



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:58 PM UTC

PDB ID : 6IQQ / pdb_00006iqq
Title : Crystal structure of Prc with S452I and L252Y mutations in complex with NlpI
Authors : Chueh, C.K.; Chang, C.I.
Deposited on : 2018-11-08
Resolution : 2.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

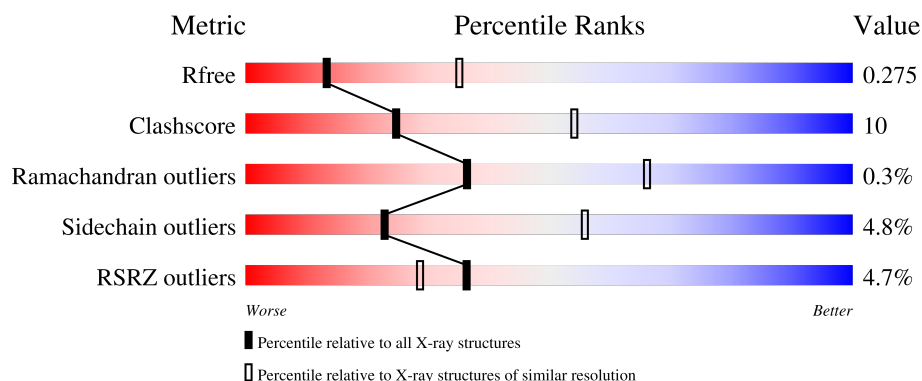
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	296	
1	B	296	
2	C	688	
2	D	688	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14502 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 Lipoprotein NlpI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2082	1331	345	403	3			
1	B	258	Total	C	N	O	S	0	0	0
			2091	1336	346	406	3			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0AFB1
A	2	GLY	-	expression tag	UNP P0AFB1
A	3	SER	-	expression tag	UNP P0AFB1
A	4	SER	-	expression tag	UNP P0AFB1
A	5	HIS	-	expression tag	UNP P0AFB1
A	6	HIS	-	expression tag	UNP P0AFB1
A	7	HIS	-	expression tag	UNP P0AFB1
A	8	HIS	-	expression tag	UNP P0AFB1
A	9	HIS	-	expression tag	UNP P0AFB1
A	10	HIS	-	expression tag	UNP P0AFB1
A	11	SER	-	expression tag	UNP P0AFB1
A	12	SER	-	expression tag	UNP P0AFB1
A	13	GLY	-	expression tag	UNP P0AFB1
A	14	LEU	-	expression tag	UNP P0AFB1
A	15	VAL	-	expression tag	UNP P0AFB1
A	16	PRO	-	expression tag	UNP P0AFB1
A	17	ARG	-	expression tag	UNP P0AFB1
A	18	GLY	-	expression tag	UNP P0AFB1
A	19	SER	-	expression tag	UNP P0AFB1
A	20	HIS	-	expression tag	UNP P0AFB1
A	21	MET	-	expression tag	UNP P0AFB1
B	1	MET	-	initiating methionine	UNP P0AFB1
B	2	GLY	-	expression tag	UNP P0AFB1
B	3	SER	-	expression tag	UNP P0AFB1
B	4	SER	-	expression tag	UNP P0AFB1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	HIS	-	expression tag	UNP P0AFB1
B	6	HIS	-	expression tag	UNP P0AFB1
B	7	HIS	-	expression tag	UNP P0AFB1
B	8	HIS	-	expression tag	UNP P0AFB1
B	9	HIS	-	expression tag	UNP P0AFB1
B	10	HIS	-	expression tag	UNP P0AFB1
B	11	SER	-	expression tag	UNP P0AFB1
B	12	SER	-	expression tag	UNP P0AFB1
B	13	GLY	-	expression tag	UNP P0AFB1
B	14	LEU	-	expression tag	UNP P0AFB1
B	15	VAL	-	expression tag	UNP P0AFB1
B	16	PRO	-	expression tag	UNP P0AFB1
B	17	ARG	-	expression tag	UNP P0AFB1
B	18	GLY	-	expression tag	UNP P0AFB1
B	19	SER	-	expression tag	UNP P0AFB1
B	20	HIS	-	expression tag	UNP P0AFB1
B	21	MET	-	expression tag	UNP P0AFB1

- Molecule 2 is a protein called Tail-specific protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	645	Total	C	N	O	S	0	0	0
			5128	3229	895	992	12			
2	D	642	Total	C	N	O	S	0	0	0
			5106	3214	891	989	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	252	TYR	LEU	engineered mutation	UNP P23865
C	452	ILE	SER	engineered mutation	UNP P23865
C	683	HIS	-	expression tag	UNP P23865
C	684	HIS	-	expression tag	UNP P23865
C	685	HIS	-	expression tag	UNP P23865
C	686	HIS	-	expression tag	UNP P23865
C	687	HIS	-	expression tag	UNP P23865
C	688	HIS	-	expression tag	UNP P23865
D	252	TYR	LEU	engineered mutation	UNP P23865
D	452	ILE	SER	engineered mutation	UNP P23865
D	683	HIS	-	expression tag	UNP P23865
D	684	HIS	-	expression tag	UNP P23865
D	685	HIS	-	expression tag	UNP P23865

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Chain	Residue	Modelled	Actual	Comment	Reference
D	686	HIS	-	expression tag	UNP P23865
D	687	HIS	-	expression tag	UNP P23865
D	688	HIS	-	expression tag	UNP P23865

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Ca 1	0	0
3	D	1	Total 1	Ca 1	0	0

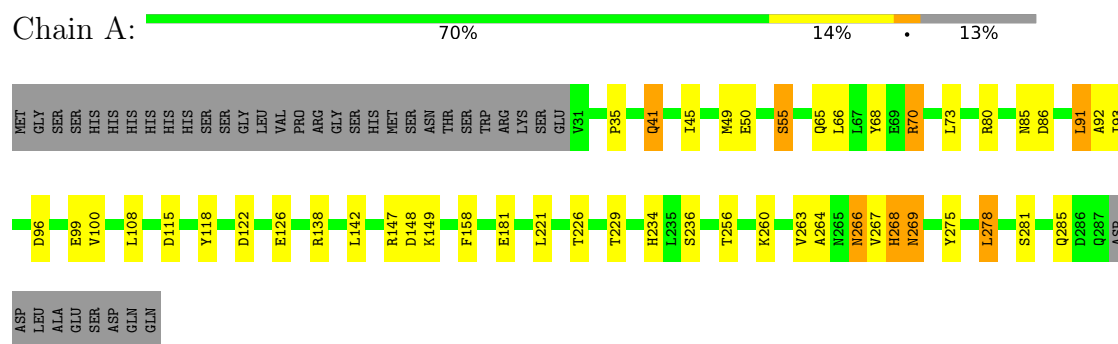
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total 16	O 16	0	0
4	B	19	Total 19	O 19	0	0
4	C	23	Total 23	O 23	0	0
4	D	35	Total 35	O 35	0	0

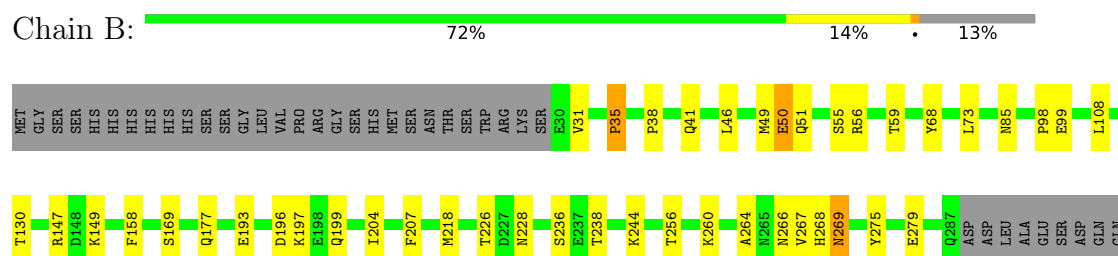
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

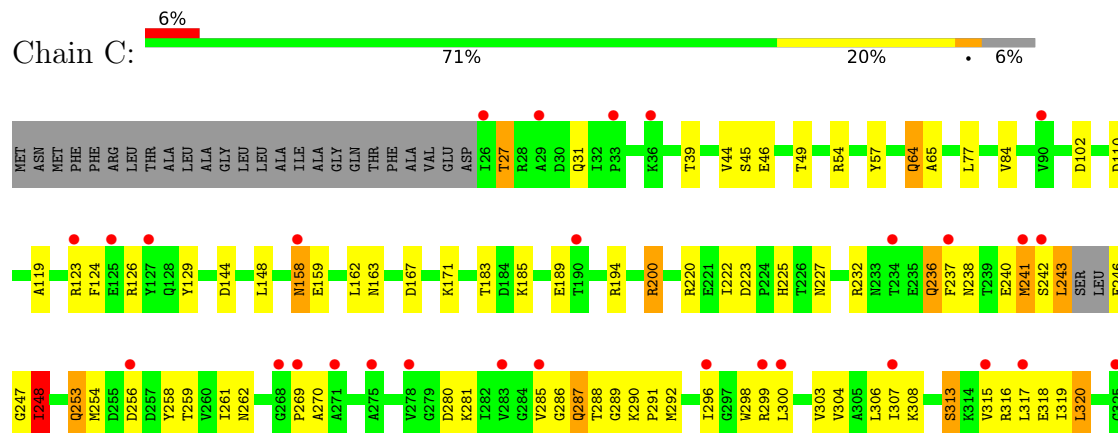
• Molecule 1: Lipoprotein NlpI



• Molecule 1: Lipoprotein NlpI



• Molecule 2: Tail-specific protease



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.94Å 143.88Å 153.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.80 29.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.98-2.80) 96.8 (29.98-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.222 , 0.278 0.224 , 0.275	Depositor DCC
R_{free} test set	3248 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14502	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0586e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.26	5/2126 (0.2%)	1.64	22/2886 (0.8%)
1	B	1.26	7/2135 (0.3%)	1.64	18/2898 (0.6%)
2	C	1.16	5/5215 (0.1%)	1.60	29/7040 (0.4%)
2	D	1.16	1/5192 (0.0%)	1.62	37/7008 (0.5%)
All	All	1.19	18/14668 (0.1%)	1.62	106/19832 (0.5%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	PRO	C-O	-8.64	1.11	1.23
1	A	267	VAL	C-O	7.71	1.33	1.24
1	B	35	PRO	C-O	-7.16	1.13	1.23
2	C	393	ARG	C-O	6.93	1.32	1.23
1	B	31	VAL	C-O	6.34	1.30	1.23
1	A	263	VAL	C-O	-5.97	1.16	1.24
1	B	130	THR	C-O	5.84	1.32	1.23
2	C	431	ASP	C-O	5.75	1.30	1.24
1	A	266	ASN	C-O	-5.75	1.16	1.23
2	C	222	ILE	C-O	5.70	1.29	1.24
2	D	501	LEU	C-O	5.51	1.30	1.23
1	B	207	PHE	C-O	-5.31	1.18	1.24
1	A	268	HIS	C-O	5.24	1.29	1.23
1	B	56	ARG	C-O	5.20	1.30	1.23
1	A	93	ILE	C-O	-5.11	1.18	1.24
2	C	225	HIS	CE1-NE2	5.04	1.37	1.32
2	C	364	GLY	C-O	5.04	1.28	1.23
1	B	98	PRO	C-O	-5.02	1.17	1.24

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ASN	CB-CA-C	8.26	123.95	110.90
2	D	120	GLN	N-CA-C	-8.16	101.66	111.69
2	D	433	ASP	CA-CB-CG	7.94	120.54	112.60
1	B	85	ASN	CB-CA-C	7.92	123.41	110.90
2	C	433	ASP	CA-CB-CG	7.69	120.29	112.60
2	C	493	MET	N-CA-C	-7.26	104.56	113.41
1	B	275	TYR	CB-CA-C	7.10	124.87	110.38
2	C	223	ASP	CA-CB-CG	7.07	119.67	112.60
2	C	522	LYS	N-CA-C	-7.07	104.52	113.43
1	A	275	TYR	CB-CA-C	6.99	124.64	110.38
1	A	268	HIS	CA-C-O	-6.95	113.50	121.15
2	D	223	ASP	CA-CB-CG	6.90	119.50	112.60
2	C	525	THR	CA-CB-OG1	-6.88	99.28	109.60
2	D	520	GLN	CB-CA-C	-6.86	99.55	109.84
2	D	521	ARG	CB-CA-C	-6.84	98.14	111.06
2	D	637	PRO	CB-CA-C	6.82	119.91	110.98
1	B	193	GLU	CB-CA-C	6.67	122.18	110.85
2	D	525	THR	CA-CB-OG1	-6.61	99.68	109.60
1	B	269	ASN	CA-CB-CG	6.51	119.11	112.60
2	D	474	THR	CA-C-N	6.48	129.28	120.54
2	D	474	THR	C-N-CA	6.48	129.28	120.54
2	D	223	ASP	CB-CA-C	6.33	118.58	110.22
1	A	158	PHE	CA-C-O	-6.32	114.19	120.82
2	D	351	THR	CA-CB-OG1	-6.31	100.13	109.60
2	C	167	ASP	N-CA-C	-6.26	104.38	111.07
1	A	85	ASN	N-CA-C	-6.24	104.40	111.14
2	C	637	PRO	CB-CA-C	6.22	119.52	110.63
2	D	401	THR	CA-CB-OG1	-6.20	100.29	109.60
1	B	85	ASN	N-CA-C	-6.17	104.47	111.14
1	A	50	GLU	CA-C-N	6.15	128.44	120.44
1	A	50	GLU	C-N-CA	6.15	128.44	120.44
2	C	571	LEU	O-C-N	6.13	128.38	122.07
2	C	474	THR	CA-C-N	6.03	128.68	120.54
2	C	474	THR	C-N-CA	6.03	128.68	120.54
1	B	41	GLN	N-CA-C	-5.99	104.83	111.36
2	D	520	GLN	N-CA-CB	5.96	118.72	109.48
1	A	278	LEU	N-CA-C	-5.87	104.81	111.14
2	D	554	ASP	CA-CB-CG	5.87	118.47	112.60
2	D	167	ASP	N-CA-C	-5.85	104.81	111.07
2	D	636	LYS	N-CA-C	-5.80	102.84	110.39
2	C	39	THR	CA-C-N	5.78	128.30	120.38
2	C	39	THR	C-N-CA	5.78	128.30	120.38
2	D	451	ALA	CA-C-O	-5.71	114.94	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	ILE	N-CA-C	-5.65	105.02	110.72
2	D	499	PRO	N-CA-C	-5.65	101.80	110.95
1	A	66	LEU	N-CA-C	-5.64	105.90	112.89
1	A	268	HIS	N-CA-C	-5.63	102.30	110.24
1	A	91	LEU	CA-C-O	-5.62	114.88	120.90
1	A	269	ASN	N-CA-CB	5.62	119.99	110.49
2	C	341	GLU	CB-CG-CD	5.59	122.10	112.60
2	D	537	THR	CB-CA-C	5.58	119.00	109.80
2	C	64	GLN	CB-CA-C	5.54	119.50	110.96
2	C	46	GLU	CA-C-N	5.52	127.61	120.44
2	C	46	GLU	C-N-CA	5.52	127.61	120.44
2	C	223	ASP	CB-CA-C	5.52	117.50	110.22
2	C	351	THR	CA-CB-OG1	-5.50	101.35	109.60
2	D	571	LEU	CA-C-O	-5.50	115.04	120.70
2	D	495	ARG	CA-C-O	5.43	125.90	120.03
2	C	571	LEU	CA-C-O	-5.41	115.14	120.82
2	D	353	GLY	CA-C-N	5.40	127.78	120.44
2	D	353	GLY	C-N-CA	5.40	127.78	120.44
1	A	92	ALA	CA-C-N	5.39	128.45	120.74
1	A	92	ALA	C-N-CA	5.39	128.45	120.74
1	A	269	ASN	CA-CB-CG	5.38	117.98	112.60
2	D	184	ASP	CA-C-N	5.38	128.26	120.79
2	D	184	ASP	C-N-CA	5.38	128.26	120.79
2	D	61	ASP	CA-CB-CG	-5.37	107.23	112.60
1	B	158	PHE	CA-C-O	-5.36	115.17	120.90
1	B	59	THR	CA-C-O	-5.35	115.90	121.99
2	D	46	GLU	CA-C-N	5.34	127.69	120.38
2	D	46	GLU	C-N-CA	5.34	127.69	120.38
2	D	216	THR	CA-CB-OG1	-5.33	101.61	109.60
1	B	55	SER	CA-C-O	-5.32	114.97	121.88
1	A	108	LEU	N-CA-C	-5.29	105.57	112.23
1	B	51	GLN	N-CA-C	-5.27	105.43	111.07
1	A	96	ASP	CB-CA-C	5.25	118.43	111.14
2	C	328	THR	CA-C-N	5.25	130.10	121.39
2	C	328	THR	C-N-CA	5.25	130.10	121.39
2	D	663	ALA	CA-C-O	-5.23	115.01	120.55
2	D	453	ALA	CA-C-N	5.22	127.27	120.28
2	D	453	ALA	C-N-CA	5.22	127.27	120.28
1	B	236	SER	N-CA-C	-5.19	105.31	110.97
1	A	236	SER	CA-C-O	-5.19	115.55	121.00
1	A	65	GLN	N-CA-C	-5.19	105.62	111.28
2	C	526	PRO	CA-C-N	5.19	127.66	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	526	PRO	C-N-CA	5.19	127.66	120.29
2	C	593	ALA	CA-C-N	5.18	127.49	120.44
2	C	593	ALA	C-N-CA	5.18	127.49	120.44
2	C	451	ALA	CA-C-N	5.18	131.30	121.97
2	C	451	ALA	C-N-CA	5.18	131.30	121.97
1	A	80	ARG	CG-CD-NE	-5.16	100.64	112.00
1	B	50	GLU	CA-C-N	5.14	127.12	120.44
1	B	50	GLU	C-N-CA	5.14	127.12	120.44
2	D	192	THR	CA-C-N	5.14	127.17	120.28
2	D	192	THR	C-N-CA	5.14	127.17	120.28
1	B	228	ASN	N-CA-C	-5.14	105.86	111.82
1	B	199	GLN	CB-CA-C	5.13	118.42	109.65
1	B	108	LEU	N-CA-C	-5.10	105.80	112.23
2	D	225	HIS	CB-CA-C	5.09	118.52	109.65
1	B	169	SER	N-CA-C	-5.09	105.82	111.36
2	C	220	ARG	CG-CD-NE	-5.07	100.86	112.00
2	D	398	GLY	CA-C-O	-5.05	117.42	120.91
2	D	310	PRO	N-CA-C	5.03	118.52	111.33
1	A	229	THR	N-CA-C	-5.02	105.72	111.14
1	A	55	SER	CA-C-O	-5.01	115.90	121.81
2	C	110	ASP	CB-CA-C	5.00	119.36	110.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2082	0	2016	26	0
1	B	2091	0	2022	23	0
2	C	5128	0	5142	143	0
2	D	5106	0	5112	102	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	16	0	0	0	0
4	B	19	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	23	0	0	0	0
4	D	35	0	0	0	0
All	All	14502	0	14292	281	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 10.

All (281) 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)
2:C:119:ALA:O	2:C:123:ARG:HG3	1.37	1.24
2:D:497:GLU:C	2:D:499:PRO:HD2	1.74	1.12
2:C:241:MET:HA	2:C:241:MET:HE2	1.36	1.08
2:C:316:ARG:HD2	2:C:332:THR:HG22	1.33	1.05
2:C:316:ARG:CD	2:C:332:THR:HG22	1.85	1.05
2:D:601:LYS:HG2	2:D:604:ILE:HB	1.42	1.02
2:D:85:LEU:HD21	2:D:119:ALA:HB2	1.45	0.99
2:D:257:ASP:OD2	2:D:297:GLY:CA	2.11	0.99
2:C:316:ARG:HD2	2:C:332:THR:CG2	1.96	0.95
2:C:290:LYS:HG3	2:C:291:PRO:CD	1.97	0.93
2:D:497:GLU:CG	2:D:497:GLU:O	2.17	0.93
2:C:316:ARG:CG	2:C:332:THR:HG22	2.00	0.92
2:D:257:ASP:OD2	2:D:297:GLY:HA3	1.67	0.92
1:A:147:ARG:CZ	2:D:54:ARG:O	2.19	0.91
2:C:232:ARG:HG2	2:C:236:GLN:NE2	1.85	0.91
2:D:346:LYS:HE2	2:D:347:MET:H	1.37	0.89
2:C:290:LYS:HG3	2:C:291:PRO:HD2	1.53	0.88
2:D:320:LEU:HD11	2:D:327:LYS:H	1.39	0.87
1:B:147:ARG:CZ	2:C:54:ARG:O	2.23	0.87
2:C:290:LYS:CG	2:C:291:PRO:HD2	2.04	0.87
2:C:438:TYR:O	2:C:439:LYS:CG	2.25	0.84
2:D:254:MET:HB2	2:D:300:LEU:HD11	1.58	0.84
2:D:601:LYS:CG	2:D:604:ILE:HB	2.09	0.81
2:D:144:ASP:OD2	2:D:171:LYS:NZ	2.13	0.81
2:C:241:MET:HA	2:C:241:MET:CE	2.09	0.81
2:C:448:ARG:NH1	2:C:472:GLU:OE2	2.12	0.80
2:C:246:GLU:O	2:C:308:LYS:HG3	1.80	0.80
2:C:253:GLN:HB3	2:C:262:ASN:HB2	1.62	0.80
2:D:497:GLU:C	2:D:499:PRO:CD	2.54	0.80
2:C:194:ARG:HD3	2:C:296:ILE:HD11	1.63	0.79
2:C:316:ARG:CD	2:C:332:THR:CG2	2.58	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:318:GLU:O	2:C:319:ILE:HD13	1.84	0.78
1:A:266:ASN:HD21	1:B:266:ASN:HD21	1.32	0.77
2:C:123:ARG:HB3	2:C:123:ARG:NH1	2.00	0.76
2:C:438:TYR:O	2:C:439:LYS:HG3	1.84	0.75
2:C:159:GLU:O	2:C:163:ASN:OD1	2.05	0.75
2:C:315:VAL:CG1	2:C:335:ARG:HH21	1.99	0.74
2:C:290:LYS:HG3	2:C:291:PRO:HD3	1.69	0.74
2:D:498:TRP:N	2:D:499:PRO:CD	2.50	0.73
2:C:269:PRO:C	2:C:333:LEU:HD11	2.13	0.73
1:A:70:ARG:CD	1:A:86:ASP:OD2	2.37	0.73
2:D:320:LEU:CD1	2:D:327:LYS:H	2.01	0.72
2:D:119:ALA:HA	2:D:122:ARG:HB2	1.71	0.72
2:D:497:GLU:O	2:D:497:GLU:HG2	1.89	0.72
2:C:287:GLN:NE2	2:C:287:GLN:HA	2.03	0.72
2:C:84:VAL:HG11	2:C:123:ARG:HG2	1.70	0.71
2:C:317:LEU:HD23	2:C:317:LEU:H	1.54	0.71
1:A:264:ALA:HB1	1:B:264:ALA:HB1	1.73	0.71
2:D:497:GLU:O	2:D:497:GLU:HG3	1.90	0.71
1:B:147:ARG:NE	2:C:54:ARG:O	2.22	0.71
1:B:218:MET:HE1	1:B:238:THR:HG21	1.70	0.71
2:D:375:VAL:O	2:D:378:GLN:HG2	1.91	0.71
2:D:336:GLU:HG2	2:D:339:ARG:HH22	1.56	0.70
2:C:194:ARG:CD	2:C:296:ILE:HD11	2.22	0.70
2:D:320:LEU:HD11	2:D:327:LYS:N	2.06	0.70
2:C:316:ARG:HG2	2:C:332:THR:HG22	1.74	0.69
2:C:253:GLN:HE21	2:C:262:ASN:CG	2.00	0.69
2:C:438:TYR:O	2:C:439:LYS:HG2	1.92	0.69
2:D:346:LYS:HE2	2:D:347:MET:N	2.07	0.68
2:D:448:ARG:HH11	2:D:537:THR:HG23	1.58	0.68
2:D:85:LEU:CD2	2:D:119:ALA:HB2	2.21	0.67
2:D:570:GLU:OE2	2:D:669:LEU:HD21	1.94	0.67
2:C:242:SER:O	2:C:243:LEU:C	2.37	0.67
2:D:294:ASP:HB3	2:D:296:ILE:CD1	2.23	0.67
2:D:314:LYS:HD3	2:D:334:THR:HG23	1.78	0.66
1:A:70:ARG:HD2	1:A:86:ASP:OD2	1.95	0.66
2:C:227:ASN:HD22	2:C:505:GLN:HE21	1.43	0.65
1:A:70:ARG:HD3	1:A:86:ASP:OD2	1.98	0.64
2:D:257:ASP:OD2	2:D:297:GLY:HA2	1.96	0.64
2:C:290:LYS:CB	2:C:291:PRO:HD2	2.28	0.63
2:C:248:ILE:HG13	2:C:248:ILE:O	1.98	0.63
2:D:44:VAL:O	2:D:48:VAL:HG13	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:369:LEU:HB3	2:C:402:GLU:HG2	1.81	0.62
1:B:149:LYS:HE2	4:B:304:HOH:O	2.00	0.62
2:C:317:LEU:HD23	2:C:317:LEU:N	2.15	0.62
2:C:315:VAL:HG12	2:C:335:ARG:HH21	1.65	0.61
2:C:286:GLY:N	2:C:316:ARG:O	2.32	0.61
1:A:147:ARG:NH2	2:D:54:ARG:O	2.34	0.60
1:A:285:GLN:OE1	2:D:425:LYS:HE3	2.01	0.60
2:C:329:ARG:HG3	2:C:329:ARG:HH11	1.66	0.60
2:D:115:LEU:O	2:D:118:LEU:O	2.19	0.60
2:D:498:TRP:N	2:D:499:PRO:HD2	2.15	0.59
2:C:232:ARG:HD2	2:C:232:ARG:N	2.17	0.59
2:D:232:ARG:HG3	2:D:236:GLN:NE2	2.18	0.59
2:D:472:GLU:OE1	2:D:532:THR:OG1	2.12	0.58
1:A:122:ASP:OD1	1:A:138:ARG:NH1	2.37	0.58
2:C:300:LEU:O	2:C:304:VAL:HG23	2.03	0.58
2:D:632:LYS:HE3	2:D:638:GLU:OE2	2.03	0.58
2:C:290:LYS:CG	2:C:291:PRO:CD	2.71	0.58
2:C:238:ASN:OD1	2:C:238:ASN:C	2.47	0.57
2:C:254:MET:HG3	2:C:258:TYR:O	2.03	0.57
2:C:315:VAL:HB	2:C:335:ARG:NH2	2.19	0.57
2:C:584:GLU:OE1	2:C:630:ARG:NH1	2.37	0.57
2:C:270:ALA:N	2:C:333:LEU:HD11	2.19	0.57
2:C:27:THR:HG22	2:C:124:PHE:HE1	1.70	0.57
2:C:77:LEU:HD23	2:C:256:ASP:OD2	2.04	0.57
2:D:49:THR:O	2:D:53:THR:OG1	2.13	0.57
1:B:268:HIS:O	1:B:269:ASN:OD1	2.22	0.57
2:D:84:VAL:HG12	2:D:122:ARG:HB3	1.85	0.57
1:A:147:ARG:NE	2:D:54:ARG:O	2.39	0.56
2:C:144:ASP:OD2	2:C:171:LYS:NZ	2.38	0.56
2:C:280:ASP:HB3	2:C:319:ILE:HG23	1.87	0.56
2:C:254:MET:HE1	2:C:298:TRP:O	2.06	0.56
2:D:118:LEU:O	2:D:119:ALA:HB3	2.06	0.56
1:B:218:MET:CE	1:B:238:THR:HG21	2.36	0.55
2:D:347:MET:HE3	2:D:380:LEU:HG	1.88	0.55
1:B:268:HIS:O	1:B:269:ASN:CB	2.54	0.55
2:C:31:GLN:CD	2:C:31:GLN:O	2.49	0.55
2:C:269:PRO:O	2:C:333:LEU:HD11	2.06	0.55
2:C:421:ASP:OD1	2:C:425:LYS:N	2.40	0.54
2:C:27:THR:HG22	2:C:124:PHE:CE1	2.41	0.54
2:C:281:LYS:HD2	2:C:320:LEU:HD22	1.90	0.54
2:C:315:VAL:CG1	2:C:335:ARG:NH2	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:233:ASN:ND2	2:D:233:ASN:H	2.03	0.54
2:D:631:PHE:CG	2:D:636:LYS:HD3	2.42	0.54
2:C:269:PRO:C	2:C:333:LEU:CD1	2.81	0.54
2:C:232:ARG:HB3	2:C:236:GLN:HB3	1.89	0.54
2:C:422:ASN:OD1	2:C:423:ASN:ND2	2.40	0.53
2:D:328:THR:O	2:D:328:THR:OG1	2.23	0.53
2:C:347:MET:HE3	2:C:380:LEU:CD2	2.38	0.53
2:D:234:THR:O	2:D:237:PHE:N	2.41	0.53
2:D:246:GLU:OE2	2:D:336:GLU:N	2.41	0.53
2:D:448:ARG:HD3	2:D:537:THR:HG21	1.90	0.53
1:A:49:MET:HE1	1:A:73:LEU:HD23	1.91	0.53
2:C:631:PHE:CG	2:C:636:LYS:HD3	2.44	0.53
1:B:49:MET:HE1	1:B:73:LEU:HD23	1.90	0.53
2:C:438:TYR:C	2:C:439:LYS:HG2	2.34	0.53
2:D:535:GLU:OE2	2:D:596:ASN:ND2	2.41	0.53
1:A:49:MET:CE	1:A:73:LEU:HD23	2.39	0.52
2:D:116:TYR:O	2:D:120:GLN:CG	2.58	0.52
2:C:290:LYS:CB	2:C:291:PRO:CD	2.88	0.52
2:C:315:VAL:HB	2:C:335:ARG:HH22	1.73	0.52
2:D:339:ARG:O	2:D:342:ASP:HB2	2.09	0.52
2:C:200:ARG:HG3	2:C:200:ARG:HH11	1.75	0.52
2:C:438:TYR:C	2:C:439:LYS:CG	2.82	0.52
2:C:632:LYS:HE3	2:C:638:GLU:CD	2.35	0.51
2:D:514:VAL:HG13	2:D:558:TYR:CD1	2.45	0.51
2:C:563:ASP:OD1	2:C:565:THR:OG1	2.24	0.51
2:D:233:ASN:ND2	2:D:233:ASN:N	2.59	0.51
2:D:85:LEU:HD21	2:D:119:ALA:CB	2.31	0.51
2:C:158:ASN:OD1	2:C:158:ASN:N	2.43	0.51
2:C:313:SER:O	2:C:335:ARG:NH1	2.44	0.51
2:D:358:GLY:HA3	2:D:380:LEU:HD22	1.92	0.51
2:D:514:VAL:HG13	2:D:558:TYR:CE1	2.45	0.51
2:C:600:ASP:OD1	2:C:601:LYS:HG2	2.11	0.50
2:D:200:ARG:O	2:D:204:GLN:HG3	2.11	0.50
1:B:49:MET:CE	1:B:73:LEU:HD23	2.41	0.50
2:C:658:GLU:HA	2:C:658:GLU:OE1	2.12	0.50
2:C:491:ASP:O	2:C:492:GLN:CB	2.58	0.50
2:D:498:TRP:O	2:D:499:PRO:C	2.54	0.50
2:C:356:LYS:HE2	2:C:383:GLN:O	2.11	0.50
2:C:194:ARG:NE	2:C:296:ILE:HD11	2.26	0.50
2:D:300:LEU:O	2:D:304:VAL:HG23	2.12	0.50
2:C:123:ARG:HB3	2:C:123:ARG:HH11	1.73	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:270:ALA:N	2:C:333:LEU:CD1	2.75	0.49
2:C:285:VAL:HG11	2:C:306:LEU:HB3	1.93	0.49
2:D:497:GLU:O	2:D:499:PRO:HD2	2.09	0.49
1:B:268:HIS:O	1:B:269:ASN:CG	2.56	0.49
2:C:631:PHE:CD1	2:C:636:LYS:HD3	2.48	0.49
2:D:119:ALA:HA	2:D:122:ARG:CB	2.42	0.49
1:A:35:PRO:HB3	1:A:264:ALA:O	2.12	0.49
2:C:246:GLU:O	2:C:308:LYS:HA	2.12	0.49
2:C:77:LEU:HA	2:C:256:ASP:OD2	2.13	0.49
2:C:248:ILE:O	2:C:270:ALA:HB2	2.13	0.49
2:C:44:VAL:HG13	2:C:486:LEU:HD13	1.96	0.48
2:C:299:ARG:O	2:C:303:VAL:HG23	2.13	0.48
2:C:433:ASP:OD1	2:C:433:ASP:O	2.31	0.48
1:A:278:LEU:O	1:A:281:SER:HB3	2.14	0.48
1:B:35:PRO:HB3	1:B:264:ALA:O	2.14	0.48
2:D:433:ASP:OD1	2:D:433:ASP:O	2.32	0.48
2:D:320:LEU:HD11	2:D:326:THR:HA	1.96	0.48
2:D:658:GLU:OE1	2:D:658:GLU:HA	2.14	0.48
2:C:315:VAL:HG12	2:C:335:ARG:NH2	2.28	0.48
2:D:601:LYS:HD2	2:D:604:ILE:HG22	1.96	0.47
1:A:126:GLU:OE1	2:D:490:TYR:OH	2.25	0.47
2:D:126:ARG:HA	2:D:126:ARG:NE	2.29	0.47
2:D:234:THR:O	2:D:237:PHE:HB3	2.14	0.47
1:A:115:ASP:OD2	2:D:422:ASN:ND2	2.43	0.47
1:B:267:VAL:HG12	1:B:267:VAL:O	2.14	0.47
2:C:289:GLY:O	2:C:290:LYS:HD3	2.15	0.47
2:C:307:ILE:O	2:C:335:ARG:HD3	2.14	0.47
2:C:316:ARG:HG2	2:C:332:THR:CG2	2.43	0.47
2:C:584:GLU:CD	2:C:630:ARG:NH1	2.73	0.47
2:C:656:LEU:O	2:C:660:VAL:HG23	2.14	0.47
2:D:563:ASP:OD1	2:D:565:THR:OG1	2.33	0.47
1:B:218:MET:HE1	1:B:238:THR:CG2	2.39	0.47
2:C:290:LYS:O	2:C:316:ARG:NH2	2.48	0.47
2:D:427:ARG:HD2	2:D:429:ASP:OD1	2.14	0.47
2:D:636:LYS:HG2	2:D:637:PRO:HD2	1.97	0.47
2:D:510:LYS:HE3	2:D:520:GLN:HG3	1.98	0.46
2:C:535:GLU:OE1	2:C:596:ASN:ND2	2.48	0.46
2:D:497:GLU:CA	2:D:499:PRO:HD2	2.44	0.46
2:C:259:THR:HG21	2:C:303:VAL:HG11	1.98	0.46
2:C:287:GLN:NE2	2:C:287:GLN:CA	2.74	0.46
2:D:351:THR:HG22	2:D:356:LYS:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:601:LYS:HG2	2:D:604:ILE:CB	2.29	0.46
1:A:41:GLN:O	1:A:45:ILE:HG12	2.15	0.46
2:C:240:GLU:O	2:C:243:LEU:HB2	2.16	0.46
2:D:358:GLY:HA3	2:D:380:LEU:CD2	2.46	0.45
2:C:451:ALA:HB1	2:C:452:ILE:HD12	1.97	0.45
2:C:480:VAL:HG23	2:C:511:PHE:CE2	2.52	0.45
2:D:254:MET:SD	2:D:256:ASP:HA	2.56	0.45
1:B:68:TYR:CZ	1:B:99:GLU:HB3	2.51	0.45
2:C:123:ARG:HH11	2:C:123:ARG:CB	2.29	0.45
1:A:91:LEU:HD23	1:A:91:LEU:HA	1.78	0.45
2:C:126:ARG:NE	2:C:126:ARG:HA	2.32	0.45
2:C:288:THR:HG22	2:C:313:SER:HB3	1.99	0.45
2:D:347:MET:HG2	2:D:348:SER:N	2.33	0.44
1:A:49:MET:HE3	1:A:70:ARG:HG3	1.99	0.44
2:C:329:ARG:HG3	2:C:329:ARG:NH1	2.32	0.44
1:A:68:TYR:CZ	1:A:99:GLU:HB3	2.52	0.44
2:C:289:GLY:O	2:C:290:LYS:HB2	2.17	0.44
2:D:636:LYS:CG	2:D:637:PRO:HD2	2.47	0.44
2:D:316:ARG:HB3	2:D:332:THR:CG2	2.47	0.44
2:D:44:VAL:HG13	2:D:486:LEU:HD13	2.00	0.43
2:D:292:MET:HE3	2:D:318:GLU:HB2	2.00	0.43
2:C:64:GLN:CD	2:C:65:ALA:H	2.26	0.43
2:D:257:ASP:CG	2:D:297:GLY:HA2	2.42	0.43
2:C:247:GLY:C	2:C:248:ILE:HG23	2.42	0.43
2:C:232:ARG:N	2:C:232:ARG:CD	2.82	0.43
2:D:182:LYS:HB3	2:D:187:ILE:HG13	2.00	0.43
2:D:400:LEU:HD11	2:D:417:VAL:HG11	1.99	0.43
2:D:521:ARG:NH2	2:D:547:ALA:O	2.48	0.43
1:B:244:LYS:NZ	1:B:279:GLU:OE2	2.48	0.43
2:C:129:TYR:CZ	2:C:163:ASN:HB3	2.53	0.43
2:C:571:LEU:HD23	2:C:665:ASP:HB3	2.01	0.43
2:C:586:GLN:O	2:C:590:LYS:HG3	2.19	0.43
2:C:397:GLY:HA2	2:C:453:ALA:HB3	2.01	0.43
2:D:571:LEU:HD23	2:D:665:ASP:HB3	2.01	0.43
2:C:241:MET:HE2	2:C:241:MET:CA	2.25	0.43
2:C:287:GLN:HE21	2:C:288:THR:H	1.65	0.43
2:C:292:MET:HG3	2:C:292:MET:O	2.18	0.43
2:C:320:LEU:C	2:C:320:LEU:HD23	2.44	0.43
2:D:656:LEU:O	2:D:660:VAL:HG23	2.19	0.43
2:D:273:SER:O	2:D:273:SER:OG	2.31	0.42
2:C:270:ALA:CA	2:C:333:LEU:HD11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:631:PHE:CD1	2:D:636:LYS:HD3	2.55	0.42
2:C:45:SER:O	2:C:49:THR:OG1	2.29	0.42
2:C:448:ARG:NH1	2:C:532:THR:HB	2.34	0.42
2:C:320:LEU:HD11	2:C:326:THR:HG22	2.00	0.42
2:D:177:LEU:O	2:D:182:LYS:HB2	2.19	0.42
2:C:270:ALA:HA	2:C:333:LEU:HD11	2.02	0.42
2:C:421:ASP:OD2	2:C:425:LYS:HB2	2.20	0.42
2:C:636:LYS:CG	2:C:637:PRO:HD2	2.49	0.42
2:D:113:TYR:CE2	2:D:210:VAL:HG11	2.54	0.42
1:A:91:LEU:HG	1:A:100:VAL:HG11	2.01	0.41
1:B:147:ARG:NH2	2:C:54:ARG:O	2.52	0.41
2:C:185:LYS:HE3	2:C:189:GLU:OE2	2.19	0.41
2:D:350:LYS:N	2:D:350:LYS:HD3	2.34	0.41
2:C:316:ARG:HD2	2:C:332:THR:HG21	1.95	0.41
2:D:84:VAL:CG1	2:D:122:ARG:HB3	2.50	0.41
2:C:422:ASN:OD1	2:C:423:ASN:CG	2.63	0.41
2:D:234:THR:HA	2:D:237:PHE:HB3	2.02	0.41
2:C:232:ARG:HG2	2:C:236:GLN:CD	2.45	0.41
1:B:46:LEU:HD23	1:B:49:MET:CE	2.51	0.41
2:C:232:ARG:HB3	2:C:236:GLN:CB	2.50	0.41
1:B:256:THR:O	1:B:260:LYS:HG3	2.20	0.41
2:C:269:PRO:HB2	2:C:333:LEU:HD13	2.02	0.41
1:A:266:ASN:HD21	1:B:266:ASN:ND2	2.09	0.41
2:C:484:ARG:HD3	2:C:484:ARG:HA	1.87	0.41
2:C:57:TYR:CD1	2:C:57:TYR:C	2.99	0.41
2:C:317:LEU:N	2:C:317:LEU:CD2	2.82	0.41
1:A:118:TYR:CZ	1:A:142:LEU:HD23	2.56	0.41
1:A:221:LEU:HG	1:A:234:HIS:HB3	2.03	0.41
1:A:256:THR:O	1:A:260:LYS:HG3	2.21	0.41
2:C:183:THR:HG23	2:C:185:LYS:HB3	2.03	0.41
2:C:461:MET:HB3	2:C:467:ALA:HB3	2.02	0.41
2:C:630:ARG:HD3	2:C:652:PRO:HG3	2.02	0.41
2:D:314:LYS:CD	2:D:334:THR:HG23	2.49	0.41
2:D:495:ARG:HA	2:D:496:PRO:HD2	1.72	0.41
2:D:327:LYS:HA	2:D:327:LYS:HD2	1.47	0.41
1:A:70:ARG:NH2	1:B:50:GLU:OE2	2.39	0.40
2:C:315:VAL:CB	2:C:335:ARG:NH2	2.82	0.40
1:B:196:ASP:C	1:B:197:LYS:HG2	2.47	0.40
2:C:286:GLY:O	2:C:315:VAL:HG23	2.21	0.40
2:C:408:GLY:HA3	2:C:431:ASP:CG	2.47	0.40
2:D:299:ARG:HG3	2:D:302:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:408:GLY:HA3	2:D:431:ASP:CG	2.46	0.40
2:D:588:ILE:HD12	2:D:588:ILE:HA	1.98	0.40
2:C:290:LYS:HB3	2:C:291:PRO:HD2	2.02	0.40
2:D:461:MET:HB3	2:D:467:ALA:HB3	2.04	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	255/296 (86%)	242 (95%)	12 (5%)	1 (0%)	30	60
1	B	256/296 (86%)	244 (95%)	12 (5%)	0	100	100
2	C	641/688 (93%)	599 (93%)	40 (6%)	2 (0%)	36	66
2	D	636/688 (92%)	603 (95%)	30 (5%)	3 (0%)	24	55
All	All	1788/1968 (91%)	1688 (94%)	94 (5%)	6 (0%)	36	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	452	ILE
2	D	452	ILE
1	A	269	ASN
2	D	497	GLU
2	C	248	ILE
2	D	313	SER

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	218/253 (86%)	210 (96%)	8 (4%)	30	65
1	B	219/253 (87%)	217 (99%)	2 (1%)	70	89
2	C	556/590 (94%)	530 (95%)	26 (5%)	23	57
2	D	554/590 (94%)	516 (93%)	38 (7%)	14	41
All	All	1547/1686 (92%)	1473 (95%)	74 (5%)	23	56

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	55	SER
1	A	70	ARG
1	A	148	ASP
1	A	149	LYS
1	A	181	GLU
1	A	226	THR
1	A	268	HIS
1	B	177	GLN
1	B	226	THR
2	C	27	THR
2	C	102	ASP
2	C	148	LEU
2	C	158	ASN
2	C	162	LEU
2	C	200	ARG
2	C	236	GLN
2	C	237	PHE
2	C	241	MET
2	C	243	LEU
2	C	248	ILE
2	C	253	GLN
2	C	261	ILE
2	C	287	GLN
2	C	313	SER
2	C	320	LEU
2	C	327	LYS
2	C	329	ARG

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Mol	Chain	Res	Type
2	C	330	THR
2	C	333	LEU
2	C	334	THR
2	C	336	GLU
2	C	497	GLU
2	C	530	MET
2	C	532	THR
2	C	554	ASP
2	D	37	GLU
2	D	48	VAL
2	D	61	ASP
2	D	69	LYS
2	D	86	LEU
2	D	145	THR
2	D	162	LEU
2	D	168	SER
2	D	210	VAL
2	D	233	ASN
2	D	235	GLU
2	D	237	PHE
2	D	240	GLU
2	D	241	MET
2	D	242	SER
2	D	243	LEU
2	D	251	VAL
2	D	272	LYS
2	D	287	GLN
2	D	288	THR
2	D	293	VAL
2	D	306	LEU
2	D	320	LEU
2	D	327	LYS
2	D	328	THR
2	D	332	THR
2	D	334	THR
2	D	336	GLU
2	D	340	LEU
2	D	343	ARG
2	D	346	LYS
2	D	381	GLU
2	D	384	ASN
2	D	401	THR

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Mol	Chain	Res	Type
2	D	514	VAL
2	D	530	MET
2	D	565	THR
2	D	605	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	266	ASN
1	A	273	HIS
1	B	132	ASN
1	B	190	GLN
1	B	265	ASN
2	C	120	GLN
2	C	204	GLN
2	C	236	GLN
2	C	253	GLN
2	C	287	GLN
2	C	423	ASN
2	C	462	GLN
2	C	505	GLN
2	C	603	ASN
2	C	650	GLN
2	C	661	ASN
2	D	120	GLN
2	D	143	ASN
2	D	233	ASN
2	D	236	GLN
2	D	253	GLN
2	D	376	GLN
2	D	378	GLN
2	D	482	GLN
2	D	534	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	257/296 (86%)	-0.43	0	100 100	18, 31, 58, 109	0
1	B	258/296 (87%)	-0.36	0	100 100	16, 33, 61, 110	0
2	C	645/688 (93%)	0.51	43 (6%)	24 17	31, 64, 134, 197	0
2	D	642/688 (93%)	0.38	41 (6%)	25 18	30, 59, 126, 184	0
All	All	1802/1968 (91%)	0.20	84 (4%)	36 29	16, 53, 125, 197	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	331	VAL	5.1
2	D	328	THR	5.1
2	D	325	GLY	5.0
2	D	243	LEU	4.9
2	C	296	ILE	4.3
2	C	315	VAL	4.3
2	C	566	ALA	4.1
2	C	333	LEU	4.0
2	C	325	GLY	4.0
2	D	498	TRP	4.0
2	C	300	LEU	3.9
2	C	603	ASN	3.8
2	D	326	THR	3.8
2	D	496	PRO	3.7
2	D	248	ILE	3.6
2	C	26	ILE	3.5
2	C	90	VAL	3.5
2	C	241	MET	3.5
2	C	283	VAL	3.4
2	D	299	ARG	3.4
2	C	268	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	327	LYS	3.3
2	D	298	TRP	3.3
2	D	331	VAL	3.2
2	C	242	SER	2.9
2	C	597	ALA	2.9
2	D	296	ILE	2.9
2	C	256	ASP	2.9
2	D	333	LEU	2.9
2	C	125	GLU	2.8
2	C	536	GLU	2.8
2	D	37	GLU	2.8
2	D	596	ASN	2.8
2	C	190	THR	2.8
2	C	317	LEU	2.7
2	C	299	ARG	2.7
2	C	340	LEU	2.7
2	C	271	ALA	2.7
2	D	237	PHE	2.6
2	C	33	PRO	2.6
2	D	90	VAL	2.6
2	C	351	THR	2.6
2	C	422	ASN	2.6
2	C	275	ALA	2.5
2	D	269	PRO	2.5
2	D	121	LYS	2.5
2	D	31	GLN	2.5
2	D	278	VAL	2.4
2	D	307	ILE	2.4
2	C	278	VAL	2.4
2	C	158	ASN	2.4
2	D	241	MET	2.4
2	D	533	GLY	2.3
2	D	119	ALA	2.3
2	C	492	GLN	2.3
2	D	315	VAL	2.3
2	D	254	MET	2.3
2	D	310	PRO	2.3
2	C	29	ALA	2.3
2	C	534	ASN	2.3
2	C	123	ARG	2.3
2	D	322	ALA	2.2
2	D	538	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	279	GLY	2.2
2	D	353	GLY	2.2
2	C	307	ILE	2.2
2	D	294	ASP	2.2
2	D	499	PRO	2.2
2	D	595	PHE	2.2
2	D	125	GLU	2.2
2	C	234	THR	2.2
2	D	671	LYS	2.2
2	C	285	VAL	2.1
2	C	421	ASP	2.1
2	D	249	GLY	2.1
2	C	269	PRO	2.1
2	D	534	ASN	2.1
2	D	306	LEU	2.1
2	C	237	PHE	2.0
2	C	535	GLU	2.0
2	C	36	LYS	2.0
2	D	242	SER	2.0
2	C	543	PHE	2.0
2	C	127	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	C	701	1/1	0.97	0.04	58,58,58,58	0
3	CA	D	701	1/1	0.97	0.06	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.