Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 03:31 PM JST

PDB ID	:	6JJO
Title	:	Crystal structure of the DegP dodecamer with a modulator
Authors	:	Cho, H.; Choi, Y.; Lee, H.H.; Kim, S.
Deposited on	:	2019-02-26
Resolution	:	4.16 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 (1)) were used in the production of this report:

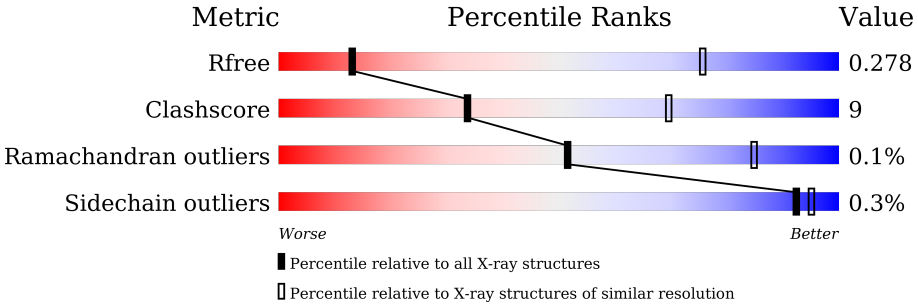
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 4.16 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	1020 (4.54-3.76)
Clashscore	141614	1028 (4.52-3.80)
Ramachandran outliers	138981	1005 (4.54-3.78)
Sidechain outliers	138945	1024 (4.54-3.76)

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%

Mol	Chain	Length	Quality of chain
1	A	469	64% 16% 19%
1	B	469	65% 18% 16%
1	C	469	64% 17% 19%
1	D	469	65% 17% 17%
1	E	469	68% 15% 17%
1	F	469	67% 14% 19%
2	G	5	80% 20%

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Mol	Chain	Length	Quality of chain
2	H	5	100%
2	I	5	100%
2	J	5	80% 20%
2	K	5	100%
2	L	5	100%
2	M	5	100%
2	N	5	100%
2	O	5	100%
2	P	5	100%
2	Q	5	80% 20%
2	R	5	100%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16906 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 Periplasmic serine endoprotease DegP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	381	2736	1703	482	538	13	0	0	0
1	B	392	2820	1752	495	560	13	0	0	0
1	C	382	2743	1709	482	539	13	0	0	0
1	D	388	2784	1731	488	553	12	0	0	0
1	E	388	2795	1737	491	554	13	0	0	0
1	F	379	2728	1700	481	534	13	0	0	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P0C0V0
A	-19	GLY	-	expression tag	UNP P0C0V0
A	-18	SER	-	expression tag	UNP P0C0V0
A	-17	SER	-	expression tag	UNP P0C0V0
A	-16	HIS	-	expression tag	UNP P0C0V0
A	-15	HIS	-	expression tag	UNP P0C0V0
A	-14	HIS	-	expression tag	UNP P0C0V0
A	-13	HIS	-	expression tag	UNP P0C0V0
A	-12	HIS	-	expression tag	UNP P0C0V0
A	-11	HIS	-	expression tag	UNP P0C0V0
A	-10	SER	-	expression tag	UNP P0C0V0
A	-9	SER	-	expression tag	UNP P0C0V0
A	-8	GLY	-	expression tag	UNP P0C0V0
A	-7	LEU	-	expression tag	UNP P0C0V0
A	-6	VAL	-	expression tag	UNP P0C0V0
A	-5	PRO	-	expression tag	UNP P0C0V0
A	-4	ARG	-	expression tag	UNP P0C0V0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P0C0V0
A	-2	SER	-	expression tag	UNP P0C0V0
A	-1	HIS	-	expression tag	UNP P0C0V0
A	0	MET	-	expression tag	UNP P0C0V0
A	210	ALA	SER	engineered mutation	UNP P0C0V0
B	-20	MET	-	expression tag	UNP P0C0V0
B	-19	GLY	-	expression tag	UNP P0C0V0
B	-18	SER	-	expression tag	UNP P0C0V0
B	-17	SER	-	expression tag	UNP P0C0V0
B	-16	HIS	-	expression tag	UNP P0C0V0
B	-15	HIS	-	expression tag	UNP P0C0V0
B	-14	HIS	-	expression tag	UNP P0C0V0
B	-13	HIS	-	expression tag	UNP P0C0V0
B	-12	HIS	-	expression tag	UNP P0C0V0
B	-11	HIS	-	expression tag	UNP P0C0V0
B	-10	SER	-	expression tag	UNP P0C0V0
B	-9	SER	-	expression tag	UNP P0C0V0
B	-8	GLY	-	expression tag	UNP P0C0V0
B	-7	LEU	-	expression tag	UNP P0C0V0
B	-6	VAL	-	expression tag	UNP P0C0V0
B	-5	PRO	-	expression tag	UNP P0C0V0
B	-4	ARG	-	expression tag	UNP P0C0V0
B	-3	GLY	-	expression tag	UNP P0C0V0
B	-2	SER	-	expression tag	UNP P0C0V0
B	-1	HIS	-	expression tag	UNP P0C0V0
B	0	MET	-	expression tag	UNP P0C0V0
B	210	ALA	SER	engineered mutation	UNP P0C0V0
C	-20	MET	-	expression tag	UNP P0C0V0
C	-19	GLY	-	expression tag	UNP P0C0V0
C	-18	SER	-	expression tag	UNP P0C0V0
C	-17	SER	-	expression tag	UNP P0C0V0
C	-16	HIS	-	expression tag	UNP P0C0V0
C	-15	HIS	-	expression tag	UNP P0C0V0
C	-14	HIS	-	expression tag	UNP P0C0V0
C	-13	HIS	-	expression tag	UNP P0C0V0
C	-12	HIS	-	expression tag	UNP P0C0V0
C	-11	HIS	-	expression tag	UNP P0C0V0
C	-10	SER	-	expression tag	UNP P0C0V0
C	-9	SER	-	expression tag	UNP P0C0V0
C	-8	GLY	-	expression tag	UNP P0C0V0
C	-7	LEU	-	expression tag	UNP P0C0V0
C	-6	VAL	-	expression tag	UNP P0C0V0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	PRO	-	expression tag	UNP P0C0V0
C	-4	ARG	-	expression tag	UNP P0C0V0
C	-3	GLY	-	expression tag	UNP P0C0V0
C	-2	SER	-	expression tag	UNP P0C0V0
C	-1	HIS	-	expression tag	UNP P0C0V0
C	0	MET	-	expression tag	UNP P0C0V0
C	210	ALA	SER	engineered mutation	UNP P0C0V0
D	-20	MET	-	expression tag	UNP P0C0V0
D	-19	GLY	-	expression tag	UNP P0C0V0
D	-18	SER	-	expression tag	UNP P0C0V0
D	-17	SER	-	expression tag	UNP P0C0V0
D	-16	HIS	-	expression tag	UNP P0C0V0
D	-15	HIS	-	expression tag	UNP P0C0V0
D	-14	HIS	-	expression tag	UNP P0C0V0
D	-13	HIS	-	expression tag	UNP P0C0V0
D	-12	HIS	-	expression tag	UNP P0C0V0
D	-11	HIS	-	expression tag	UNP P0C0V0
D	-10	SER	-	expression tag	UNP P0C0V0
D	-9	SER	-	expression tag	UNP P0C0V0
D	-8	GLY	-	expression tag	UNP P0C0V0
D	-7	LEU	-	expression tag	UNP P0C0V0
D	-6	VAL	-	expression tag	UNP P0C0V0
D	-5	PRO	-	expression tag	UNP P0C0V0
D	-4	ARG	-	expression tag	UNP P0C0V0
D	-3	GLY	-	expression tag	UNP P0C0V0
D	-2	SER	-	expression tag	UNP P0C0V0
D	-1	HIS	-	expression tag	UNP P0C0V0
D	0	MET	-	expression tag	UNP P0C0V0
D	210	ALA	SER	engineered mutation	UNP P0C0V0
E	-20	MET	-	expression tag	UNP P0C0V0
E	-19	GLY	-	expression tag	UNP P0C0V0
E	-18	SER	-	expression tag	UNP P0C0V0
E	-17	SER	-	expression tag	UNP P0C0V0
E	-16	HIS	-	expression tag	UNP P0C0V0
E	-15	HIS	-	expression tag	UNP P0C0V0
E	-14	HIS	-	expression tag	UNP P0C0V0
E	-13	HIS	-	expression tag	UNP P0C0V0
E	-12	HIS	-	expression tag	UNP P0C0V0
E	-11	HIS	-	expression tag	UNP P0C0V0
E	-10	SER	-	expression tag	UNP P0C0V0
E	-9	SER	-	expression tag	UNP P0C0V0
E	-8	GLY	-	expression tag	UNP P0C0V0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	LEU	-	expression tag	UNP P0C0V0
E	-6	VAL	-	expression tag	UNP P0C0V0
E	-5	PRO	-	expression tag	UNP P0C0V0
E	-4	ARG	-	expression tag	UNP P0C0V0
E	-3	GLY	-	expression tag	UNP P0C0V0
E	-2	SER	-	expression tag	UNP P0C0V0
E	-1	HIS	-	expression tag	UNP P0C0V0
E	0	MET	-	expression tag	UNP P0C0V0
E	210	ALA	SER	engineered mutation	UNP P0C0V0
F	-20	MET	-	expression tag	UNP P0C0V0
F	-19	GLY	-	expression tag	UNP P0C0V0
F	-18	SER	-	expression tag	UNP P0C0V0
F	-17	SER	-	expression tag	UNP P0C0V0
F	-16	HIS	-	expression tag	UNP P0C0V0
F	-15	HIS	-	expression tag	UNP P0C0V0
F	-14	HIS	-	expression tag	UNP P0C0V0
F	-13	HIS	-	expression tag	UNP P0C0V0
F	-12	HIS	-	expression tag	UNP P0C0V0
F	-11	HIS	-	expression tag	UNP P0C0V0
F	-10	SER	-	expression tag	UNP P0C0V0
F	-9	SER	-	expression tag	UNP P0C0V0
F	-8	GLY	-	expression tag	UNP P0C0V0
F	-7	LEU	-	expression tag	UNP P0C0V0
F	-6	VAL	-	expression tag	UNP P0C0V0
F	-5	PRO	-	expression tag	UNP P0C0V0
F	-4	ARG	-	expression tag	UNP P0C0V0
F	-3	GLY	-	expression tag	UNP P0C0V0
F	-2	SER	-	expression tag	UNP P0C0V0
F	-1	HIS	-	expression tag	UNP P0C0V0
F	0	MET	-	expression tag	UNP P0C0V0
F	210	ALA	SER	engineered mutation	UNP P0C0V0

- Molecule 2 is a protein called TMB-CYRKL modulator.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	G	5	25	15	5	5	0	0	0
2	M	5	25	15	5	5	0	0	0
2	H	5	25	15	5	5	0	0	0
2	N	5	25	15	5	5	0	0	0

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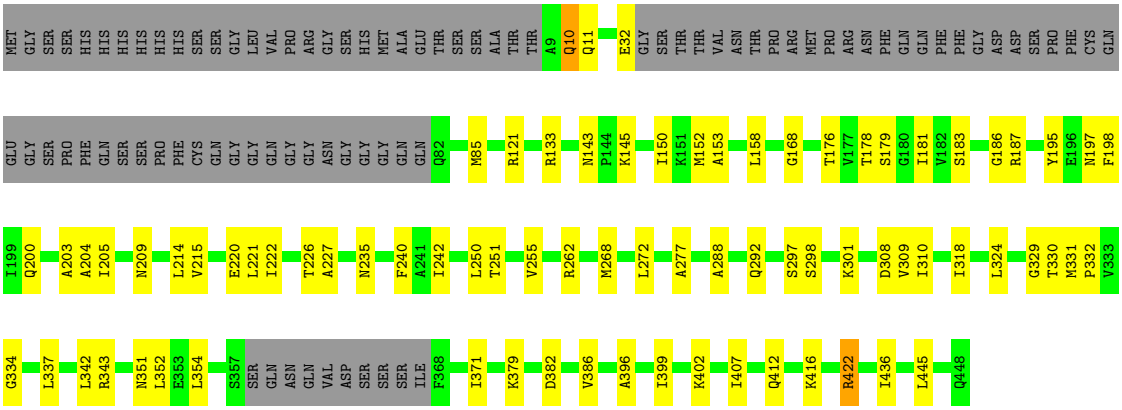
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	5	25	15	5	5	0	0	0
			Total	C	N	O			
2	O	5	25	15	5	5	0	0	0
			Total	C	N	O			
2	J	5	25	15	5	5	0	0	0
			Total	C	N	O			
2	P	5	25	15	5	5	0	0	0
			Total	C	N	O			
2	K	5	25	15	5	5	0	0	0
			Total	C	N	O			
2	Q	5	25	15	5	5	0	0	0
			Total	C	N	O			
2	L	5	25	15	5	5	0	0	0
			Total	C	N	O			
2	R	5	25	15	5	5	0	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. 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. 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.

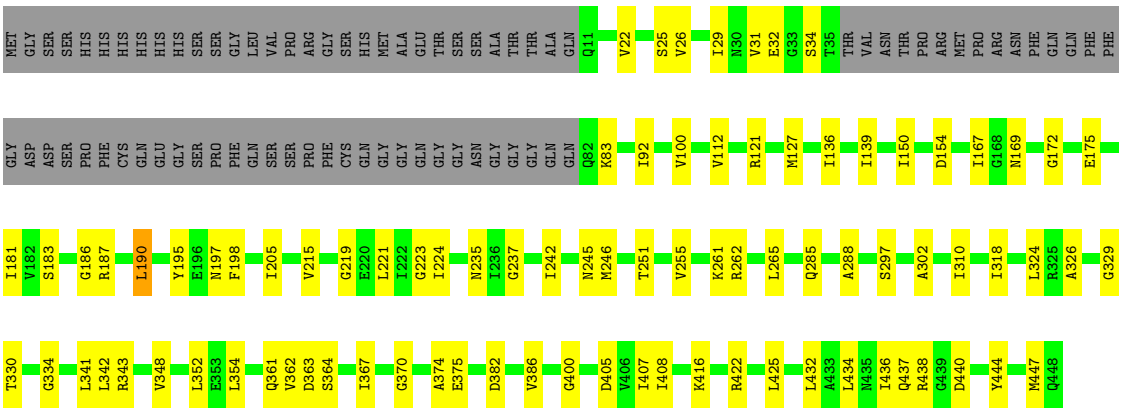
- Molecule 1: Periplasmic serine endoprotease DegP

Chain A: 64% 16% 19%



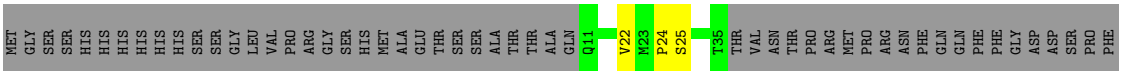
- Molecule 1: Periplasmic serine endoprotease DegP

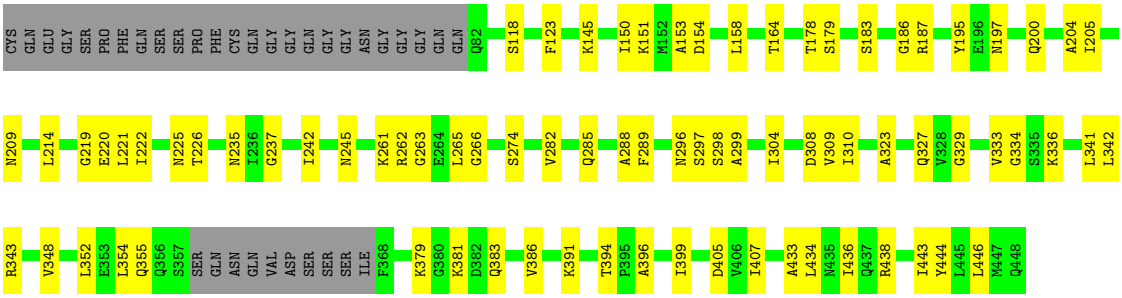
Chain B: 65% 18% 16%



- Molecule 1: Periplasmic serine endoprotease DegP

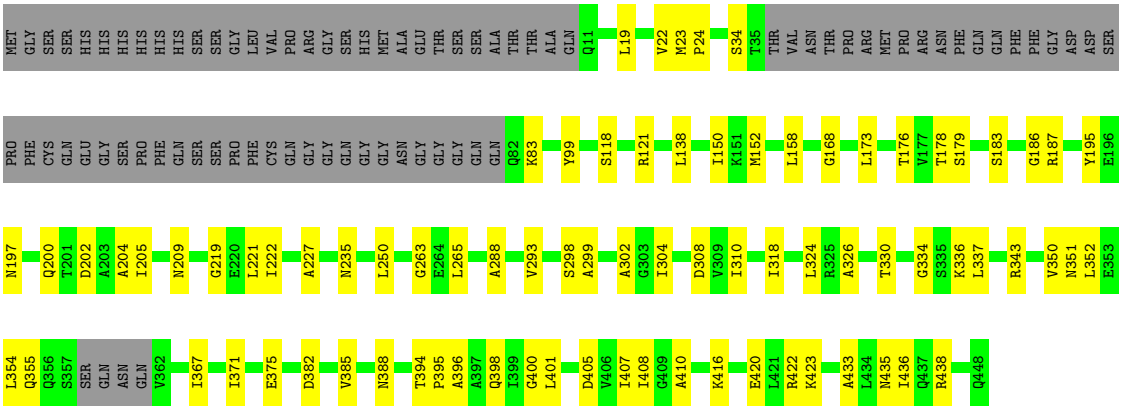
Chain C: 64% 17% 19%





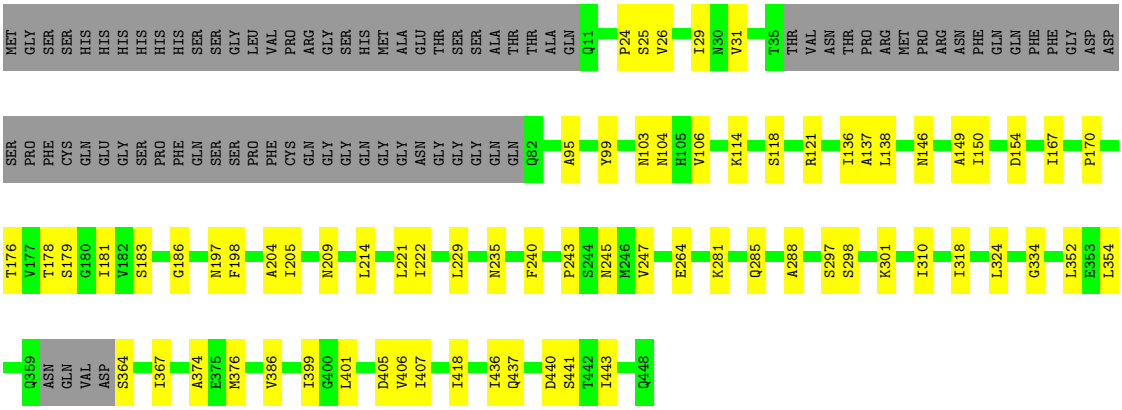
- Molecule 1: Periplasmic serine endoprotease DegP

Chain D:



- Molecule 1: Periplasmic serine endoprotease DegP

Chain E:



- Molecule 1: Periplasmic serine endoprotease DegP

Chain F:

PRO PHE CYS GLN GLU GLY SER PRO PHE GLN SER SER PRO PHE CYS GLN GLY GLY GLN GLY GLY ASN GLY GLY GLY GLN GLN Q82 I92 V100 N103 N104 H105 R121 K122 F123 K126 D135 I136 I141 K145 I150 K151 M152 A153 D154 L158 Y163

I167 T176 V177 T178 I181 V182 S183 R207 L217 E220 L221 I222 I242 N245 L265 G266 Q285 A288 S297 S298 A299 I304 V309 I310 I318 L324 V328 M331 L341 L342 V348 L352 Q356 S357 SER GLN ASN GLN VAL

ASP SER SER SER ILE F368 I371 E372 G373 A374 V390 A396 L401 D405 V406 I407 L432 A433 L434 N435 I436 I443 Y444 L445 L446 M447 Q448

- Molecule 2: TMB-CYRKL modulator

Chain G: 80% 20%

C460 Y461 R462 K463 L464

- Molecule 2: TMB-CYRKL modulator

Chain M: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: TMB-CYRKL modulator

Chain H: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: TMB-CYRKL modulator

Chain N: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: TMB-CYRKL modulator

Chain I: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: TMB-CYRKL modulator

Chain O: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: TMB-CYRKL modulator

Chain J: 80% 20%

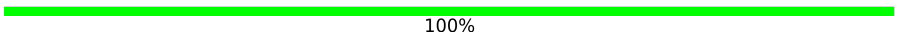
C460 Y461 R462 K463 L464

- Molecule 2: TMB-CYRKL modulator

Chain P:

There are no outlier residues recorded for this chain.

- Molecule 2: TMB-CYRKL modulator

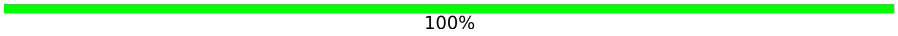
Chain K: 

There are no outlier residues recorded for this chain.

- Molecule 2: TMB-CYRKL modulator

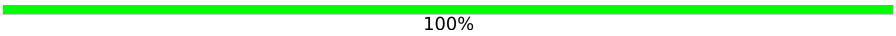
Chain Q:

- Molecule 2: TMB-CYRKL modulator

Chain L: 

There are no outlier residues recorded for this chain.

- Molecule 2: TMB-CYRKL modulator

Chain R: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	217.15Å 123.52Å 140.56Å 90.00° 118.00° 90.00°	Depositor
Resolution (Å)	35.61 – 4.16 35.61 – 4.16	Depositor EDS
% Data completeness (in resolution range)	98.5 (35.61-4.16) 98.4 (35.61-4.16)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.44 (at 4.12Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.216 , 0.278 0.216 , 0.278	Depositor DCC
R_{free} test set	1262 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	151.8	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 105.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	16906	wwPDB-VP
Average B, all atoms (Å^2)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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 (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	0.27	0/2759	0.47	0/3735
1	B	0.26	0/2845	0.47	0/3853
1	C	0.27	0/2766	0.48	0/3742
1	D	0.26	0/2808	0.48	0/3804
1	E	0.26	0/2819	0.48	0/3815
1	F	0.26	0/2751	0.47	0/3722
2	G	0.23	0/24	0.41	0/32
2	H	0.20	0/24	0.45	0/32
2	I	0.22	0/24	0.45	0/32
2	J	0.24	0/24	0.44	0/32
2	K	0.22	0/24	0.43	0/32
2	L	0.33	0/24	0.36	0/32
2	M	0.22	0/24	0.37	0/32
2	N	0.35	0/24	0.47	0/32
2	O	0.25	0/24	0.61	0/32
2	P	0.22	0/24	0.38	0/32
2	Q	0.31	0/24	0.41	0/32
2	R	0.26	0/24	0.38	0/32
All	All	0.26	0/17036	0.47	0/23055

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	2736	0	2768	52	0
1	B	2820	0	2849	58	0
1	C	2743	0	2793	53	0
1	D	2784	0	2807	50	0
1	E	2795	0	2831	48	0
1	F	2728	0	2778	43	0
2	G	25	0	9	1	0
2	H	25	0	9	0	0
2	I	25	0	9	0	0
2	J	25	0	9	1	0
2	K	25	0	9	0	0
2	L	25	0	9	0	0
2	M	25	0	9	0	0
2	N	25	0	9	0	0
2	O	25	0	9	0	0
2	P	25	0	9	0	0
2	Q	25	0	9	1	0
2	R	25	0	9	0	0
All	All	16906	0	16934	288	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 9.

All (288) 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:D:420:GLU:HA	1:D:423:LYS:HD3	1.63	0.81
1:C:158:LEU:HD11	1:C:222:ILE:HD12	1.65	0.77
1:B:341:LEU:HB2	1:B:348:VAL:HB	1.68	0.75
1:E:288:ALA:HB3	1:E:310:ILE:HB	1.68	0.75
1:D:34:SER:HA	1:D:83:LYS:HA	1.68	0.75
1:D:334:GLY:H	1:D:354:LEU:HB2	1.50	0.74
1:B:262:ARG:NH1	1:B:329:GLY:O	2.22	0.73
1:F:154:ASP:OD1	1:F:245:ASN:ND2	2.17	0.73
1:F:432:LEU:HB3	1:F:447:MET:HB2	1.71	0.72
1:C:262:ARG:NH1	1:C:329:GLY:O	2.23	0.70
1:B:150:ILE:HD13	1:B:221:LEU:HB2	1.74	0.69
1:B:367:ILE:HG22	1:B:425:LEU:HD12	1.74	0.69
1:D:183:SER:HB3	1:F:176:THR:HG23	1.74	0.69
1:A:176:THR:HG23	1:B:183:SER:HB3	1.75	0.69
1:D:158:LEU:HD11	1:D:222:ILE:HD12	1.73	0.68
1:D:187:ARG:NH1	1:D:200:GLN:OE1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:PHE:HE1	1:C:145:LYS:HE3	1.59	0.68
1:E:364:SER:N	1:E:374:ALA:O	2.28	0.67
1:B:400:GLY:O	1:B:438:ARG:NH2	2.19	0.66
1:B:432:LEU:HB3	1:B:447:MET:HB2	1.78	0.65
1:E:121:ARG:HH12	1:E:146:ASN:HB3	1.61	0.65
1:D:400:GLY:O	1:D:438:ARG:NH2	2.23	0.65
1:E:318:ILE:HD11	1:E:324:LEU:HD13	1.78	0.64
1:D:367:ILE:HG23	1:D:422:ARG:HD3	1.80	0.63
1:F:407:ILE:HG12	1:F:436:ILE:HG22	1.79	0.63
1:F:341:LEU:HB2	1:F:348:VAL:HB	1.80	0.63
1:F:288:ALA:HB3	1:F:310:ILE:HB	1.82	0.62
1:C:261:LYS:HB3	1:C:333:VAL:HG23	1.83	0.61
1:B:121:ARG:HA	1:C:285:GLN:HG2	1.83	0.60
1:D:179:SER:HB3	1:E:181:ILE:HD13	1.83	0.60
1:D:178:THR:HG21	1:D:204:ALA:HB3	1.82	0.60
1:D:202:ASP:HB3	1:F:178:THR:HG22	1.84	0.59
1:D:385:VAL:HB	1:D:407:ILE:HB	1.85	0.59
1:A:179:SER:HB3	1:B:181:ILE:HD13	1.85	0.59
1:A:32:GLU:HG2	1:A:85:MET:HG2	1.85	0.58
1:A:133:ARG:HD2	1:A:195:TYR:HE1	1.68	0.58
1:C:266:GLY:HA3	1:C:297:SER:HB2	1.85	0.58
1:D:173:LEU:HD11	1:E:229:LEU:HD22	1.85	0.58
1:B:288:ALA:HB3	1:B:310:ILE:HB	1.85	0.58
1:F:158:LEU:HD11	1:F:222:ILE:HD12	1.86	0.57
1:C:341:LEU:HB2	1:C:348:VAL:HB	1.87	0.57
1:A:379:LYS:HB2	1:A:386:VAL:HB	1.85	0.57
1:F:265:LEU:HD23	1:F:352:LEU:HD13	1.86	0.57
1:B:361:GLN:HG2	1:B:362:VAL:HG23	1.87	0.57
1:D:22:VAL:HG21	1:D:219:GLY:HA3	1.87	0.57
1:A:121:ARG:HA	1:B:285:GLN:HG2	1.86	0.57
1:B:190:LEU:HD21	1:B:198:PHE:HE2	1.69	0.56
1:E:436:ILE:HD11	1:E:443:ILE:HD11	1.87	0.56
1:F:371:ILE:HG22	1:F:372:GLU:HG2	1.86	0.56
1:A:262:ARG:NH1	1:A:329:GLY:O	2.38	0.56
1:A:150:ILE:HD13	1:A:221:LEU:HB2	1.87	0.56
1:C:263:GLY:HA3	1:C:354:LEU:HD13	1.88	0.56
1:D:263:GLY:HA3	1:D:354:LEU:HD13	1.87	0.56
1:E:364:SER:HA	1:E:376:MET:HE3	1.88	0.56
1:A:407:ILE:HG12	1:A:436:ILE:HG22	1.88	0.55
1:D:308:ASP:OD2	1:D:343:ARG:NH2	2.38	0.55
1:B:22:VAL:HG21	1:B:219:GLY:HA3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ASN:O	1:C:355:GLN:NE2	2.37	0.55
1:C:308:ASP:OD2	1:C:343:ARG:NH2	2.39	0.55
1:C:323:ALA:O	1:C:327:GLN:HG2	2.06	0.55
1:D:299:ALA:HB1	1:D:304:ILE:HD12	1.89	0.55
1:F:390:VAL:HG21	1:F:401:LEU:O	2.08	0.54
1:C:150:ILE:HD13	1:C:221:LEU:HB2	1.90	0.54
1:C:153:ALA:HB2	1:C:220:GLU:HB3	1.90	0.54
1:E:154:ASP:OD1	1:E:245:ASN:ND2	2.35	0.54
1:D:405:ASP:HB3	1:D:436:ILE:HD12	1.90	0.54
1:E:186:GLY:HA2	1:E:197:ASN:OD1	2.07	0.54
1:C:151:LYS:NZ	1:C:220:GLU:OE1	2.32	0.53
1:E:170:PRO:HD2	1:E:176:THR:HB	1.89	0.53
1:A:318:ILE:HG12	1:A:324:LEU:HB2	1.91	0.53
1:D:302:ALA:HB1	1:D:350:VAL:HG21	1.91	0.53
1:A:412:GLN:HG3	1:E:281:LYS:HB2	1.91	0.53
1:D:152:MET:HG2	1:D:221:LEU:HD23	1.91	0.52
1:D:396:ALA:HB1	1:D:401:LEU:HD12	1.91	0.52
1:B:215:VAL:HG12	1:B:221:LEU:HA	1.91	0.52
1:C:436:ILE:HD11	1:C:443:ILE:HD11	1.90	0.52
1:B:190:LEU:HD21	1:B:198:PHE:CE2	2.44	0.52
1:C:235:ASN:OD1	1:C:237:GLY:N	2.37	0.52
1:F:266:GLY:HA3	1:F:297:SER:HB2	1.90	0.52
1:C:298:SER:N	1:C:355:GLN:OE1	2.42	0.52
1:D:375:GLU:O	1:D:388:ASN:N	2.41	0.52
1:B:34:SER:HA	1:B:83:LYS:HA	1.92	0.52
1:A:143:ASN:HB3	1:A:145:LYS:HE2	1.90	0.52
1:A:309:VAL:HB	1:A:342:LEU:HB3	1.92	0.52
1:D:176:THR:HG23	1:E:183:SER:HB3	1.92	0.52
1:B:386:VAL:HA	1:B:405:ASP:O	2.10	0.52
1:C:299:ALA:HB1	1:C:304:ILE:HD12	1.92	0.52
1:C:407:ILE:HG12	1:C:436:ILE:HG22	1.91	0.52
1:F:434:LEU:O	1:F:444:TYR:HA	2.10	0.51
1:B:154:ASP:OD1	1:B:245:ASN:ND2	2.33	0.51
1:D:99:TYR:HB3	1:D:138:LEU:HD11	1.93	0.51
1:E:103:ASN:HB2	1:E:106:VAL:HG23	1.93	0.51
1:D:318:ILE:HD13	1:D:324:LEU:HD22	1.92	0.51
1:F:432:LEU:O	1:F:446:LEU:HA	2.10	0.51
1:B:407:ILE:HA	1:B:436:ILE:HA	1.92	0.51
1:A:186:GLY:HA2	1:A:197:ASN:OD1	2.10	0.51
1:D:186:GLY:HA2	1:D:197:ASN:OD1	2.10	0.51
1:A:205:ILE:H	1:A:235:ASN:ND2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ASP:OD1	1:C:245:ASN:ND2	2.31	0.50
1:C:214:LEU:HB2	1:C:225:ASN:OD1	2.11	0.50
1:E:178:THR:HG21	1:E:204:ALA:HB3	1.93	0.50
1:A:133:ARG:HB3	1:A:195:TYR:CD1	2.47	0.50
1:C:434:LEU:O	1:C:444:TYR:HA	2.11	0.50
1:E:104:ASN:HA	1:E:137:ALA:HB2	1.94	0.50
1:D:318:ILE:HG21	1:D:324:LEU:HB2	1.93	0.49
1:E:121:ARG:HA	1:F:285:GLN:HG2	1.93	0.49
1:D:250:LEU:HG	1:D:330:THR:HB	1.92	0.49
1:D:265:LEU:HB3	1:D:299:ALA:HB2	1.94	0.49
1:D:121:ARG:HG2	1:E:285:GLN:HG2	1.94	0.49
1:E:214:LEU:O	1:E:222:ILE:HG12	2.13	0.49
1:F:163:TYR:HB2	1:F:217:LEU:HD11	1.94	0.49
1:F:436:ILE:HD11	1:F:443:ILE:HD11	1.94	0.49
1:B:432:LEU:HD21	1:B:434:LEU:HD21	1.94	0.49
1:C:334:GLY:H	1:C:354:LEU:HB2	1.78	0.49
1:C:405:ASP:HB3	1:C:436:ILE:HD12	1.96	0.48
1:F:105:HIS:HD1	1:F:135:ASP:CG	2.16	0.48
1:D:150:ILE:HD13	1:D:221:LEU:HB2	1.94	0.48
1:C:381:LYS:O	1:C:383:GLN:NE2	2.35	0.48
1:B:25:SER:OG	1:B:150:ILE:HB	2.14	0.48
1:D:336:LYS:HA	1:D:352:LEU:O	2.14	0.48
1:F:153:ALA:HB2	1:F:220:GLU:HB3	1.95	0.48
1:B:363:ASP:HA	1:B:375:GLU:HA	1.95	0.48
1:E:150:ILE:HD13	1:E:221:LEU:HB2	1.94	0.48
1:E:198:PHE:HB3	1:E:240:PHE:HB3	1.96	0.47
1:C:186:GLY:HA2	1:C:197:ASN:OD1	2.14	0.47
1:B:251:THR:O	1:B:255:VAL:HG23	2.14	0.47
1:E:405:ASP:HB3	1:E:436:ILE:HD12	1.97	0.47
1:A:205:ILE:HG23	1:A:209:ASN:CB	2.45	0.47
1:A:205:ILE:HG23	1:A:209:ASN:HB2	1.97	0.47
1:D:298:SER:HB3	1:D:355:GLN:HG2	1.96	0.47
1:E:170:PRO:HG3	1:E:209:ASN:OD1	2.15	0.47
1:F:356:GLN:HG2	1:F:357:SER:N	2.29	0.47
1:D:371:ILE:HA	1:D:395:PRO:HB2	1.97	0.47
1:D:227:ALA:HB1	2:J:462:ARG:O	2.15	0.47
1:F:299:ALA:HB1	1:F:304:ILE:HD12	1.96	0.47
1:A:298:SER:HB2	1:A:352:LEU:HD22	1.96	0.47
1:F:19:LEU:HD11	1:F:177:VAL:HG11	1.96	0.47
1:E:26:VAL:HG11	1:E:167:ILE:HG22	1.96	0.46
1:C:396:ALA:O	1:C:399:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:LEU:O	1:D:351:ASN:HA	2.15	0.46
1:F:151:LYS:NZ	1:F:220:GLU:OE1	2.45	0.46
1:A:181:ILE:HD13	1:C:179:SER:HB3	1.97	0.46
1:B:136:ILE:HD11	1:B:242:ILE:HD12	1.97	0.46
1:B:221:LEU:HD21	1:B:224:ILE:HD11	1.97	0.46
1:B:367:ILE:HG23	1:B:422:ARG:HD3	1.98	0.46
1:B:334:GLY:H	1:B:354:LEU:HB2	1.80	0.46
1:E:334:GLY:H	1:E:354:LEU:HB2	1.80	0.46
1:B:25:SER:HA	1:B:92:ILE:HD12	1.97	0.46
1:B:187:ARG:HA	1:B:187:ARG:HD3	1.68	0.46
1:F:318:ILE:HD12	1:F:318:ILE:HA	1.78	0.46
1:A:251:THR:O	1:A:255:VAL:HG23	2.16	0.46
1:B:26:VAL:HG11	1:B:167:ILE:HG22	1.98	0.46
1:B:175:GLU:O	1:C:187:ARG:NH2	2.49	0.46
1:E:176:THR:HG23	1:F:183:SER:HB3	1.98	0.46
1:A:178:THR:HG21	1:A:204:ALA:HB3	1.96	0.46
1:B:246:MET:HE3	1:B:330:THR:HG21	1.98	0.45
1:D:205:ILE:HG23	1:D:209:ASN:CB	2.47	0.45
1:F:352:LEU:HA	1:F:352:LEU:HD23	1.77	0.45
1:A:187:ARG:HA	1:A:187:ARG:HD3	1.82	0.45
1:B:195:TYR:HB3	1:B:326:ALA:HA	1.98	0.45
1:C:352:LEU:HA	1:C:352:LEU:HD23	1.73	0.45
1:E:179:SER:HB3	1:F:181:ILE:HD13	1.96	0.45
1:D:24:PRO:HA	1:D:118:SER:OG	2.16	0.45
1:D:352:LEU:HA	1:D:352:LEU:HD23	1.73	0.45
1:A:183:SER:HB2	1:A:200:GLN:HG2	1.99	0.45
1:A:308:ASP:OD2	1:A:343:ARG:NH2	2.50	0.45
1:D:293:VAL:HG11	1:D:304:ILE:O	2.17	0.45
1:B:169:ASN:ND2	1:B:172:GLY:HA2	2.32	0.45
1:A:152:MET:HG2	1:A:221:LEU:HD23	1.98	0.45
1:A:158:LEU:HD11	1:A:222:ILE:HB	1.99	0.45
1:F:318:ILE:HD11	1:F:324:LEU:HB2	1.98	0.45
1:C:336:LYS:HA	1:C:352:LEU:O	2.17	0.45
1:A:214:LEU:O	1:A:222:ILE:HG12	2.17	0.44
1:A:215:VAL:HG12	1:A:221:LEU:HA	1.98	0.44
1:A:371:ILE:HD11	1:A:422:ARG:HH12	1.80	0.44
1:D:265:LEU:HD23	1:D:352:LEU:HD13	1.98	0.44
1:C:282:VAL:HG13	1:C:342:LEU:HD23	1.99	0.44
1:B:261:LYS:HB3	1:B:261:LYS:HE2	1.77	0.44
1:E:205:ILE:HG23	1:E:209:ASN:HB2	1.98	0.44
1:F:309:VAL:O	1:F:342:LEU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ALA:HB2	1:A:220:GLU:HB3	1.99	0.44
1:B:235:ASN:OD1	1:B:237:GLY:N	2.46	0.44
1:A:187:ARG:NH1	1:A:200:GLN:OE1	2.51	0.44
1:C:265:LEU:HD23	1:C:352:LEU:HD13	2.00	0.44
1:A:198:PHE:HB3	1:A:240:PHE:HB3	1.99	0.44
1:B:92:ILE:HA	1:B:100:VAL:HG22	1.99	0.44
1:C:379:LYS:HB2	1:C:386:VAL:HB	1.99	0.44
1:E:25:SER:OG	1:E:150:ILE:HB	2.17	0.44
1:B:32:GLU:HB2	1:B:112:VAL:HB	2.00	0.44
1:D:382:ASP:HB3	1:D:416:LYS:HD3	1.99	0.44
1:E:407:ILE:HG12	1:E:436:ILE:HG22	2.00	0.44
1:F:126:LYS:HA	1:F:126:LYS:HD3	1.66	0.43
1:A:382:ASP:HB3	1:A:416:LYS:HB3	1.99	0.43
1:B:186:GLY:HA2	1:B:197:ASN:OD1	2.18	0.43
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.64	0.43
1:C:391:LYS:O	1:C:394:THR:OG1	2.36	0.43
1:A:226:THR:OG1	1:A:242:ILE:HG13	2.18	0.43
1:C:226:THR:OG1	1:C:242:ILE:HG13	2.18	0.43
1:A:399:ILE:O	1:A:445:LEU:HD22	2.19	0.43
1:C:214:LEU:O	1:C:222:ILE:HG12	2.19	0.43
1:C:433:ALA:HA	1:C:446:LEU:HD23	1.99	0.43
1:E:386:VAL:HA	1:E:406:VAL:HA	2.00	0.43
1:B:364:SER:HB3	1:B:374:ALA:HB3	2.00	0.43
1:A:297:SER:O	1:A:301:LYS:HG3	2.19	0.43
1:B:265:LEU:O	1:B:297:SER:HB2	2.18	0.43
1:B:29:ILE:HG22	1:B:31:VAL:HG23	2.00	0.43
1:B:302:ALA:HB2	1:B:352:LEU:HD21	2.00	0.43
1:B:382:ASP:HB3	1:B:416:LYS:HB3	2.00	0.43
1:C:22:VAL:HG21	1:C:219:GLY:HA3	2.01	0.43
1:C:205:ILE:O	1:C:235:ASN:HB2	2.18	0.43
1:D:195:TYR:HB3	1:D:326:ALA:HA	2.00	0.42
1:A:227:ALA:HB1	2:G:462:ARG:O	2.19	0.42
1:C:205:ILE:HG23	1:C:209:ASN:CB	2.49	0.42
1:D:410:ALA:HA	1:D:433:ALA:O	2.19	0.42
1:A:396:ALA:O	1:A:399:ILE:HG12	2.18	0.42
1:B:190:LEU:HD23	1:B:190:LEU:H	1.84	0.42
1:B:318:ILE:HG12	1:B:324:LEU:HB2	2.01	0.42
1:B:364:SER:N	1:B:374:ALA:O	2.52	0.42
1:B:434:LEU:O	1:B:444:TYR:HA	2.19	0.42
1:C:274:SER:HA	1:C:285:GLN:HG3	2.02	0.42
1:D:168:GLY:HA3	1:D:209:ASN:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:ALA:HB3	1:D:310:ILE:HB	2.01	0.42
1:F:374:ALA:HB2	1:F:396:ALA:HB1	2.01	0.42
1:B:440:ASP:OD1	1:B:440:ASP:N	2.53	0.42
1:F:25:SER:OG	1:F:150:ILE:HB	2.20	0.42
1:A:179:SER:O	1:A:203:ALA:HA	2.20	0.42
1:C:289:PHE:HD1	1:C:309:VAL:HG22	1.84	0.42
1:F:328:VAL:HA	1:F:331:MET:HG3	2.00	0.42
1:C:309:VAL:HB	1:C:342:LEU:HB3	2.02	0.42
1:E:401:LEU:HD21	1:E:436:ILE:HG21	2.02	0.42
1:F:136:ILE:HD13	1:F:136:ILE:HA	1.91	0.42
1:E:24:PRO:HA	1:E:118:SER:OG	2.20	0.42
1:E:367:ILE:HD13	1:E:418:ILE:HG23	2.02	0.42
1:F:121:ARG:NH1	1:F:145:LYS:O	2.47	0.42
1:B:223:GLY:HA2	1:B:242:ILE:O	2.20	0.41
1:C:178:THR:HG21	1:C:204:ALA:HB3	2.01	0.41
1:C:288:ALA:HB3	1:C:310:ILE:HB	2.01	0.41
1:D:205:ILE:H	1:D:235:ASN:ND2	2.18	0.41
1:A:334:GLY:H	1:A:354:LEU:HB2	1.86	0.41
1:A:337:LEU:O	1:A:351:ASN:HA	2.20	0.41
1:C:183:SER:N	1:C:200:GLN:O	2.47	0.41
1:F:374:ALA:HB2	1:F:396:ALA:CB	2.50	0.41
1:A:288:ALA:HB3	1:A:310:ILE:HB	2.02	0.41
1:A:10:GLN:HG3	1:A:11:GLN:H	1.86	0.41
1:B:205:ILE:H	1:B:235:ASN:ND2	2.18	0.41
1:D:19:LEU:HB3	1:D:23:MET:SD	2.60	0.41
1:D:408:ILE:HB	1:D:435:ASN:O	2.21	0.41
1:E:29:ILE:HG22	1:E:31:VAL:HG23	2.02	0.41
1:F:92:ILE:HG12	1:F:100:VAL:HG22	2.03	0.41
1:A:402:LYS:HB3	1:A:402:LYS:HE3	1.90	0.41
1:B:343:ARG:HH11	1:B:348:VAL:HG21	1.86	0.41
1:E:99:TYR:HB3	1:E:138:LEU:HD11	2.02	0.41
1:D:394:THR:O	1:D:398:GLN:N	2.50	0.41
1:E:297:SER:O	1:E:301:LYS:HG3	2.21	0.41
1:E:298:SER:HB2	1:E:352:LEU:HD22	2.02	0.41
1:E:367:ILE:HD12	1:E:376:MET:HE3	2.03	0.41
1:E:399:ILE:HD11	1:E:401:LEU:HD12	2.02	0.41
1:F:167:ILE:HG12	1:F:177:VAL:HG22	2.02	0.41
1:A:250:LEU:HD21	1:A:330:THR:HG22	2.03	0.41
1:C:24:PRO:HA	1:C:118:SER:OG	2.20	0.41
1:E:136:ILE:HD13	1:E:136:ILE:HA	1.92	0.41
1:E:264:GLU:HB2	2:Q:475:LEU:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:SER:N	1:A:200:GLN:O	2.53	0.41
1:A:268:MET:HB2	1:A:292:GLN:HG3	2.02	0.41
1:B:407:ILE:HG12	1:B:436:ILE:HG22	2.02	0.41
1:C:25:SER:OG	1:C:150:ILE:HB	2.21	0.41
1:E:205:ILE:H	1:E:235:ASN:ND2	2.19	0.41
1:F:123:PHE:HB3	1:F:141:ILE:HG23	2.01	0.41
1:F:401:LEU:HA	1:F:405:ASP:OD2	2.20	0.41
1:A:272:LEU:HD11	1:A:277:ALA:HB2	2.03	0.41
1:B:408:ILE:HD11	1:B:437:GLN:CD	2.41	0.41
1:E:95:ALA:HB2	1:E:149:ALA:HB2	2.03	0.41
1:C:195:TYR:CE2	1:C:329:GLY:HA3	2.56	0.40
1:E:318:ILE:HG12	1:E:324:LEU:HD22	2.02	0.40
1:A:331:MET:HA	1:A:332:PRO:HD3	1.95	0.40
1:B:342:LEU:HD12	1:B:342:LEU:HA	1.99	0.40
1:B:343:ARG:NH1	1:B:348:VAL:HG21	2.36	0.40
1:C:309:VAL:O	1:C:342:LEU:N	2.55	0.40
1:E:437:GLN:HB2	1:E:441:SER:O	2.21	0.40
1:F:158:LEU:HD23	1:F:158:LEU:HA	1.87	0.40
1:E:243:PRO:O	1:E:247:VAL:HG23	2.21	0.40
1:F:136:ILE:HD11	1:F:242:ILE:HD12	2.02	0.40
1:E:440:ASP:OD1	1:E:440:ASP:N	2.54	0.40
1:A:168:GLY:HA3	1:A:209:ASN:HD22	1.86	0.40
1:B:127:MET:HA	1:B:139:ILE:HG22	2.03	0.40
1:C:164:THR:HB	1:C:214:LEU:HD11	2.04	0.40
1:C:342:LEU:HD12	1:C:342:LEU:HA	1.93	0.40
1:F:103:ASN:ND2	1:F:135:ASP:O	2.41	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	375/469 (80%)	362 (96%)	12 (3%)	1 (0%)	41	76
1	B	388/469 (83%)	376 (97%)	11 (3%)	1 (0%)	41	76
1	C	376/469 (80%)	362 (96%)	14 (4%)	0	100	100
1	D	382/469 (81%)	369 (97%)	13 (3%)	0	100	100
1	E	382/469 (81%)	375 (98%)	7 (2%)	0	100	100
1	F	373/469 (80%)	359 (96%)	14 (4%)	0	100	100
2	G	3/5 (60%)	3 (100%)	0	0	100	100
2	H	3/5 (60%)	3 (100%)	0	0	100	100
2	I	3/5 (60%)	3 (100%)	0	0	100	100
2	J	3/5 (60%)	3 (100%)	0	0	100	100
2	K	3/5 (60%)	3 (100%)	0	0	100	100
2	L	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
2	M	3/5 (60%)	3 (100%)	0	0	100	100
2	N	3/5 (60%)	3 (100%)	0	0	100	100
2	O	3/5 (60%)	3 (100%)	0	0	100	100
2	P	3/5 (60%)	3 (100%)	0	0	100	100
2	Q	3/5 (60%)	3 (100%)	0	0	100	100
2	R	3/5 (60%)	3 (100%)	0	0	100	100
All	All	2312/2874 (80%)	2238 (97%)	72 (3%)	2 (0%)	51	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	B	370	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	287/374 (77%)	286 (100%)	1 (0%)	92	95
1	B	300/374 (80%)	299 (100%)	1 (0%)	92	95
1	C	290/374 (78%)	289 (100%)	1 (0%)	92	95
1	D	295/374 (79%)	295 (100%)	0	100	100
1	E	298/374 (80%)	297 (100%)	1 (0%)	92	95
1	F	288/374 (77%)	287 (100%)	1 (0%)	92	95
All	All	1758/2244 (78%)	1753 (100%)	5 (0%)	92	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	ARG
1	B	190	LEU
1	C	438	ARG
1	E	114	LYS
1	F	207	ARG

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

Mol	Chain	Res	Type
1	E	369	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 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.