



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 10:13 PM JST

PDB ID : 6IQQ  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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

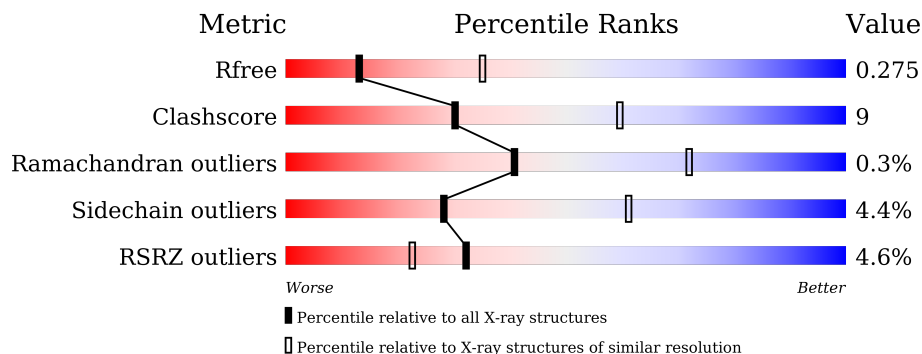
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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  $\geq 3$ , 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	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">74%      11%      •      13%</p>
1	B	296	<div style="display: flex; align-items: center;"> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">79%      8%      •      13%</p>
2	C	688	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">6%      74%      17%      •      6%</p>
2	D	688	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5%      74%      16%      •      7%</p>

## 2 Entry composition i

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
			Total	C	N	O	S			
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 (three-letter code: CA) (formula: Ca).

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

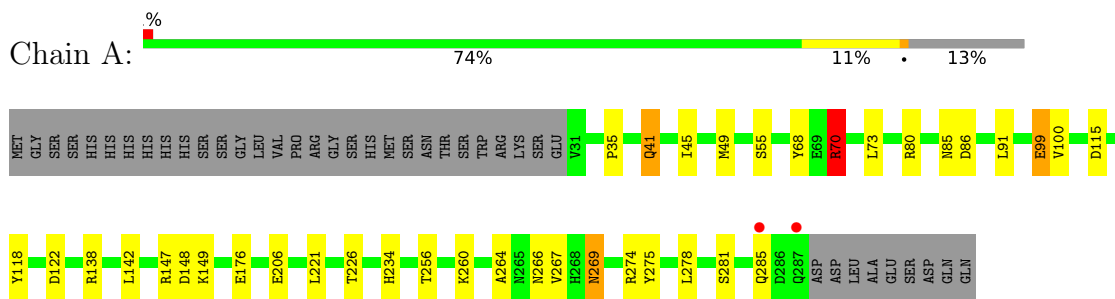
- Molecule 4 is water.

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

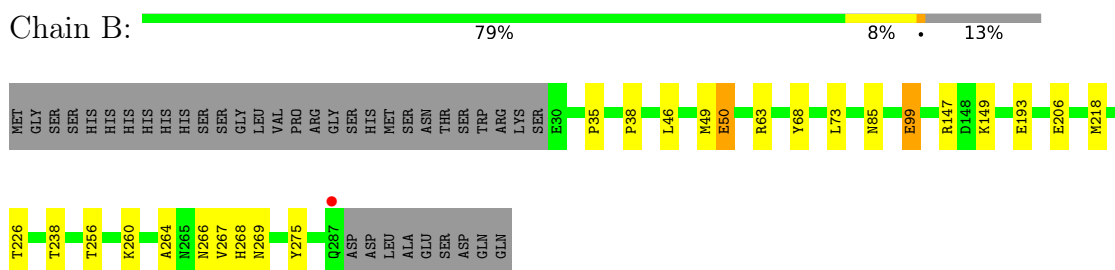
### 3 Residue-property plots

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.

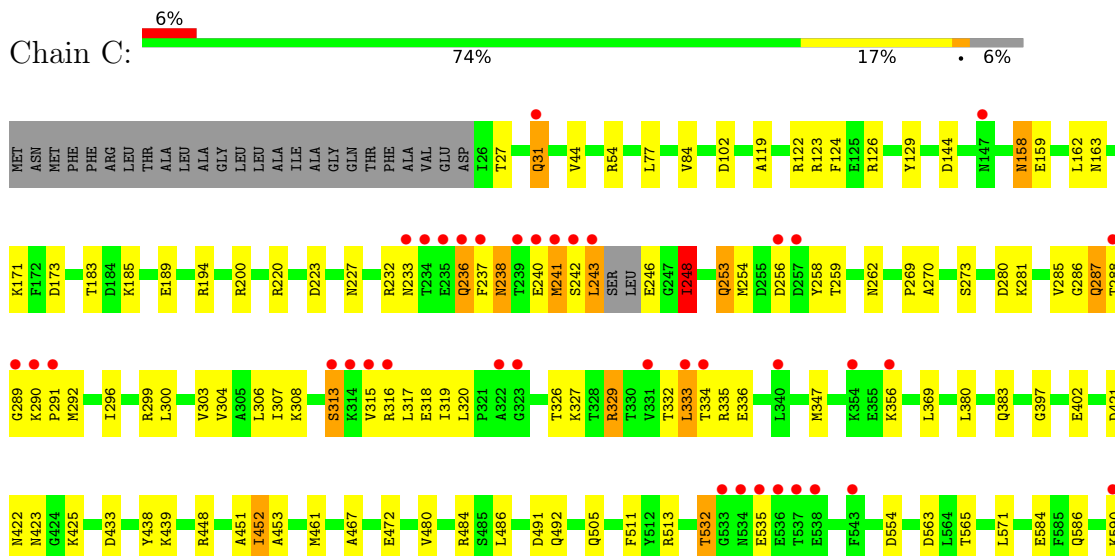
- Molecule 1: Lipoprotein NlpI

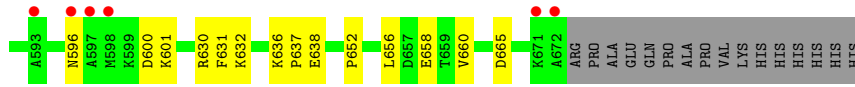


- Molecule 1: Lipoprotein NlpI

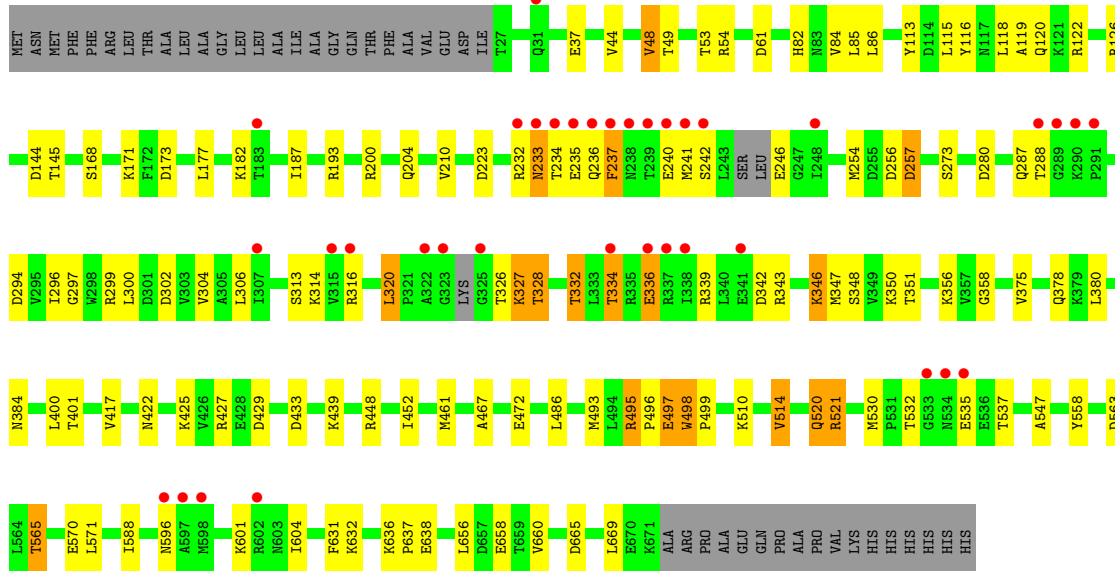
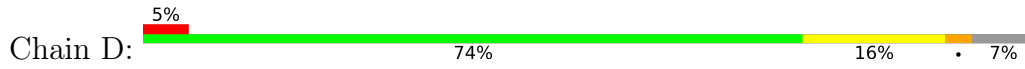


- Molecule 2: Tail-specific protease





• 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, $\alpha$ , $\beta$ , $\gamma$	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) 97.0 (29.98-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 2.80Å)	Xtrriage
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 (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtrriage
Anisotropy	0.069	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14502	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.90	4/2126 (0.2%)	1.05	6/2886 (0.2%)
1	B	0.92	4/2135 (0.2%)	1.04	4/2898 (0.1%)
2	C	0.79	0/5215	0.99	2/7040 (0.0%)
2	D	0.79	0/5192	1.02	4/7008 (0.1%)
All	All	0.83	8/14668 (0.1%)	1.02	16/19832 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	50	GLU	CD-OE2	-6.42	1.18	1.25
1	A	99	GLU	CD-OE2	-6.08	1.19	1.25
1	A	206	GLU	CD-OE2	6.06	1.32	1.25
1	B	38	PRO	C-O	-5.74	1.11	1.23
1	B	99	GLU	CD-OE2	-5.68	1.19	1.25
1	A	176	GLU	CD-OE1	5.56	1.31	1.25
1	B	206	GLU	CD-OE2	5.50	1.31	1.25
1	A	267	VAL	C-O	5.21	1.33	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	495	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	B	275	TYR	CB-CA-C	7.24	124.87	110.40
1	A	275	TYR	CB-CA-C	7.12	124.64	110.40
1	A	85	ASN	CB-CA-C	6.77	123.95	110.40
1	B	85	ASN	CB-CA-C	6.51	123.41	110.40
2	D	521	ARG	CB-CA-C	-6.13	98.14	110.40
2	C	513	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	193	GLU	CB-CA-C	5.89	122.18	110.40
1	B	63	ARG	NE-CZ-NH2	5.85	123.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	70	ARG	NE-CZ-NH2	-5.48	117.56	120.30
2	D	520	GLN	CB-CA-C	-5.43	99.55	110.40
1	A	80	ARG	CG-CD-NE	-5.32	100.64	111.80
1	A	269	ASN	N-CA-CB	5.22	119.99	110.60
2	C	220	ARG	CG-CD-NE	-5.21	100.86	111.80
2	D	495	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	2082	0	2016	25	0
1	B	2091	0	2022	21	0
2	C	5128	0	5142	135	0
2	D	5106	0	5112	99	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
4	C	23	0	0	1	0
4	D	35	0	0	0	0
All	All	14502	0	14292	268	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 (268) 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	1.07
2:C:316:ARG:HD2	2:C:332:THR:HG22	1.33	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:241:MET:HA	2:C:241:MET:CE	2.09	0.82
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: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: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
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:D:497:GLU:C	2:D:499:PRO:CD	2.54	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:438:TYR:O	2:C:439:LYS:HG2	1.92	0.69
2:C:269:PRO:C	2:C:333:LEU:HD11	2.13	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:C:241:MET:HA	2:C:241:MET:HE1	1.76	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: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
2:C:253:GLN:HE21	2:C:262:ASN:CG	2.00	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
2:C:242:SER:O	2:C:243:LEU:C	2.37	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:218:MET:CE	1:B:238:THR:HG21	2.36	0.56
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:D:118:LEU:O	2:D:119:ALA:HB3	2.06	0.56
1:B:268:HIS:O	1:B:269:ASN:CB	2.54	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
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: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: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
2:C:238:ASN:OD1	2:C:238:ASN:C	2.47	0.53
2:C:631:PHE:CG	2:C:636:LYS:HD3	2.44	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:D:514:VAL:HG13	2:D:558:TYR:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:31:GLN:CD	2:C:31:GLN:O	2.49	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
1:B:49:MET:HE1	1:B:73:LEU:HD23	1.92	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: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
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
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:269:PRO:C	2:C:333:LEU:CD1	2.81	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:C:438:TYR:C	2:C:439:LYS:HG2	2.34	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
2:C:273:SER:O	2:C:273:SER:OG	2.30	0.47
2:D:126:ARG:HA	2:D:126:ARG:NE	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:218:MET:HE1	1:B:238:THR:HG21	1.96	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:438:TYR:C	2:C:439:LYS:CG	2.82	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
2:C:290:LYS:O	2:C:316:ARG:NH2	2.48	0.47
2:C:632:LYS:HE3	2:C:638:GLU:CD	2.35	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
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:D:498:TRP:O	2:D:499:PRO:C	2.54	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:D:347:MET:HE2	2:D:380:LEU:CD2	2.47	0.45
1:B:268:HIS:O	1:B:269:ASN:CG	2.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:MET:HE1	1:B:238:THR:CG2	2.48	0.43
2:D:44:VAL:HG13	2:D:486:LEU:HD13	2.00	0.43
1:A:49:MET:HE2	1:A:73:LEU:HD23	1.99	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
2:C:129:TYR:CZ	2:C:163:ASN:HB3	2.53	0.43
2:C:292:MET:HG3	2:C:292:MET:O	2.18	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
1:A:49:MET:HE1	1:A:73:LEU:HD23	2.00	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:287:GLN:HE21	2:C:288:THR:H	1.65	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
2:D:631:PHE:CD1	2:D:636:LYS:HD3	2.55	0.42
2:C:448:ARG:NH1	2:C:532:THR:HB	2.34	0.42
2:C:584:GLU:CD	2:C:630:ARG:NH1	2.73	0.42
2:C:320:LEU:HD11	2:C:326:THR:HG22	2.00	0.42
2:C:347:MET:HE2	2:C:380:LEU:HD21	2.01	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:D:234:THR:HA	2:D:237:PHE:HB3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:317:LEU:N	2:C:317:LEU:CD2	2.82	0.41
2:D:347:MET:HE2	2:D:380:LEU:HD21	2.03	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:281:LYS:NZ	4:C:802:HOH:O	2.53	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
2:C:286:GLY:O	2:C:315:VAL:HG23	2.21	0.40
2:D:299:ARG:HG3	2:D:302:ASP:OD2	2.21	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%)	34 66
1	B	256/296 (86%)	244 (95%)	12 (5%)	0	100 100
2	C	641/688 (93%)	599 (93%)	40 (6%)	2 (0%)	41 72
2	D	636/688 (92%)	603 (95%)	30 (5%)	3 (0%)	29 61
All	All	1788/1968 (91%)	1688 (94%)	94 (5%)	6 (0%)	41 72

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%)	212 (97%)	6 (3%)	43 77
1	B	219/253 (87%)	218 (100%)	1 (0%)	88 96
2	C	556/590 (94%)	532 (96%)	24 (4%)	29 62
2	D	554/590 (94%)	517 (93%)	37 (7%)	16 43
All	All	1547/1686 (92%)	1479 (96%)	68 (4%)	28 61

All (68) 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	226	THR
1	B	226	THR
2	C	31	GLN
2	C	102	ASP
2	C	122	ARG
2	C	158	ASN
2	C	162	LEU
2	C	173	ASP
2	C	223	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	233	ASN
2	C	236	GLN
2	C	237	PHE
2	C	238	ASN
2	C	241	MET
2	C	243	LEU
2	C	248	ILE
2	C	253	GLN
2	C	287	GLN
2	C	313	SER
2	C	327	LYS
2	C	329	ARG
2	C	333	LEU
2	C	334	THR
2	C	336	GLU
2	C	532	THR
2	C	554	ASP
2	D	37	GLU
2	D	48	VAL
2	D	61	ASP
2	D	82	HIS
2	D	86	LEU
2	D	145	THR
2	D	168	SER
2	D	173	ASP
2	D	193	ARG
2	D	223	ASP
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	257	ASP
2	D	280	ASP
2	D	287	GLN
2	D	288	THR
2	D	306	LEU
2	D	320	LEU
2	D	327	LYS
2	D	328	THR
2	D	332	THR

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Mol	Chain	Res	Type
2	D	334	THR
2	D	336	GLU
2	D	343	ARG
2	D	346	LYS
2	D	384	ASN
2	D	401	THR
2	D	439	LYS
2	D	493	MET
2	D	498	TRP
2	D	514	VAL
2	D	530	MET
2	D	565	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	ASN
1	A	273	HIS
2	C	236	GLN
2	C	253	GLN
2	C	287	GLN
2	C	423	ASN
2	C	505	GLN
2	D	120	GLN
2	D	143	ASN
2	D	233	ASN
2	D	236	GLN

### 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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	257/296 (86%)	-0.57	2 (0%) 86 81	18, 31, 58, 109	0
1	B	258/296 (87%)	-0.55	1 (0%) 92 91	16, 33, 61, 110	0
2	C	645/688 (93%)	0.12	44 (6%) 17 10	31, 64, 134, 197	0
2	D	642/688 (93%)	-0.04	36 (5%) 24 16	30, 59, 126, 184	0
All	All	1802/1968 (91%)	-0.13	83 (4%) 32 22	16, 53, 125, 197	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	323	GLY	10.0
2	D	241	MET	7.4
2	C	323	GLY	6.1
2	C	241	MET	6.0
2	C	322	ALA	5.2
2	C	233	ASN	5.2
2	C	535	GLU	5.1
2	C	290	LYS	4.5
2	D	236	GLN	4.4
2	D	322	ALA	4.4
2	C	537	THR	4.4
2	C	235	GLU	4.3
2	C	239	THR	4.3
2	C	534	ASN	4.2
2	C	242	SER	4.2
2	C	536	GLU	4.1
2	C	315	VAL	4.1
2	D	289	GLY	4.0
2	C	538	GLU	4.0
2	C	598	MET	4.0
2	D	240	GLU	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	240	GLU	3.7
2	D	233	ASN	3.6
2	D	316	ARG	3.6
2	D	334	THR	3.5
2	D	238	ASN	3.4
2	C	147	ASN	3.4
2	C	243	LEU	3.4
2	C	234	THR	3.4
2	D	596	ASN	3.4
2	D	248	ILE	3.3
2	D	315	VAL	3.2
2	C	236	GLN	3.2
2	C	288	THR	3.2
2	C	316	ARG	3.2
2	C	597	ALA	3.2
2	D	533	GLY	3.1
2	D	239	THR	3.1
2	C	354	LYS	3.1
2	C	672	ALA	3.1
2	C	333	LEU	3.0
2	C	313	SER	3.0
2	D	237	PHE	2.9
2	D	288	THR	2.9
2	D	535	GLU	2.8
2	D	232	ARG	2.8
2	D	534	ASN	2.8
2	C	533	GLY	2.8
2	D	183	THR	2.7
2	C	671	LYS	2.7
2	D	234	THR	2.7
2	D	31	GLN	2.7
2	C	291	PRO	2.7
2	D	598	MET	2.7
2	D	602	ARG	2.7
2	C	314	LYS	2.6
2	C	356	LYS	2.6
2	D	290	LYS	2.6
2	D	597	ALA	2.5
2	D	242	SER	2.4
2	D	235	GLU	2.4
2	D	307	ILE	2.4
2	C	31	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	336	GLU	2.3
1	B	287	GLN	2.3
2	D	341	GLU	2.3
2	D	291	PRO	2.3
2	C	543	PHE	2.2
2	C	256	ASP	2.2
2	C	289	GLY	2.1
2	D	338	ILE	2.1
2	D	325	GLY	2.1
1	A	287	GLN	2.1
2	C	331	VAL	2.1
2	C	237	PHE	2.1
2	C	334	THR	2.1
2	C	257	ASP	2.1
2	C	593	ALA	2.1
2	D	337	ARG	2.0
2	C	590	LYS	2.0
2	C	340	LEU	2.0
2	C	596	ASN	2.0
1	A	285	GLN	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 monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	D	701	1/1	0.91	0.18	48,48,48,48	0
3	CA	C	701	1/1	0.92	0.14	58,58,58,58	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.