Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:22 pm BST

PDB ID	:	2HA9
Title	:	Crystal structure of protein SP0239 from Streptococcus pneumoniae
Authors	:	Chang, C.; Hatzos, C.; Abdullah, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2006-06-12
Resolution	:	2.70 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 ⓘ symbol.

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

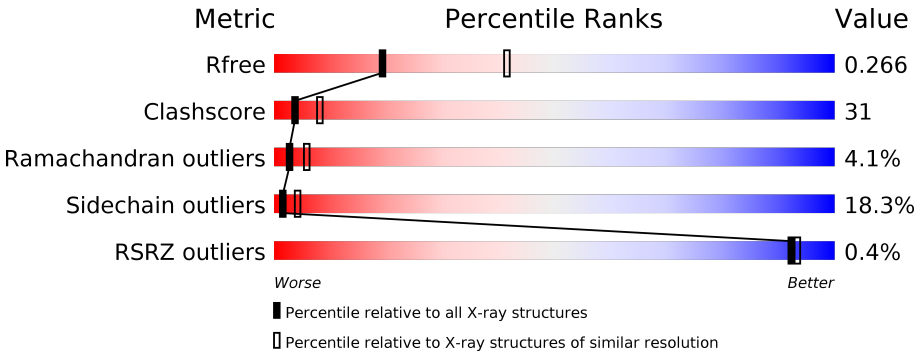
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	446	49% 31% 10% • 7%
1	B	446	47% 33% 10% • 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6011 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 UPF0210 protein SP0239.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	Se	0	0	0
			2978	1867	504	586	4	17			
1	B	415	Total	C	N	O	S	Se	0	0	0
			2979	1865	508	587	3	16			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	CLONING ARTIFACT	UNP Q97ST4
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
A	12	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
A	25	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
A	158	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
A	164	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
A	177	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
A	195	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
A	255	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
A	288	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
A	315	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
A	336	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
A	353	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
A	363	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
A	378	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
A	390	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
A	406	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
A	419	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
B	0	ALA	-	CLONING ARTIFACT	UNP Q97ST4
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
B	12	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
B	25	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
B	158	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
B	164	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
B	177	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	195	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
B	255	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
B	288	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
B	315	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
B	336	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
B	353	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
B	363	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
B	378	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
B	390	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
B	406	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4
B	419	MSE	MET	MODIFIED RESIDUE	UNP Q97ST4

- Molecule 2 is water.

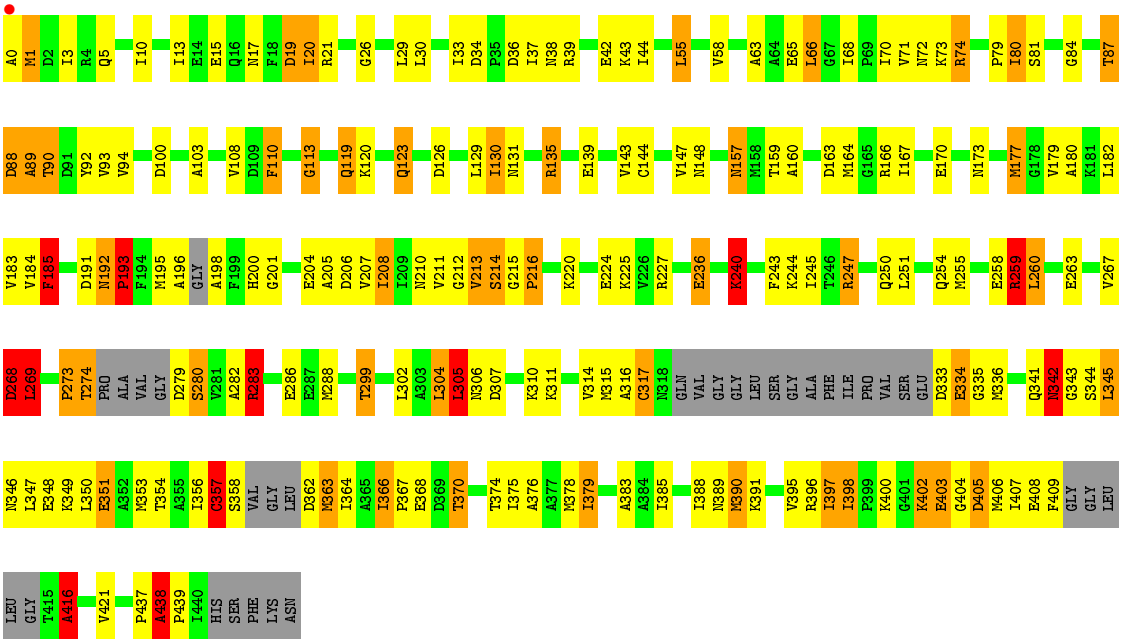
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	27	Total O 27 27	0	0
2	B	27	Total O 27 27	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

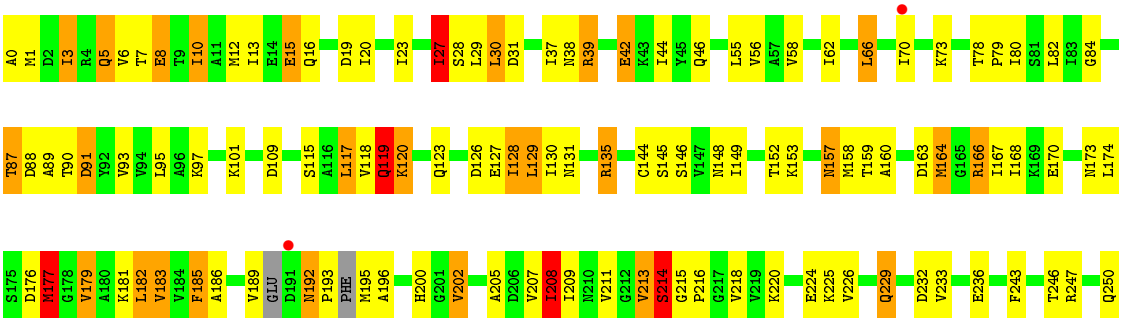
- Molecule 1: UPF0210 protein SP0239

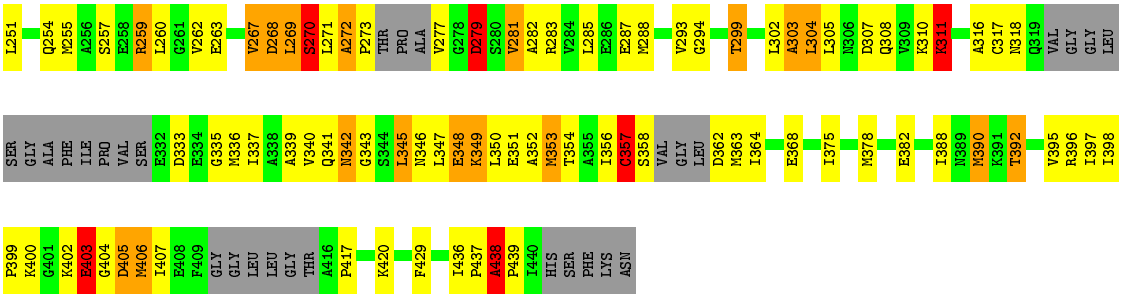
Chain A:



- Molecule 1: UPF0210 protein SP0239

Chain B:




L251 Q254 M255 A256 S257 E258 R259 L260 G261 V262 E263 V267 D268 L269 S270 L271 A272 P273 THR PRO ALA V277 G278 D279 S280 V281 A282 R283 V284 L285 E286 E287 M288 V293 G294 T299 L302 A303 L304 L305 N306 D307 Q308 V309 K310 K311 A316 C317 N318 Q319 VAL GLY GLY LEU
SER GLY ALA PHE ILE PRO VAL SER E332 D333 E334 G335 M336 I337 A338 A339 V340 Q341 N342 G343 S344 L345 N346 L347 E348 K349 L350 E351 A352 M353 T354 A355 I356 C357 S358 VAL GLY LEU D362 M363 I364 E368 I375 M378 E382 I388 N389 M390 K391 T392 V395 R396 I397 I398
P399 K400 G401 K402 E403 G404 D405 M406 I407 E408 F409 GLY GLY LEU LEU GLY THR A416 P417 K420 F429 I436 P437 A438 P439 I440 HIS SER PHE LYS ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.91Å 139.96Å 148.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 43.58 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.70) 95.4 (43.58-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.271 0.191 , 0.266	Depositor DCC
R_{free} test set	1672 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	59.2	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6011	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.51	22/2982 (0.7%)	1.39	28/4004 (0.7%)
1	B	1.59	31/2982 (1.0%)	1.43	31/4002 (0.8%)
All	All	1.55	53/5964 (0.9%)	1.41	59/8006 (0.7%)

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	A	0	5
1	B	0	3
All	All	0	8

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	PHE	CB-CG	-11.41	1.31	1.51
1	B	123	GLN	CG-CD	8.77	1.71	1.51
1	B	185	PHE	CB-CG	-8.31	1.37	1.51
1	B	144	CYS	CB-SG	-8.30	1.68	1.82
1	A	334	GLU	CG-CD	7.95	1.63	1.51
1	A	383	ALA	CA-CB	-7.91	1.35	1.52
1	B	220	LYS	CD-CE	7.88	1.71	1.51
1	B	177	MSE	CG-SE	7.04	2.19	1.95
1	B	183	VAL	CB-CG1	-6.98	1.38	1.52
1	B	123	GLN	CD-NE2	6.95	1.50	1.32
1	B	357	CYS	CB-SG	-6.89	1.70	1.82
1	A	143	VAL	CB-CG2	-6.38	1.39	1.52
1	B	101	LYS	CD-CE	6.27	1.67	1.51
1	B	438	ALA	N-CA	6.21	1.58	1.46
1	B	27	ILE	CA-CB	6.17	1.69	1.54
1	B	8	GLU	CB-CG	-6.16	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	LYS	CD-CE	6.11	1.66	1.51
1	A	314	VAL	CB-CG2	-5.93	1.40	1.52
1	B	214	SER	CA-CB	5.81	1.61	1.52
1	B	403	GLU	CG-CD	5.76	1.60	1.51
1	A	283	ARG	CZ-NH1	5.74	1.40	1.33
1	A	183	VAL	CB-CG2	-5.70	1.40	1.52
1	B	420	LYS	CA-CB	5.66	1.66	1.53
1	A	351	GLU	CG-CD	5.63	1.60	1.51
1	B	236	GLU	CD-OE1	5.59	1.31	1.25
1	B	186	ALA	CA-CB	-5.56	1.40	1.52
1	B	119	GLN	CB-CG	-5.56	1.37	1.52
1	A	438	ALA	CA-C	-5.52	1.38	1.52
1	B	185	PHE	CA-CB	-5.51	1.41	1.53
1	A	438	ALA	N-CA	5.45	1.57	1.46
1	B	202	VAL	CA-CB	-5.44	1.43	1.54
1	B	39	ARG	CG-CD	5.44	1.65	1.51
1	A	185	PHE	CD1-CE1	-5.42	1.28	1.39
1	B	303	ALA	CA-CB	-5.42	1.41	1.52
1	B	236	GLU	CG-CD	5.42	1.60	1.51
1	A	139	GLU	CD-OE1	5.39	1.31	1.25
1	B	185	PHE	CD2-CE2	-5.35	1.28	1.39
1	B	243	PHE	CE1-CZ	5.29	1.47	1.37
1	A	263	GLU	CD-OE2	5.28	1.31	1.25
1	A	42	GLU	CG-CD	5.26	1.59	1.51
1	A	224	GLU	CB-CG	5.25	1.62	1.52
1	A	236	GLU	CG-CD	5.25	1.59	1.51
1	A	103	ALA	CA-CB	-5.24	1.41	1.52
1	B	42	GLU	CB-CG	5.17	1.61	1.52
1	A	123	GLN	CD-NE2	5.16	1.45	1.32
1	B	220	LYS	CE-NZ	5.16	1.61	1.49
1	B	135	ARG	CG-CD	5.15	1.64	1.51
1	B	118	VAL	CB-CG2	5.14	1.63	1.52
1	A	110	PHE	CB-CG	-5.13	1.42	1.51
1	B	220	LYS	CB-CG	5.12	1.66	1.52
1	A	240	LYS	CD-CE	5.11	1.64	1.51
1	A	376	ALA	CA-CB	-5.07	1.41	1.52
1	B	101	LYS	CE-NZ	5.04	1.61	1.49

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	185	PHE	CB-CA-C	-10.06	90.28	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	208	ILE	CG1-CB-CG2	-9.71	90.05	111.40
1	A	185	PHE	CB-CA-C	-9.63	91.14	110.40
1	A	163	ASP	CB-CG-OD1	9.37	126.73	118.30
1	B	126	ASP	CB-CG-OD2	-9.17	110.05	118.30
1	B	208	ILE	CB-CA-C	-9.03	93.54	111.60
1	A	269	LEU	CA-CB-CG	8.90	135.78	115.30
1	B	438	ALA	C-N-CD	-8.76	101.33	120.60
1	B	417	PRO	N-CA-CB	8.45	113.44	103.30
1	B	398	ILE	C-N-CD	8.36	145.96	128.40
1	B	164	MSE	CG-SE-CE	-8.15	80.97	98.90
1	A	268	ASP	N-CA-C	7.97	132.53	111.00
1	B	166	ARG	NE-CZ-NH1	-7.85	116.37	120.30
1	B	353	MSE	CG-SE-CE	7.78	116.02	98.90
1	B	126	ASP	CB-CG-OD1	7.45	125.00	118.30
1	A	129	LEU	CA-CB-CG	-7.25	98.62	115.30
1	B	82	LEU	CB-CG-CD1	-7.13	98.88	111.00
1	A	317	CYS	CA-CB-SG	-7.11	101.19	114.00
1	A	247	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	B	357	CYS	CA-CB-SG	-7.03	101.34	114.00
1	A	283	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	A	213	VAL	CB-CA-C	-6.76	98.55	111.40
1	B	390	MSE	CA-CB-CG	-6.70	101.92	113.30
1	B	213	VAL	CB-CA-C	-6.69	98.69	111.40
1	A	173	ASN	N-CA-CB	6.64	122.55	110.60
1	B	438	ALA	C-N-CA	6.46	149.14	122.00
1	A	304	LEU	CB-CG-CD1	-6.43	100.07	111.00
1	B	263	GLU	CB-CA-C	-6.41	97.57	110.40
1	A	20	ILE	CG1-CB-CG2	-6.39	97.35	111.40
1	A	305	LEU	CA-CB-CG	6.30	129.78	115.30
1	B	129	LEU	CA-CB-CG	-6.02	101.45	115.30
1	B	357	CYS	N-CA-C	6.00	127.20	111.00
1	A	438	ALA	N-CA-C	-5.95	94.93	111.00
1	B	270	SER	N-CA-C	5.88	126.86	111.00
1	A	177	MSE	CG-SE-CE	5.79	111.64	98.90
1	B	220	LYS	CD-CE-NZ	5.74	124.90	111.70
1	B	27	ILE	CA-CB-CG1	5.72	121.86	111.00
1	A	193	PRO	N-CA-C	5.70	126.91	112.10
1	B	311	LYS	CD-CE-NZ	-5.66	98.68	111.70
1	B	145	SER	N-CA-CB	-5.63	102.06	110.50
1	B	46	GLN	C-N-CA	-5.60	107.70	121.70
1	B	31	ASP	CB-CG-OD1	-5.56	113.30	118.30
1	B	97	LYS	CD-CE-NZ	-5.54	98.95	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	119	GLN	CB-CA-C	-5.50	99.39	110.40
1	B	438	ALA	N-CA-C	-5.50	96.14	111.00
1	B	163	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	220	LYS	CD-CE-NZ	5.46	124.25	111.70
1	B	117	LEU	CB-CG-CD2	5.41	120.19	111.00
1	A	259	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	55	LEU	CB-CG-CD2	5.29	120.00	111.00
1	B	123	GLN	CB-CA-C	5.27	120.93	110.40
1	A	100	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	88	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	A	90	THR	N-CA-CB	-5.20	100.42	110.30
1	A	144	CYS	CA-CB-SG	-5.14	104.74	114.00
1	A	247	ARG	CG-CD-NE	-5.13	101.03	111.80
1	A	385	ILE	CG1-CB-CG2	-5.12	100.13	111.40
1	B	88	ASP	CB-CG-OD1	-5.06	113.74	118.30
1	A	398	ILE	CB-CA-C	-5.04	101.53	111.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	ASN	Peptide
1	A	268	ASP	Peptide
1	A	269	LEU	Peptide
1	A	416	ALA	Peptide
1	A	437	PRO	Peptide
1	B	268	ASP	Peptide
1	B	269	LEU	Peptide
1	B	437	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	2978	0	3041	205	0
1	B	2979	0	3035	193	0
2	A	27	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	0	5	0
All	All	6011	0	6076	375	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 31.

All (375) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ILE:CD1	1:A:208:ILE:CG1	1.74	1.60
1:B:364:ILE:CG1	1:B:364:ILE:CD1	1.84	1.50
1:B:177:MSE:CG	1:B:177:MSE:SE	2.19	1.39
1:B:251:LEU:HG	1:B:255:MSE:CE	1.68	1.22
1:A:438:ALA:HB2	1:B:311:LYS:HZ3	1.10	1.13
1:B:251:LEU:HG	1:B:255:MSE:HE2	1.18	1.11
1:B:208:ILE:HD13	1:B:208:ILE:N	1.54	1.10
1:A:177:MSE:HE2	1:A:409:PHE:CB	1.82	1.09
1:B:3:ILE:H	1:B:3:ILE:HD13	1.15	1.09
1:A:251:LEU:HD11	1:A:255:MSE:HE3	1.17	1.09
1:A:438:ALA:HB2	1:B:311:LYS:NZ	1.69	1.07
1:B:273:PRO:HD2	1:B:279:ASP:HB2	1.11	1.06
1:B:251:LEU:CG	1:B:255:MSE:HE2	1.85	1.06
1:B:349:LYS:HG3	1:B:353:MSE:CE	1.85	1.06
1:B:273:PRO:CD	1:B:279:ASP:HB2	1.84	1.05
1:B:176:ASP:O	1:B:400:LYS:HE3	1.57	1.04
1:B:375:ILE:HA	1:B:378:MSE:HE3	1.40	1.04
1:A:251:LEU:CD1	1:A:255:MSE:HE3	1.91	1.01
1:B:87:THR:HG23	1:B:89:ALA:H	1.24	1.00
1:A:349:LYS:HG3	1:A:353:MSE:HE3	1.42	0.99
1:B:349:LYS:HG3	1:B:353:MSE:HE3	1.41	0.99
1:B:375:ILE:HA	1:B:378:MSE:CE	1.93	0.97
1:A:19:ASP:CB	1:A:214:SER:HB3	1.94	0.96
1:A:438:ALA:CB	1:A:439:PRO:HA	1.96	0.96
1:A:251:LEU:HD11	1:A:255:MSE:CE	1.95	0.96
1:A:19:ASP:HB3	1:A:214:SER:HB3	1.49	0.95
1:A:342:ASN:HD21	1:A:344:SER:HB3	1.26	0.95
1:B:0:ALA:HB3	1:B:251:LEU:HD13	1.47	0.95
1:A:341:GLN:HE21	1:A:406:MSE:HE1	1.30	0.92
1:A:311:LYS:NZ	1:B:438:ALA:CB	2.33	0.91
1:A:438:ALA:CB	1:A:439:PRO:CA	2.50	0.90
1:A:71:VAL:HG12	1:A:72:ASN:ND2	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ILE:HG22	1:A:167:ILE:HD13	1.53	0.89
1:A:374:THR:HG22	1:A:378:MSE:CE	2.03	0.89
1:A:65:GLU:OE1	1:A:259:ARG:NH2	2.06	0.88
1:A:438:ALA:HB1	1:A:439:PRO:CA	2.04	0.87
1:B:0:ALA:N	1:B:5:GLN:HE22	1.71	0.87
1:A:342:ASN:ND2	1:A:344:SER:HB3	1.90	0.86
1:A:273:PRO:CD	1:A:279:ASP:O	2.24	0.85
1:A:311:LYS:NZ	1:B:438:ALA:HB2	1.90	0.84
1:B:0:ALA:HB1	1:B:6:VAL:HA	1.57	0.84
1:B:66:LEU:HD21	1:B:255:MSE:HE1	1.59	0.84
1:B:251:LEU:CD1	1:B:255:MSE:HE2	2.07	0.84
1:A:438:ALA:CB	1:B:311:LYS:NZ	2.40	0.84
1:B:273:PRO:CG	1:B:277:VAL:HA	2.08	0.84
1:A:311:LYS:HZ1	1:B:438:ALA:CB	1.90	0.84
1:A:438:ALA:HB1	1:A:439:PRO:HA	1.57	0.83
1:A:342:ASN:ND2	1:A:344:SER:CB	2.41	0.83
1:B:131:ASN:HD21	1:B:166:ARG:HH22	1.24	0.83
1:A:341:GLN:HE21	1:A:406:MSE:CE	1.92	0.82
1:B:87:THR:CG2	1:B:89:ALA:H	1.91	0.82
1:B:0:ALA:N	1:B:5:GLN:NE2	2.27	0.82
1:A:438:ALA:CB	1:B:311:LYS:HZ3	1.90	0.82
1:A:349:LYS:HG3	1:A:353:MSE:CE	2.09	0.82
1:A:268:ASP:O	1:A:269:LEU:HD23	1.80	0.80
1:B:282:ALA:HB3	1:B:335:GLY:HA3	1.63	0.80
1:B:333:ASP:CB	2:B:446:HOH:O	2.27	0.80
1:A:20:ILE:CG2	1:A:70:ILE:HG12	2.12	0.79
1:A:282:ALA:O	1:A:286:GLU:HG3	1.82	0.79
1:B:3:ILE:N	1:B:3:ILE:HD13	1.97	0.79
1:A:367:PRO:O	1:A:370:THR:HG23	1.82	0.79
1:B:0:ALA:HA	1:B:5:GLN:NE2	1.98	0.79
1:A:438:ALA:HB3	1:A:439:PRO:HA	1.65	0.78
1:B:208:ILE:CD1	1:B:208:ILE:N	2.43	0.78
1:A:374:THR:HG22	1:A:378:MSE:HE1	1.65	0.78
1:B:349:LYS:O	1:B:353:MSE:HG3	1.83	0.78
1:B:349:LYS:HG3	1:B:353:MSE:HE2	1.64	0.78
1:B:207:VAL:HG12	1:B:262:VAL:HG13	1.65	0.78
1:B:3:ILE:H	1:B:3:ILE:CD1	1.92	0.78
1:B:395:VAL:HG12	1:B:397:ILE:HG13	1.66	0.78
1:B:247:ARG:NH1	1:B:316:ALA:HB1	1.99	0.77
1:B:192:ASN:CB	1:B:193:PRO:HD3	2.15	0.76
1:B:208:ILE:H	1:B:208:ILE:HD13	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLY:O	1:A:87:THR:HB	1.85	0.76
1:B:0:ALA:CA	1:B:5:GLN:NE2	2.49	0.75
1:A:208:ILE:CD1	1:A:208:ILE:CG2	2.63	0.75
1:B:200:HIS:CE1	1:B:208:ILE:HD11	2.21	0.75
1:B:350:LEU:O	1:B:354:THR:HG23	1.85	0.75
1:B:247:ARG:HH11	1:B:250:GLN:HE22	1.33	0.75
1:A:273:PRO:HD2	1:A:279:ASP:O	1.87	0.74
1:B:0:ALA:H1	1:B:5:GLN:HE22	1.34	0.74
1:A:208:ILE:CD1	1:A:208:ILE:HG21	2.18	0.73
1:B:157:ASN:HD22	1:B:157:ASN:C	1.88	0.73
1:B:157:ASN:HD21	1:B:159:THR:HB	1.53	0.73
1:B:207:VAL:HG12	1:B:262:VAL:CG1	2.19	0.73
1:A:131:ASN:HD21	1:A:166:ARG:HH12	1.36	0.73
1:B:56:VAL:HG13	1:B:73:LYS:CD	2.18	0.72
1:A:345:LEU:HD21	1:A:353:MSE:HE1	1.71	0.72
1:B:0:ALA:CB	1:B:251:LEU:HD13	2.19	0.72
1:A:406:MSE:SE	1:A:416:ALA:HB1	2.40	0.71
1:A:205:ALA:HB3	1:A:208:ILE:CG1	2.21	0.71
1:A:20:ILE:HG21	1:A:70:ILE:HG12	1.71	0.71
1:B:247:ARG:HH12	1:B:316:ALA:HB1	1.56	0.71
1:A:306:ASN:HB2	1:A:357:CYS:SG	2.31	0.70
1:A:311:LYS:HZ3	1:B:438:ALA:CB	2.04	0.70
1:B:342:ASN:HD22	1:B:342:ASN:C	1.94	0.70
1:A:311:LYS:NZ	1:B:438:ALA:HB1	2.08	0.69
1:A:208:ILE:HG21	1:A:208:ILE:HD13	1.73	0.69
1:A:346:ASN:HD22	1:B:348:GLU:HG3	1.57	0.69
1:B:362:ASP:HA	1:B:364:ILE:HD12	1.75	0.68
1:B:257:SER:OG	1:B:262:VAL:O	2.07	0.67
1:A:43:LYS:NZ	2:A:450:HOH:O	2.27	0.67
1:B:247:ARG:NH1	1:B:250:GLN:HE22	1.92	0.67
1:B:0:ALA:HA	1:B:5:GLN:CD	2.15	0.67
1:A:21:ARG:NH2	1:A:273:PRO:HB3	2.10	0.66
1:B:0:ALA:CB	1:B:6:VAL:HA	2.26	0.66
1:A:21:ARG:NH2	1:A:214:SER:HB2	2.10	0.66
1:B:131:ASN:ND2	1:B:166:ARG:HH22	1.94	0.66
1:A:37:ILE:HD12	1:A:87:THR:HG21	1.77	0.65
1:A:19:ASP:OD2	1:A:21:ARG:NE	2.29	0.65
1:A:157:ASN:HD21	1:A:159:THR:HB	1.61	0.65
1:A:71:VAL:CG1	1:A:72:ASN:ND2	2.59	0.65
1:A:157:ASN:HD22	1:A:157:ASN:C	1.99	0.65
1:A:93:VAL:O	1:A:93:VAL:HG12	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:PRO:HD3	1:A:279:ASP:O	1.95	0.64
1:A:195:MSE:HA	1:A:198:ALA:HB2	1.79	0.64
1:B:37:ILE:HG23	1:B:38:ASN:N	2.11	0.64
1:A:311:LYS:HZ3	1:B:438:ALA:HB2	1.62	0.64
1:A:10:ILE:O	1:A:13:ILE:HG13	1.99	0.63
1:A:364:ILE:O	1:A:364:ILE:HD12	1.99	0.63
1:A:195:MSE:O	1:A:196:ALA:HB3	1.99	0.63
1:B:192:ASN:CB	1:B:193:PRO:CD	2.76	0.63
1:B:176:ASP:O	1:B:400:LYS:CE	2.41	0.62
1:A:195:MSE:HA	1:A:198:ALA:CB	2.28	0.62
1:A:374:THR:HG22	1:A:378:MSE:HE3	1.80	0.62
1:A:388:ILE:HD12	1:A:388:ILE:C	2.19	0.62
1:B:392:THR:O	1:B:392:THR:HG22	1.98	0.62
1:B:395:VAL:CG1	1:B:397:ILE:HG13	2.29	0.62
1:B:268:ASP:C	1:B:268:ASP:OD2	2.36	0.62
1:A:341:GLN:C	1:A:343:GLY:H	2.03	0.62
1:B:273:PRO:HG2	1:B:277:VAL:HA	1.80	0.62
1:B:402:LYS:O	1:B:404:GLY:N	2.33	0.62
1:B:349:LYS:CG	1:B:353:MSE:HE3	2.23	0.62
1:A:84:GLY:HA3	1:A:92:TYR:CE2	2.34	0.61
1:B:273:PRO:HG3	1:B:277:VAL:HA	1.83	0.61
1:A:19:ASP:CB	1:A:214:SER:CB	2.76	0.61
1:A:157:ASN:ND2	1:A:160:ALA:H	1.99	0.61
1:B:0:ALA:HB1	1:B:6:VAL:CA	2.29	0.61
1:A:19:ASP:HB2	1:A:214:SER:HB3	1.83	0.60
1:B:157:ASN:ND2	1:B:157:ASN:C	2.55	0.60
1:A:208:ILE:CG2	1:A:208:ILE:HD13	2.30	0.60
1:A:1:MSE:HA	1:A:254:GLN:OE1	2.02	0.60
1:A:87:THR:CG2	1:A:89:ALA:H	2.14	0.60
1:B:56:VAL:HG13	1:B:73:LYS:HD3	1.83	0.60
1:A:349:LYS:CG	1:A:353:MSE:HE3	2.24	0.60
1:A:135:ARG:HG2	1:A:135:ARG:HH11	1.67	0.59
1:A:87:THR:HG23	1:A:89:ALA:H	1.66	0.59
1:A:346:ASN:HD22	1:B:348:GLU:CG	2.16	0.59
1:A:247:ARG:HH11	1:A:250:GLN:HE22	1.49	0.59
1:A:333:ASP:O	1:A:336:MSE:HB2	2.03	0.59
1:B:304:LEU:O	1:B:304:LEU:HD12	2.01	0.59
1:A:0:ALA:H3	1:A:251:LEU:HD13	1.68	0.59
1:B:229:GLN:HG2	1:B:233:VAL:HG11	1.85	0.58
1:B:251:LEU:HG	1:B:255:MSE:HE1	1.77	0.58
1:B:247:ARG:HH11	1:B:250:GLN:NE2	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ILE:CG2	1:B:38:ASN:N	2.66	0.58
1:B:0:ALA:HB1	1:B:6:VAL:HG22	1.86	0.58
1:B:362:ASP:HB2	1:B:396:ARG:HB2	1.84	0.58
1:A:131:ASN:ND2	1:A:166:ARG:HH12	2.01	0.57
1:B:368:GLU:HB2	1:B:400:LYS:HA	1.86	0.57
1:A:315:MSE:HG2	1:A:315:MSE:O	2.04	0.57
1:A:71:VAL:HG12	1:A:72:ASN:CG	2.23	0.57
1:B:193:PRO:O	1:B:195:MSE:CB	2.52	0.57
1:A:130:ILE:HG22	1:A:167:ILE:CD1	2.32	0.57
1:B:157:ASN:ND2	1:B:160:ALA:H	2.02	0.57
1:B:287:GLU:O	1:B:287:GLU:HG3	2.03	0.57
1:A:438:ALA:HB3	1:A:439:PRO:CA	2.28	0.57
1:B:345:LEU:HD23	1:B:346:ASN:H	1.69	0.57
1:B:375:ILE:HA	1:B:378:MSE:HE2	1.85	0.57
1:B:0:ALA:H1	1:B:5:GLN:NE2	1.94	0.57
1:A:135:ARG:HH11	1:A:135:ARG:CG	2.18	0.57
1:A:374:THR:CG2	1:A:378:MSE:CE	2.80	0.57
1:A:438:ALA:HB2	1:B:311:LYS:HZ1	1.68	0.57
1:B:268:ASP:O	1:B:268:ASP:OD2	2.23	0.57
1:B:56:VAL:HG13	1:B:73:LYS:HD2	1.86	0.57
1:B:20:ILE:HB	1:B:70:ILE:HG12	1.86	0.56
1:A:177:MSE:HE3	1:A:180:ALA:HB2	1.86	0.56
1:A:93:VAL:CG1	1:A:93:VAL:O	2.51	0.56
1:B:19:ASP:OD2	1:B:214:SER:HB3	2.05	0.56
1:A:130:ILE:HD12	1:A:164:MSE:HE1	1.87	0.56
1:A:438:ALA:CB	1:B:311:LYS:HZ1	2.17	0.56
1:A:251:LEU:HD21	1:A:255:MSE:HE1	1.87	0.56
1:B:91:ASP:HA	1:B:128:ILE:HG23	1.89	0.55
1:A:200:HIS:CE1	1:A:204:GLU:HB3	2.41	0.55
1:A:227:ARG:HG3	1:A:227:ARG:HH11	1.71	0.55
1:A:307:ASP:OD2	1:B:439:PRO:HA	2.07	0.55
1:A:19:ASP:HB2	1:A:214:SER:CB	2.37	0.55
1:B:388:ILE:C	1:B:388:ILE:HD12	2.28	0.54
1:A:157:ASN:C	1:A:157:ASN:ND2	2.61	0.54
1:A:342:ASN:ND2	1:A:344:SER:HB2	2.21	0.54
1:B:84:GLY:O	1:B:87:THR:HB	2.08	0.54
1:A:195:MSE:CA	1:A:198:ALA:HB2	2.37	0.54
1:A:366:ILE:CD1	1:A:397:ILE:CG2	2.86	0.54
1:A:363:MSE:SE	1:A:396:ARG:HH11	2.41	0.54
1:A:0:ALA:N	1:A:251:LEU:HD13	2.22	0.54
1:B:196:ALA:HB1	1:B:396:ARG:HH12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ASP:O	1:B:311:LYS:HG2	2.08	0.54
1:A:66:LEU:HD21	1:A:255:MSE:SE	2.58	0.53
1:B:66:LEU:HD21	1:B:255:MSE:CE	2.34	0.53
1:A:130:ILE:CG2	1:A:167:ILE:HD13	2.31	0.53
1:B:29:LEU:HD13	1:B:44:ILE:HG12	1.91	0.53
1:B:196:ALA:CB	1:B:396:ARG:HH12	2.21	0.53
1:A:404:GLY:O	1:A:405:ASP:O	2.27	0.53
1:A:356:ILE:HG22	1:B:388:ILE:HG12	1.90	0.53
1:B:182:LEU:O	1:B:396:ARG:HG2	2.09	0.53
1:A:126:ASP:O	1:A:130:ILE:HG12	2.08	0.53
1:A:205:ALA:HB3	1:A:208:ILE:HG13	1.90	0.52
1:A:356:ILE:HG22	1:B:388:ILE:CG1	2.39	0.52
1:A:240:LYS:HD2	1:A:244:LYS:HE3	1.92	0.52
1:A:368:GLU:CG	1:A:368:GLU:O	2.56	0.52
1:A:304:LEU:HD13	1:B:436:ILE:HG23	1.91	0.52
1:B:153:LYS:HG2	1:B:153:LYS:O	2.10	0.52
1:B:247:ARG:NH1	1:B:316:ALA:CB	2.72	0.52
1:B:56:VAL:HA	1:B:73:LYS:HD3	1.91	0.52
1:A:395:VAL:HG11	1:A:397:ILE:HD11	1.91	0.52
1:B:403:GLU:OE1	1:B:403:GLU:O	2.28	0.52
1:B:87:THR:CG2	1:B:89:ALA:N	2.67	0.52
1:A:195:MSE:HG3	1:A:196:ALA:N	2.24	0.52
1:A:375:ILE:O	1:A:379:ILE:HG13	2.10	0.51
1:A:243:PHE:CE1	1:A:315:MSE:O	2.64	0.51
1:A:71:VAL:HG12	1:A:72:ASN:HD21	1.73	0.51
1:B:127:GLU:HB2	2:B:451:HOH:O	2.10	0.51
1:A:282:ALA:HB3	1:A:335:GLY:HA3	1.93	0.51
1:B:207:VAL:C	1:B:208:ILE:HD13	2.27	0.50
1:A:131:ASN:ND2	1:A:166:ARG:NH1	2.60	0.50
1:B:164:MSE:O	1:B:168:ILE:HD12	2.11	0.50
1:A:299:THR:HG21	1:B:351:GLU:OE2	2.11	0.50
1:A:341:GLN:C	1:A:343:GLY:N	2.65	0.50
1:B:120:LYS:HG3	2:B:470:HOH:O	2.11	0.50
1:A:29:LEU:HD13	1:A:44:ILE:HD13	1.94	0.50
1:A:36:ASP:CG	1:A:39:ARG:HG3	2.32	0.50
1:A:438:ALA:HB1	1:A:439:PRO:C	2.32	0.49
1:B:119:GLN:CD	1:B:119:GLN:H	2.15	0.49
1:B:148:ASN:HA	1:B:185:PHE:HB2	1.94	0.49
1:A:73:LYS:C	1:A:74:ARG:HG2	2.32	0.49
1:A:346:ASN:HB3	1:A:349:LYS:H	1.76	0.49
1:B:29:LEU:O	1:B:30:LEU:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ILE:HD13	1:A:397:ILE:HG22	1.95	0.49
1:B:117:LEU:HD13	1:B:189:VAL:HG23	1.95	0.49
1:B:19:ASP:CG	1:B:214:SER:HB3	2.34	0.49
1:A:87:THR:CG2	1:A:88:ASP:N	2.75	0.49
1:B:362:ASP:O	1:B:363:MSE:HB2	2.13	0.49
1:A:36:ASP:OD2	1:A:39:ARG:HG3	2.13	0.48
1:B:12:MSE:HA	1:B:15:GLU:OE2	2.13	0.48
1:B:226:VAL:O	1:B:229:GLN:HB2	2.12	0.48
1:B:304:LEU:C	1:B:304:LEU:HD12	2.32	0.48
1:B:115:SER:HB3	1:B:146:SER:O	2.13	0.48
1:A:212:GLY:HA2	1:A:268:ASP:HB2	1.96	0.48
1:A:273:PRO:HG2	1:A:279:ASP:N	2.29	0.48
1:A:201:GLY:O	1:A:204:GLU:HB2	2.13	0.48
1:A:205:ALA:HB3	1:A:208:ILE:HG12	1.96	0.48
1:A:402:LYS:O	1:A:404:GLY:N	2.47	0.47
1:A:273:PRO:HB2	1:A:274:THR:H	1.29	0.47
1:A:342:ASN:HD22	1:A:344:SER:CB	2.27	0.47
1:A:251:LEU:CG	1:A:255:MSE:HE3	2.43	0.47
1:B:336:MSE:O	1:B:340:VAL:HG23	2.14	0.47
1:A:388:ILE:HD12	1:A:389:ASN:N	2.30	0.47
1:B:342:ASN:ND2	1:B:342:ASN:C	2.65	0.47
1:A:215:GLY:O	1:A:216:PRO:C	2.52	0.47
1:A:58:VAL:HG11	1:A:260:LEU:HD22	1.97	0.47
1:B:250:GLN:HE22	1:B:316:ALA:HB1	1.80	0.47
1:B:149:ILE:C	1:B:149:ILE:HD12	2.35	0.47
1:B:170:GLU:O	1:B:174:LEU:HB2	2.15	0.47
1:B:375:ILE:CA	1:B:378:MSE:CE	2.82	0.47
1:A:63:ALA:HB2	1:A:70:ILE:HD12	1.96	0.46
1:A:311:LYS:HZ3	1:B:438:ALA:HB1	1.72	0.46
1:A:208:ILE:CD1	1:A:208:ILE:CB	2.78	0.46
1:B:272:ALA:HB2	1:B:281:VAL:HG23	1.97	0.46
1:B:211:VAL:O	1:B:267:VAL:HA	2.15	0.46
1:B:30:LEU:HD13	1:B:78:THR:HG21	1.97	0.46
1:B:346:ASN:OD1	1:B:348:GLU:OE2	2.32	0.46
1:A:280:SER:H	1:A:283:ARG:HG3	1.80	0.46
1:A:389:ASN:C	1:A:390:MSE:CG	2.81	0.46
1:A:20:ILE:CB	1:A:70:ILE:HG12	2.46	0.46
1:A:193:PRO:HG2	1:A:210:ASN:HD22	1.80	0.46
1:A:357:CYS:HB3	1:A:358:SER:H	1.27	0.46
1:B:157:ASN:HD22	1:B:158:MSE:N	2.14	0.46
1:B:285:LEU:O	1:B:288:MSE:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HB3	1:A:356:ILE:HD11	1.97	0.46
1:A:126:ASP:O	1:A:130:ILE:CG1	2.64	0.46
1:A:26:GLY:O	1:A:207:VAL:HA	2.15	0.46
1:B:382:GLU:HG3	1:B:395:VAL:HG22	1.98	0.46
1:A:84:GLY:HA3	1:A:92:TYR:CD2	2.51	0.46
1:A:195:MSE:CG	1:A:196:ALA:H	2.28	0.45
1:B:273:PRO:HG2	1:B:277:VAL:CA	2.45	0.45
1:B:27:ILE:HG22	1:B:28:SER:O	2.16	0.45
1:A:184:VAL:HG12	1:A:185:PHE:N	2.32	0.45
1:A:74:ARG:HH21	1:A:195:MSE:CB	2.29	0.45
1:A:366:ILE:HD13	1:A:397:ILE:CG2	2.47	0.45
1:A:402:LYS:O	1:A:403:GLU:C	2.55	0.45
1:A:363:MSE:SE	1:A:396:ARG:HD2	2.67	0.45
1:B:246:THR:O	1:B:250:GLN:HG3	2.17	0.45
1:B:129:LEU:HG	1:B:129:LEU:O	2.11	0.44
1:B:177:MSE:HE3	1:B:181:LYS:HD3	1.99	0.44
1:B:0:ALA:H2	1:B:5:GLN:HE22	1.59	0.44
1:A:21:ARG:HH11	1:A:21:ARG:HG3	1.80	0.44
1:A:195:MSE:O	1:A:196:ALA:CB	2.65	0.44
1:A:71:VAL:CG1	1:A:72:ASN:HD21	2.29	0.44
1:B:10:ILE:HG21	1:B:10:ILE:HD12	1.47	0.44
1:A:130:ILE:HG21	1:A:164:MSE:HE1	2.00	0.44
1:B:294:GLY:O	1:B:349:LYS:HE3	2.18	0.44
1:B:80:ILE:HD13	1:B:80:ILE:HA	1.77	0.44
1:B:93:VAL:HG21	1:B:135:ARG:HE	1.82	0.44
1:A:389:ASN:C	1:A:390:MSE:HG3	2.39	0.44
1:B:229:GLN:HG2	1:B:233:VAL:HG21	2.00	0.43
1:B:37:ILE:HD12	1:B:87:THR:HG21	1.99	0.43
1:B:293:VAL:CG1	1:B:339:ALA:CB	2.96	0.43
1:B:341:GLN:C	1:B:343:GLY:H	2.21	0.43
1:B:58:VAL:O	1:B:62:ILE:HG13	2.18	0.43
1:B:23:ILE:HG21	1:B:23:ILE:HD13	1.73	0.43
1:B:304:LEU:HD12	1:B:308:GLN:HG2	2.00	0.43
1:A:191:ASP:O	1:A:192:ASN:C	2.57	0.43
1:A:21:ARG:NH1	1:A:214:SER:HA	2.34	0.43
1:A:299:THR:HG22	1:A:349:LYS:HZ1	1.84	0.43
1:A:79:PRO:HA	1:A:113:GLY:O	2.19	0.43
1:B:390:MSE:H	1:B:390:MSE:HG3	1.60	0.43
1:A:147:VAL:HG11	1:A:164:MSE:HE3	2.00	0.43
1:A:368:GLU:HG2	1:A:368:GLU:O	2.18	0.43
1:A:341:GLN:NE2	1:A:406:MSE:HE1	2.14	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ARG:HG2	1:B:259:ARG:H	1.53	0.43
1:A:73:LYS:O	1:A:108:VAL:HB	2.19	0.43
1:A:131:ASN:HD21	1:A:166:ARG:NH1	2.09	0.43
1:A:87:THR:CG2	1:A:89:ALA:N	2.80	0.43
1:B:202:VAL:HG23	1:B:202:VAL:H	1.43	0.43
1:B:3:ILE:N	1:B:3:ILE:CD1	2.67	0.43
1:A:299:THR:HG22	1:A:349:LYS:NZ	2.34	0.42
1:B:215:GLY:O	1:B:218:VAL:HB	2.19	0.42
1:A:148:ASN:HA	1:A:185:PHE:HB2	2.01	0.42
1:B:78:THR:O	1:B:79:PRO:C	2.56	0.42
1:A:130:ILE:CG2	1:A:164:MSE:HE1	2.49	0.42
1:A:306:ASN:CB	1:A:357:CYS:SG	3.06	0.42
1:B:149:ILE:HG13	1:B:185:PHE:O	2.19	0.42
1:A:243:PHE:CD1	1:A:315:MSE:O	2.73	0.42
1:A:80:ILE:O	1:A:81:SER:C	2.56	0.42
1:B:215:GLY:HA3	1:B:216:PRO:HD3	1.83	0.42
1:A:37:ILE:HG23	1:A:38:ASN:N	2.35	0.42
1:B:273:PRO:CD	1:B:279:ASP:CB	2.77	0.42
1:B:308:GLN:HA	1:B:311:LYS:HG3	2.02	0.42
1:A:195:MSE:HG3	1:A:196:ALA:H	1.83	0.42
1:B:375:ILE:HG12	1:B:378:MSE:HE1	2.02	0.42
1:A:398:ILE:HG22	1:A:400:LYS:HG3	2.02	0.42
1:B:152:THR:HG21	1:B:390:MSE:HG2	2.02	0.42
1:B:282:ALA:CB	1:B:335:GLY:HA3	2.41	0.42
1:B:345:LEU:HD21	1:B:353:MSE:CE	2.50	0.41
1:B:303:ALA:N	1:B:356:ILE:HD13	2.35	0.41
1:A:350:LEU:O	1:A:354:THR:HG23	2.19	0.41
1:A:94:VAL:HG12	2:A:455:HOH:O	2.20	0.41
1:A:135:ARG:NH1	1:A:135:ARG:HG2	2.32	0.41
1:A:193:PRO:HG2	1:A:210:ASN:ND2	2.36	0.41
1:A:299:THR:CG2	1:B:351:GLU:OE2	2.67	0.41
1:B:10:ILE:HA	1:B:13:ILE:HG12	2.03	0.41
1:B:179:VAL:HG22	2:B:471:HOH:O	2.19	0.41
1:A:351:GLU:OE2	1:B:299:THR:HG21	2.19	0.41
1:A:341:GLN:O	1:A:343:GLY:N	2.53	0.41
1:A:244:LYS:O	1:A:245:ILE:C	2.58	0.41
1:A:268:ASP:HB3	1:A:269:LEU:H	1.75	0.41
1:A:346:ASN:HD21	1:B:346:ASN:HD21	1.67	0.41
1:A:37:ILE:CD1	1:A:87:THR:HG21	2.47	0.41
1:A:206:ASP:O	1:A:207:VAL:HG23	2.20	0.41
1:A:74:ARG:HD3	1:A:74:ARG:HH11	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:LYS:O	1:B:352:ALA:HB3	2.21	0.41
1:B:405:ASP:O	1:B:406:MSE:HG2	2.21	0.41
1:A:204:GLU:OE1	1:A:208:ILE:HD12	2.21	0.41
1:A:123:GLN:HA	1:A:123:GLN:NE2	2.35	0.41
1:B:270:SER:O	1:B:270:SER:OG	2.30	0.41
1:B:356:ILE:O	1:B:357:CYS:HB2	2.21	0.41
1:B:302:LEU:HD23	1:B:356:ILE:HD11	2.03	0.40
1:B:56:VAL:H	1:B:56:VAL:HG23	1.65	0.40
1:A:74:ARG:HH21	1:A:195:MSE:HB2	1.86	0.40
1:A:288:MSE:HE1	1:A:305:LEU:HB2	2.03	0.40
1:A:33:ILE:CG2	1:A:34:ASP:N	2.84	0.40
1:A:74:ARG:HD2	1:A:110:PHE:HB2	2.02	0.40
1:B:128:ILE:HD13	2:B:460:HOH:O	2.22	0.40
1:B:130:ILE:HD13	1:B:164:MSE:HE1	2.03	0.40
1:B:95:LEU:HA	1:B:95:LEU:HD23	1.82	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	402/446 (90%)	356 (89%)	31 (8%)	15 (4%)	3	7
1	B	401/446 (90%)	357 (89%)	26 (6%)	18 (4%)	2	5
All	All	803/892 (90%)	713 (89%)	57 (7%)	33 (4%)	3	6

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	PRO
1	A	214	SER
1	A	273	PRO

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Mol	Chain	Res	Type
1	A	403	GLU
1	A	405	ASP
1	A	407	ILE
1	A	416	ALA
1	A	438	ALA
1	B	192	ASN
1	B	214	SER
1	B	269	LEU
1	B	279	ASP
1	B	317	CYS
1	B	357	CYS
1	B	403	GLU
1	B	405	ASP
1	B	406	MSE
1	B	407	ILE
1	B	438	ALA
1	A	316	ALA
1	A	342	ASN
1	A	357	CYS
1	B	205	ALA
1	B	271	LEU
1	A	1	MSE
1	A	89	ALA
1	B	429	PHE
1	B	399	PRO
1	A	317	CYS
1	B	272	ALA
1	B	318	ASN
1	A	113	GLY
1	B	281	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	310/329 (94%)	253 (82%)	57 (18%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	308/329 (94%)	252 (82%)	56 (18%)	1 4
All	All	618/658 (94%)	505 (82%)	113 (18%)	1 4

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	5	GLN
1	A	15	GLU
1	A	17	ASN
1	A	19	ASP
1	A	30	LEU
1	A	55	LEU
1	A	66	LEU
1	A	68	ILE
1	A	74	ARG
1	A	80	ILE
1	A	87	THR
1	A	90	THR
1	A	119	GLN
1	A	120	LYS
1	A	130	ILE
1	A	135	ARG
1	A	157	ASN
1	A	170	GLU
1	A	179	VAL
1	A	182	LEU
1	A	185	PHE
1	A	193	PRO
1	A	211	VAL
1	A	213	VAL
1	A	216	PRO
1	A	225	LYS
1	A	236	GLU
1	A	240	LYS
1	A	258	GLU
1	A	259	ARG
1	A	260	LEU
1	A	267	VAL
1	A	269	LEU
1	A	274	THR
1	A	280	SER

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Mol	Chain	Res	Type
1	A	283	ARG
1	A	299	THR
1	A	305	LEU
1	A	310	LYS
1	A	334	GLU
1	A	342	ASN
1	A	345	LEU
1	A	347	LEU
1	A	348	GLU
1	A	357	CYS
1	A	362	ASP
1	A	363	MSE
1	A	366	ILE
1	A	370	THR
1	A	379	ILE
1	A	390	MSE
1	A	391	LYS
1	A	397	ILE
1	A	402	LYS
1	A	408	GLU
1	A	421	VAL
1	B	1	MSE
1	B	3	ILE
1	B	5	GLN
1	B	7	THR
1	B	8	GLU
1	B	10	ILE
1	B	15	GLU
1	B	16	GLN
1	B	27	ILE
1	B	30	LEU
1	B	39	ARG
1	B	42	GLU
1	B	55	LEU
1	B	66	LEU
1	B	87	THR
1	B	90	THR
1	B	91	ASP
1	B	109	ASP
1	B	119	GLN
1	B	120	LYS
1	B	128	ILE

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Mol	Chain	Res	Type
1	B	157	ASN
1	B	167	ILE
1	B	173	ASN
1	B	177	MSE
1	B	179	VAL
1	B	182	LEU
1	B	183	VAL
1	B	208	ILE
1	B	209	ILE
1	B	213	VAL
1	B	224	GLU
1	B	225	LYS
1	B	229	GLN
1	B	232	ASP
1	B	254	GLN
1	B	259	ARG
1	B	260	LEU
1	B	267	VAL
1	B	270	SER
1	B	279	ASP
1	B	283	ARG
1	B	299	THR
1	B	304	LEU
1	B	305	LEU
1	B	310	LYS
1	B	311	LYS
1	B	337	ILE
1	B	342	ASN
1	B	345	LEU
1	B	347	LEU
1	B	348	GLU
1	B	349	LYS
1	B	358	SER
1	B	392	THR
1	B	403	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	72	ASN
1	A	123	GLN

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Mol	Chain	Res	Type
1	A	131	ASN
1	A	157	ASN
1	A	250	GLN
1	A	308	GLN
1	A	341	GLN
1	A	342	ASN
1	A	346	ASN
1	A	389	ASN
1	B	5	GLN
1	B	72	ASN
1	B	131	ASN
1	B	157	ASN
1	B	250	GLN
1	B	308	GLN
1	B	342	ASN
1	B	389	ASN

5.3.3 RNA

There are no RNA molecules 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

There are no ligands in this entry.

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	397/446 (89%)	-0.51	1 (0%)	94	95	23, 40, 74, 93	0
1	B	398/446 (89%)	-0.49	2 (0%)	91	92	22, 37, 71, 86	0
All	All	795/892 (89%)	-0.50	3 (0%)	92	93	22, 39, 72, 93	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	ILE	3.1
1	A	0	ALA	2.7
1	B	191	ASP	2.4

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.