLU
1	E	143	LEU
1	E	144	GLU
1	E	146	THR
1	E	149	ASP
1	E	151	SER
1	E	155	ARG
1	E	156	LEU
1	E	186	GLU
1	E	188	LEU
1	E	189	LEU
1	E	190	LYS
1	E	191	LYS
1	E	206	THR
1	E	224	LYS
1	E	226	PHE
1	E	228	LYS
1	E	230	ILE
1	E	232	ARG
1	E	234	LEU
1	E	240	ILE
1	E	242	ASP
1	E	279	LYS
1	E	281	LEU
1	E	284	ASP
1	E	316	THR
1	F	14	ILE
1	F	17	ASP
1	F	19	ASP
1	F	20	ARG
1	F	22	GLU

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Mol	Chain	Res	Type
1	F	27	ILE
1	F	34	VAL
1	F	37	LEU
1	F	40	ASP
1	F	52	ILE
1	F	54	ARG
1	F	57	LYS
1	F	60	GLU
1	F	64	ARG
1	F	69	HIS
1	F	73	ARG
1	F	77	ILE
1	F	81	LYS
1	F	82	GLU
1	F	83	VAL
1	F	85	LEU
1	F	89	HIS
1	F	111	ARG
1	F	139	ARG
1	F	141	LEU
1	F	142	LYS
1	F	144	GLU
1	F	151	SER
1	F	155	ARG
1	F	156	LEU
1	F	163	TYR
1	F	179	THR
1	F	188	LEU
1	F	190	LYS
1	F	191	LYS
1	F	206	THR
1	F	219	ASP
1	F	221	GLU
1	F	222	GLU
1	F	225	ASN
1	F	229	THR
1	F	242	ASP
1	F	246	ILE
1	F	261	ASP
1	F	279	LYS
1	F	303	GLN
1	F	310	GLN

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Mol	Chain	Res	Type
1	F	314	GLU
1	F	316	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	303	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	275/317 (86%)	0.21	11 (4%) 36 36	30, 53, 102, 178	0
1	B	278/317 (87%)	0.04	4 (1%) 72 74	32, 53, 103, 134	0
1	C	261/317 (82%)	0.08	7 (2%) 52 52	26, 50, 100, 121	0
1	D	279/317 (88%)	0.21	11 (3%) 37 36	31, 58, 105, 158	0
1	E	255/317 (80%)	0.36	23 (9%) 10 8	32, 63, 118, 161	0
1	F	273/317 (86%)	0.23	14 (5%) 27 26	31, 55, 106, 128	0
All	All	1621/1902 (85%)	0.19	70 (4%) 34 33	26, 55, 106, 178	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	GLU	6.4
1	E	87	PRO	4.3
1	F	163	TYR	4.0
1	E	302	GLY	3.9
1	A	189	LEU	3.9
1	D	299	ASP	3.9
1	A	12	LEU	3.8
1	D	162	GLY	3.8
1	E	56	GLU	3.7
1	D	31	ASN	3.6
1	A	162	GLY	3.6
1	C	34	VAL	3.5
1	E	52	ILE	3.5
1	F	31	ASN	3.4
1	D	29	ALA	3.4
1	D	300	GLN	3.4
1	D	163	TYR	3.3
1	E	62	VAL	3.2
1	B	224	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	56	GLU	3.2
1	F	317	VAL	3.1
1	F	62	VAL	3.1
1	E	34	VAL	3.0
1	F	60	GLU	3.0
1	E	143	LEU	2.9
1	C	28	GLY	2.9
1	F	52	ILE	2.9
1	A	88	THR	2.9
1	F	34	VAL	2.9
1	E	304	SER	2.9
1	E	53	GLU	2.9
1	E	152	PRO	2.8
1	A	161	PHE	2.7
1	C	52	ILE	2.7
1	D	32	PHE	2.7
1	A	31	ASN	2.6
1	E	303	GLN	2.6
1	E	67	ILE	2.6
1	E	305	ILE	2.6
1	F	29	ALA	2.6
1	C	160	ASP	2.5
1	A	192	GLU	2.5
1	D	317	VAL	2.5
1	B	226	PHE	2.5
1	E	27	ILE	2.5
1	A	34	VAL	2.4
1	E	13	PRO	2.4
1	B	18	SER	2.4
1	E	60	GLU	2.4
1	F	224	LYS	2.4
1	E	51	TYR	2.4
1	E	28	GLY	2.3
1	A	32	PHE	2.3
1	A	152	PRO	2.2
1	E	230	ILE	2.2
1	E	311	ILE	2.2
1	F	136	VAL	2.2
1	E	63	LYS	2.2
1	D	161	PHE	2.2
1	B	84	ILE	2.2
1	F	56	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	131	ALA	2.2
1	E	73	ARG	2.1
1	F	152	PRO	2.1
1	F	57	LYS	2.1
1	E	179	THR	2.1
1	D	283	ALA	2.1
1	D	73	ARG	2.0
1	C	12	LEU	2.0
1	C	50	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CL	C	318	1/1	0.23	6.34	86,86,86,86	0
2	CL	F	318	1/1	0.26	6.04	88,88,88,88	0
2	CL	D	318	1/1	0.19	0.78	91,91,91,91	0
2	CL	B	318	1/1	0.12	-0.58	87,87,87,87	0
2	CL	A	318	1/1	0.09	-1.41	83,83,83,83	0
2	CL	E	318	1/1	0.09	-2.40	86,86,86,86	0

6.5 Other polymers ⓘ

There are no such residues in this entry.