



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:46 AM UTC

PDB ID : 6IQR / pdb_00006iqr
Title : Crystal structure of Prc with S452I and L252Y mutations
Authors : Chueh, C.K.; Chang, C.I.
Deposited on : 2018-11-08
Resolution : 3.42 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

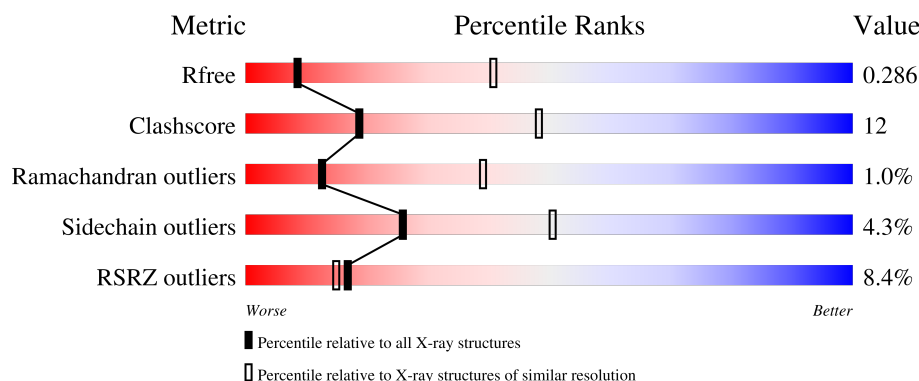
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	688	8% 63% 25% 5% 7%
1	B	688	8% 66% 22% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10145 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 Tail-specific protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	0	0
			5080	3201	884	983	12			
1	B	636	Total	C	N	O	S	0	0	0
			5063	3192	884	975	12			

There are 16 discrepancies between the modelled and reference sequences:

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

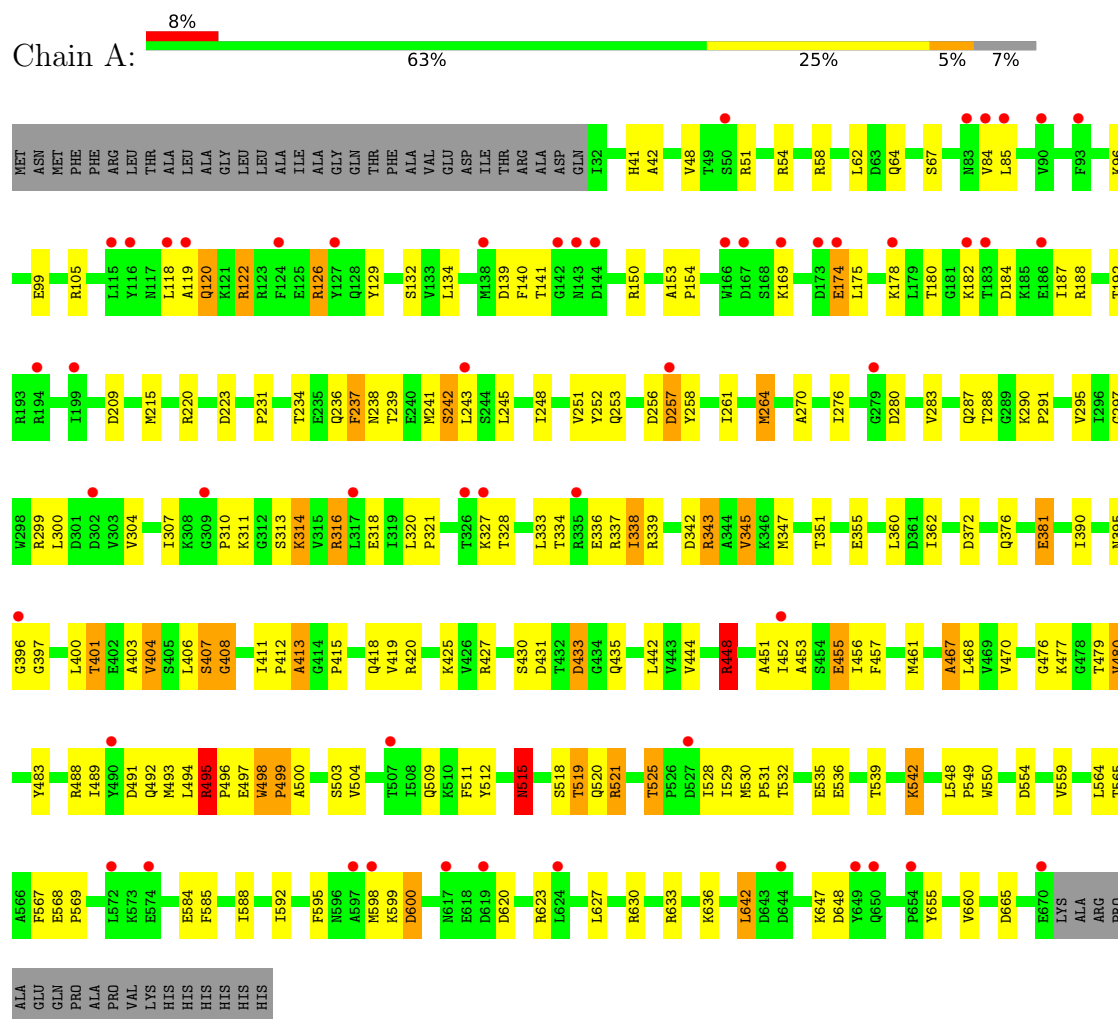
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		
2	B	1	Total	O	0	0
			1	1		

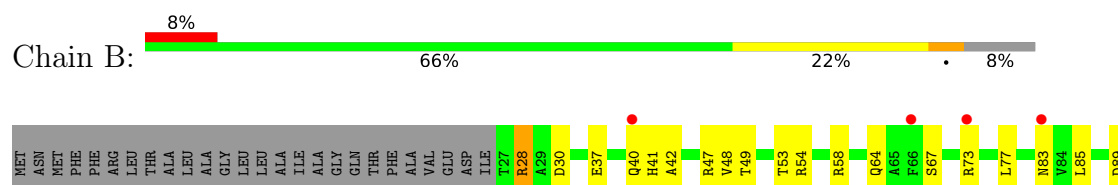
3 Residue-property plots

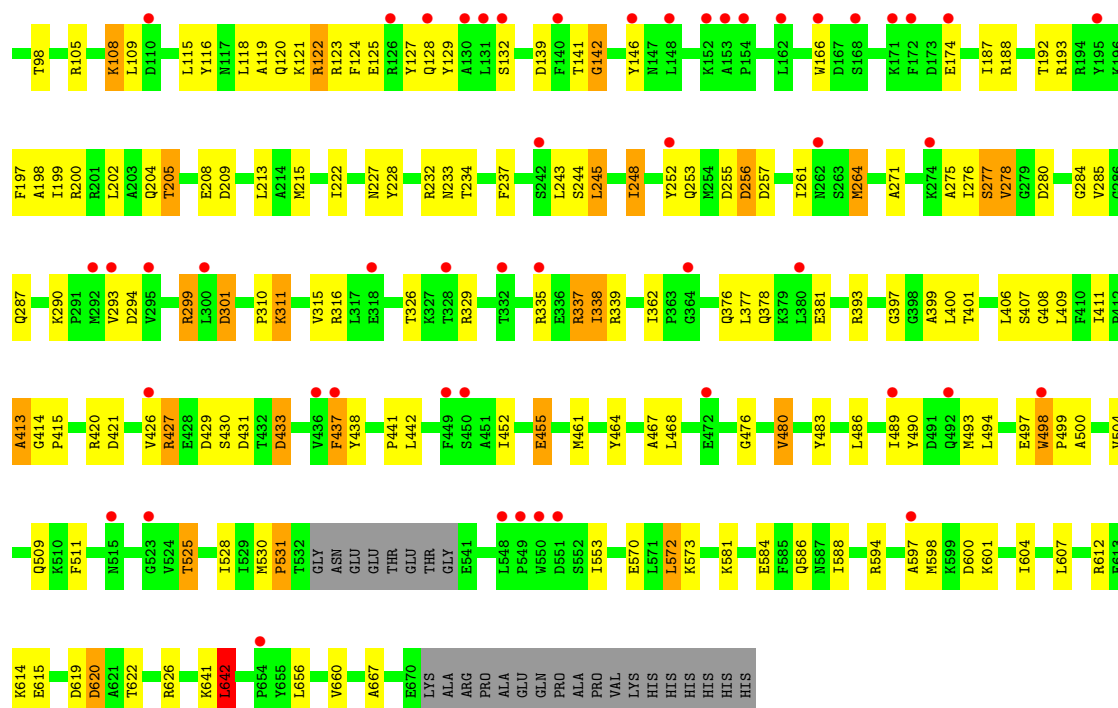
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Tail-specific protease



• Molecule 1: Tail-specific protease





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.28Å 129.28Å 236.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.97 – 3.42 29.97 – 3.42	Depositor EDS
% Data completeness (in resolution range)	90.9 (29.97-3.42) 90.9 (29.97-3.42)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	39.63 (at 3.39Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.239 , 0.288 0.244 , 0.286	Depositor DCC
R_{free} test set	1515 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	77.1	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.099 for -h,-k,l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10145	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	1.06	16/5168 (0.3%)	1.43	30/6979 (0.4%)
1	B	1.01	13/5150 (0.3%)	1.34	19/6953 (0.3%)
All	All	1.04	29/10318 (0.3%)	1.39	49/13932 (0.4%)

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	15
1	B	0	15
All	All	0	30

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	362	ILE	N-CA	-11.07	1.37	1.46
1	A	435	GLN	C-O	-11.02	1.09	1.24
1	A	519	THR	C-O	-7.95	1.13	1.24
1	A	408	GLY	C-O	-7.93	1.15	1.23
1	A	642	LEU	N-CA	7.61	1.56	1.46
1	A	467	ALA	C-O	-7.47	1.14	1.23
1	B	245	LEU	N-CA	7.34	1.55	1.46
1	B	414	GLY	N-CA	7.03	1.54	1.44
1	A	479	THR	N-CA	-6.14	1.38	1.45
1	B	248	ILE	N-CA	5.86	1.53	1.46
1	B	498	TRP	N-CA	-5.78	1.41	1.46
1	B	660	VAL	N-CA	5.74	1.53	1.46
1	A	407	SER	C-O	-5.70	1.17	1.24
1	A	248	ILE	N-CA	5.69	1.53	1.46
1	A	564	LEU	N-CA	-5.68	1.39	1.46
1	A	565	THR	N-CA	5.63	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	490	TYR	N-CA	5.59	1.53	1.46
1	A	251	VAL	N-CA	-5.56	1.39	1.46
1	B	572	LEU	C-O	5.48	1.30	1.24
1	B	264	MET	N-CA	-5.45	1.39	1.46
1	A	264	MET	N-CA	-5.41	1.39	1.46
1	B	204	GLN	N-CA	5.33	1.53	1.46
1	A	660	VAL	N-CA	5.29	1.52	1.46
1	B	642	LEU	N-CA	5.23	1.53	1.46
1	B	455	GLU	C-O	-5.17	1.18	1.24
1	A	455	GLU	C-O	-5.09	1.18	1.24
1	A	515	ASN	C-O	-5.08	1.17	1.24
1	A	521	ARG	N-CA	5.06	1.52	1.46
1	B	233	ASN	N-CA	5.06	1.52	1.46

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	GLN	N-CA-C	-10.32	100.55	113.55
1	A	120	GLN	N-CA-C	-8.91	102.32	113.55
1	A	337	ARG	CB-CA-C	8.73	125.69	109.71
1	A	433	ASP	CB-CA-C	-8.58	96.97	109.84
1	B	525	THR	CB-CA-C	8.36	118.45	110.17
1	B	413	ALA	N-CA-C	8.32	122.51	111.28
1	A	525	THR	CB-CA-C	7.96	118.05	110.17
1	A	499	PRO	N-CA-C	-7.86	103.62	113.84
1	A	342	ASP	CB-CA-C	7.73	123.99	110.85
1	A	174	GLU	CB-CG-CD	7.54	125.42	112.60
1	A	234	THR	CB-CA-C	-7.41	98.08	110.68
1	A	245	LEU	CA-C-N	6.97	132.54	122.85
1	A	245	LEU	C-N-CA	6.97	132.54	122.85
1	A	536	GLU	CB-CG-CD	6.58	123.79	112.60
1	B	397	GLY	CA-C-N	6.42	129.26	120.72
1	B	397	GLY	C-N-CA	6.42	129.26	120.72
1	A	491	ASP	CA-CB-CG	6.34	118.94	112.60
1	B	244	SER	CA-C-N	6.31	133.60	121.54
1	B	244	SER	C-N-CA	6.31	133.60	121.54
1	B	205	THR	CB-CA-C	6.27	122.23	109.76
1	A	381	GLU	N-CA-C	-6.24	105.80	113.41
1	B	499	PRO	N-CA-C	-6.23	105.74	113.84
1	A	520	GLN	CB-CA-C	5.89	119.32	109.89
1	B	381	GLU	N-CA-C	-5.85	106.28	113.41
1	B	243	LEU	CA-C-O	-5.84	114.54	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	VAL	CA-C-N	5.80	127.99	120.44
1	A	404	VAL	C-N-CA	5.80	127.99	120.44
1	B	437	PHE	CA-CB-CG	-5.78	108.02	113.80
1	A	372	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	237	PHE	CA-CB-CG	-5.69	108.11	113.80
1	B	311	LYS	CB-CA-C	-5.63	99.21	110.42
1	A	345	VAL	CA-C-O	-5.58	115.22	121.36
1	A	477	LYS	CB-CG-CD	5.52	124.00	111.30
1	A	252	TYR	CA-C-O	-5.39	115.06	121.16
1	B	310	PRO	N-CA-C	5.35	119.61	111.15
1	A	519	THR	N-CA-C	-5.35	106.53	113.16
1	B	139	ASP	CB-CA-C	5.27	119.72	109.33
1	B	301	ASP	CB-CA-C	-5.24	102.04	110.74
1	A	665	ASP	CA-CB-CG	5.24	117.83	112.60
1	A	401	THR	CA-CB-OG1	-5.19	101.81	109.60
1	A	554	ASP	N-CA-C	-5.18	102.01	110.20
1	A	395	ASN	CA-CB-CG	5.14	117.74	112.60
1	B	586	GLN	N-CA-C	-5.12	105.59	111.07
1	B	294	ASP	CA-CB-CG	5.11	117.71	112.60
1	B	399	ALA	CA-C-O	-5.09	115.12	120.92
1	A	435	GLN	CA-C-N	5.05	129.69	123.12
1	A	435	GLN	C-N-CA	5.05	129.69	123.12
1	A	223	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	567	PHE	CA-CB-CG	5.02	118.82	113.80

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	ARG	Sidechain
1	A	126	ARG	Sidechain
1	A	150	ARG	Sidechain
1	A	220	ARG	Sidechain
1	A	231	PRO	Peptide
1	A	316	ARG	Sidechain
1	A	343	ARG	Sidechain
1	A	397	GLY	Peptide
1	A	448	ARG	Sidechain
1	A	488	ARG	Sidechain
1	A	495	ARG	Sidechain
1	A	496	PRO	Peptide
1	A	54	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	623	ARG	Sidechain
1	A	633	ARG	Sidechain
1	B	105	ARG	Sidechain
1	B	108	LYS	Peptide
1	B	122	ARG	Sidechain
1	B	123	ARG	Sidechain
1	B	200	ARG	Sidechain
1	B	232	ARG	Sidechain
1	B	28	ARG	Sidechain
1	B	287	GLN	Peptide
1	B	299	ARG	Sidechain
1	B	326	THR	Peptide
1	B	337	ARG	Sidechain
1	B	427	ARG	Sidechain
1	B	54	ARG	Sidechain
1	B	594	ARG	Sidechain
1	B	626	ARG	Sidechain

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	5080	0	5093	145	0
1	B	5063	0	5085	101	0
2	A	1	0	0	4	0
2	B	1	0	0	2	0
All	All	10145	0	10178	242	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 12.

All (242) 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:B:408:GLY:HA3	1:B:431:ASP:OD2	1.45	1.14
1:B:408:GLY:CA	1:B:431:ASP:OD2	1.98	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ASP:O	2:B:701:HOH:O	1.74	1.04
1:A:209:ASP:OD2	1:A:299:ARG:NH1	1.94	0.99
1:B:411:ILE:O	2:B:701:HOH:O	1.85	0.94
1:A:448:ARG:NH2	1:A:532:THR:HG22	1.85	0.91
1:B:28:ARG:HH11	1:B:128:GLN:CD	1.80	0.90
1:A:448:ARG:NH2	1:A:532:THR:CG2	2.36	0.88
1:B:85:LEU:HD21	1:B:119:ALA:HB2	1.53	0.88
1:B:209:ASP:OD2	1:B:299:ARG:NH1	2.05	0.88
1:A:48:VAL:HG11	1:A:215:MET:SD	2.18	0.84
1:B:48:VAL:HG11	1:B:215:MET:SD	2.17	0.84
1:B:248:ILE:HD11	1:B:252:TYR:OH	1.78	0.82
1:A:498:TRP:N	1:A:499:PRO:CD	2.41	0.82
1:B:28:ARG:NH1	1:B:128:GLN:NE2	2.30	0.80
1:A:492:GLN:NE2	1:A:497:GLU:O	2.17	0.78
1:B:28:ARG:NH1	1:B:128:GLN:HE22	1.82	0.76
1:A:338:ILE:HG22	1:A:338:ILE:O	1.84	0.76
1:A:448:ARG:HH21	1:A:532:THR:HG22	1.52	0.75
1:A:287:GLN:O	1:A:316:ARG:NH1	2.19	0.73
1:B:49:THR:O	1:B:53:THR:HG23	1.88	0.73
1:B:530:MET:HB3	1:B:531:PRO:HD2	1.70	0.72
1:B:408:GLY:HA2	1:B:431:ASP:OD2	1.87	0.71
1:B:118:LEU:O	1:B:119:ALA:HB3	1.88	0.71
1:A:257:ASP:HA	1:A:297:GLY:HA2	1.73	0.71
1:A:498:TRP:O	1:A:498:TRP:CE3	2.45	0.70
1:A:461:MET:HE2	1:A:461:MET:HA	1.71	0.70
1:B:408:GLY:HA3	1:B:431:ASP:CG	2.17	0.69
1:A:376:GLN:OE1	1:A:376:GLN:HA	1.91	0.69
1:B:493:MET:HE2	1:B:494:LEU:HD21	1.75	0.69
1:A:188:ARG:O	1:A:192:THR:OG1	2.08	0.69
1:A:433:ASP:CB	2:A:701:HOH:O	2.39	0.69
1:A:448:ARG:HH22	1:A:532:THR:CG2	2.04	0.69
1:A:600:ASP:OD2	1:B:525:THR:HG21	1.91	0.69
1:A:118:LEU:O	1:A:119:ALA:HB3	1.93	0.68
1:B:280:ASP:OD2	1:B:329:ARG:NH2	2.26	0.68
1:A:178:LYS:NZ	1:A:184:ASP:OD1	2.27	0.68
1:A:498:TRP:N	1:A:499:PRO:HD3	2.10	0.67
1:B:28:ARG:NH1	1:B:128:GLN:CD	2.51	0.66
1:B:461:MET:HE2	1:B:461:MET:HA	1.78	0.66
1:B:480:VAL:HG22	1:B:509:GLN:HB2	1.79	0.65
1:A:468:LEU:HD21	1:A:528:ILE:HD12	1.78	0.65
1:B:275:ALA:O	1:B:329:ARG:NH2	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ASP:HB3	2:A:701:HOH:O	1.96	0.64
1:B:122:ARG:NH1	1:B:125:GLU:OE2	2.30	0.64
1:A:470:VAL:CG1	1:A:530:MET:HE2	2.28	0.63
1:B:40:GLN:NE2	1:B:497:GLU:O	2.24	0.63
1:A:174:GLU:HG2	1:A:187:ILE:HG21	1.81	0.63
1:A:480:VAL:HG22	1:A:509:GLN:HB2	1.80	0.63
1:B:174:GLU:HG3	1:B:187:ILE:HG21	1.80	0.63
1:B:58:ARG:NH1	1:B:222:ILE:O	2.31	0.62
1:A:418:GLN:HB2	1:A:512:TYR:HB2	1.80	0.62
1:A:498:TRP:O	1:A:498:TRP:HE3	1.83	0.62
1:A:320:LEU:HD12	1:A:327:LYS:O	2.00	0.62
1:A:139:ASP:OD1	1:A:141:THR:CB	2.48	0.61
1:A:400:LEU:HD22	1:A:511:PHE:CE1	2.36	0.61
1:A:84:VAL:O	1:A:122:ARG:HG2	2.00	0.61
1:A:493:MET:HG2	1:A:494:LEU:HD23	1.81	0.61
1:A:85:LEU:CD2	1:A:119:ALA:HB2	2.32	0.60
1:A:139:ASP:OD1	1:A:141:THR:HB	2.02	0.59
1:A:433:ASP:HB2	2:A:701:HOH:O	2.00	0.59
1:B:498:TRP:HA	1:B:498:TRP:CE3	2.37	0.59
1:A:408:GLY:HA3	1:A:431:ASP:CG	2.28	0.59
1:A:62:LEU:O	1:A:105:ARG:NH2	2.36	0.59
1:B:376:GLN:HA	1:B:376:GLN:OE1	2.00	0.59
1:B:28:ARG:HH11	1:B:128:GLN:NE2	1.95	0.58
1:A:236:GLN:OE1	1:A:239:THR:HB	2.04	0.58
1:A:390:ILE:HB	1:A:444:VAL:HG22	1.84	0.58
1:A:140:PHE:CE1	1:A:175:LEU:HB2	2.39	0.57
1:B:188:ARG:O	1:B:192:THR:OG1	2.15	0.57
1:B:337:ARG:O	1:B:338:ILE:HB	2.04	0.57
1:A:595:PHE:O	1:A:599:LYS:HB3	2.05	0.57
1:B:441:PRO:HG2	1:B:667:ALA:HA	1.86	0.57
1:B:124:PHE:CZ	1:B:128:GLN:NE2	2.74	0.56
1:A:237:PHE:C	1:A:237:PHE:CD2	2.83	0.56
1:A:498:TRP:C	1:A:500:ALA:H	2.14	0.56
1:A:153:ALA:HB1	1:A:154:PRO:HD2	1.86	0.56
1:A:494:LEU:O	1:A:495:ARG:HG3	2.06	0.56
1:A:345:VAL:HG23	1:A:362:ILE:HG12	1.88	0.55
1:B:208:GLU:OE2	1:B:228:TYR:OH	2.13	0.55
1:A:535:GLU:HG3	1:A:592:ILE:HG23	1.89	0.55
1:A:530:MET:HB3	1:A:531:PRO:HD2	1.89	0.55
1:A:412:PRO:O	1:A:413:ALA:O	2.24	0.55
1:B:83:ASN:O	1:B:166:TRP:NE1	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASP:CG	1:A:299:ARG:HH11	2.10	0.55
1:A:238:ASN:O	1:A:242:SER:HB2	2.07	0.55
1:A:455:GLU:OE2	1:A:476:GLY:N	2.39	0.55
1:A:396:GLY:HA2	1:A:451:ALA:HB3	1.89	0.54
1:A:345:VAL:HG13	1:A:345:VAL:O	2.07	0.54
1:A:139:ASP:OD1	1:A:141:THR:OG1	2.25	0.54
1:B:28:ARG:HD3	1:B:128:GLN:OE1	2.07	0.54
1:A:134:LEU:O	1:A:188:ARG:NH1	2.40	0.54
1:A:236:GLN:OE1	1:A:236:GLN:HA	2.08	0.54
1:A:518:SER:O	1:A:550:TRP:NE1	2.40	0.54
1:A:532:THR:OG1	1:A:655:TYR:OH	2.25	0.54
1:A:237:PHE:CE2	1:A:241:MET:HG2	2.42	0.54
1:A:345:VAL:O	1:A:345:VAL:CG1	2.56	0.53
1:A:498:TRP:C	1:A:500:ALA:N	2.63	0.53
1:B:285:VAL:O	1:B:293:VAL:HG12	2.08	0.53
1:A:413:ALA:N	1:A:433:ASP:O	2.41	0.53
1:B:146:TYR:HB2	1:B:607:LEU:HD21	1.90	0.53
1:B:468:LEU:HD21	1:B:528:ILE:CD1	2.39	0.53
1:A:84:VAL:O	1:A:122:ARG:CG	2.57	0.52
1:B:28:ARG:NH1	1:B:128:GLN:OE1	2.23	0.52
1:A:313:SER:OG	1:A:314:LYS:N	2.42	0.52
1:B:468:LEU:HD21	1:B:528:ILE:HD12	1.91	0.52
1:A:85:LEU:HD21	1:A:119:ALA:CB	2.40	0.52
1:A:470:VAL:HG11	1:A:530:MET:HE2	1.92	0.51
1:A:343:ARG:O	1:A:343:ARG:HG2	2.11	0.51
1:B:530:MET:HB3	1:B:531:PRO:CD	2.40	0.51
1:A:85:LEU:CD2	1:A:119:ALA:CB	2.89	0.51
1:B:620:ASP:CG	1:B:642:LEU:HD12	2.36	0.51
1:A:318:GLU:HG2	1:A:328:THR:HG21	1.92	0.51
1:B:427:ARG:NH1	1:B:429:ASP:OD1	2.44	0.51
1:A:620:ASP:CG	1:A:642:LEU:HD23	2.36	0.50
1:A:419:VAL:HG21	1:A:427:ARG:HH21	1.76	0.50
1:A:525:THR:HG21	1:B:600:ASP:OD2	2.12	0.50
1:B:409:LEU:HD22	1:B:437:PHE:CD1	2.47	0.50
1:B:480:VAL:HG21	1:B:509:GLN:HE21	1.77	0.50
1:B:261:ILE:CD1	1:B:276:ILE:HG23	2.42	0.50
1:A:498:TRP:H	1:A:499:PRO:HD3	1.76	0.49
1:A:600:ASP:CG	1:B:525:THR:HG21	2.37	0.49
1:A:419:VAL:HG21	1:A:427:ARG:NH2	2.28	0.49
1:B:315:VAL:HG11	1:B:335:ARG:NH2	2.27	0.49
1:A:318:GLU:HG2	1:A:328:THR:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ASP:OD1	1:B:256:ASP:N	2.45	0.49
1:B:290:LYS:O	1:B:316:ARG:NH2	2.43	0.49
1:A:347:MET:HG2	1:A:360:LEU:CD2	2.42	0.49
1:B:413:ALA:HB1	1:B:431:ASP:O	2.13	0.49
1:A:243:LEU:HD13	1:A:311:LYS:HE2	1.95	0.48
1:A:532:THR:CB	1:A:655:TYR:OH	2.62	0.48
1:B:28:ARG:CD	1:B:128:GLN:OE1	2.60	0.48
1:B:480:VAL:CG2	1:B:509:GLN:HE21	2.26	0.48
1:B:49:THR:O	1:B:53:THR:CG2	2.60	0.48
1:A:559:VAL:HG12	1:A:559:VAL:O	2.13	0.48
1:A:310:PRO:O	1:A:313:SER:CB	2.61	0.48
1:B:89:ASP:HB3	1:B:118:LEU:HD21	1.95	0.48
1:B:277:SER:O	1:B:278:VAL:C	2.56	0.48
1:A:290:LYS:O	1:A:316:ARG:NH2	2.42	0.48
1:A:236:GLN:O	1:A:237:PHE:C	2.56	0.48
1:B:420:ARG:O	1:B:509:GLN:HA	2.14	0.48
1:A:493:MET:HE2	1:A:494:LEU:HD21	1.95	0.47
1:A:584:GLU:O	1:A:588:ILE:HG13	2.14	0.47
1:B:584:GLU:O	1:B:588:ILE:HG13	2.14	0.47
1:A:420:ARG:O	1:A:509:GLN:HA	2.13	0.47
1:B:234:THR:O	1:B:237:PHE:HB3	2.14	0.47
1:B:455:GLU:OE2	1:B:476:GLY:N	2.42	0.47
1:A:264:MET:HE2	1:A:270:ALA:HB1	1.97	0.47
1:A:444:VAL:HG21	1:A:457:PHE:HE2	1.80	0.47
1:B:601:LYS:O	1:B:604:ILE:HG22	2.15	0.47
1:A:468:LEU:HD21	1:A:528:ILE:CD1	2.44	0.46
1:A:442:LEU:HB3	1:A:467:ALA:HB2	1.97	0.46
1:A:304:VAL:HA	1:A:307:ILE:HD12	1.98	0.46
1:B:393:ARG:HH22	1:B:656:LEU:HB2	1.79	0.46
1:A:256:ASP:O	1:A:258:TYR:N	2.48	0.46
1:A:448:ARG:HH21	1:A:532:THR:CG2	2.15	0.46
1:A:180:THR:HG21	1:A:182:LYS:HE2	1.98	0.46
1:A:521:ARG:HD3	1:A:549:PRO:HA	1.98	0.46
1:A:174:GLU:CG	1:A:187:ILE:HG21	2.46	0.46
1:A:351:THR:HA	1:A:355:GLU:O	2.16	0.46
1:B:261:ILE:HD13	1:B:276:ILE:HG23	1.97	0.46
1:B:498:TRP:C	1:B:500:ALA:N	2.74	0.46
1:A:261:ILE:HD12	1:A:276:ILE:CG2	2.47	0.45
1:A:497:GLU:C	1:A:499:PRO:CD	2.88	0.45
1:A:535:GLU:HG3	1:A:592:ILE:CG2	2.46	0.45
1:B:37:GLU:OE1	1:B:109:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLU:CA	1:A:499:PRO:HD3	2.46	0.45
1:B:442:LEU:O	1:B:467:ALA:HB1	2.16	0.45
1:A:320:LEU:CD1	1:A:327:LYS:O	2.65	0.45
1:A:411:ILE:HG13	1:A:411:ILE:O	2.16	0.45
1:B:129:TYR:O	1:B:132:SER:HB3	2.16	0.45
1:A:129:TYR:O	1:A:132:SER:HB3	2.16	0.45
1:A:336:GLU:HB3	1:A:339:ARG:HH21	1.82	0.45
1:A:58:ARG:HD2	1:A:548:LEU:HD21	2.00	0.44
1:A:530:MET:HB2	1:A:655:TYR:CE2	2.52	0.44
1:B:127:TYR:CZ	1:B:198:ALA:HB1	2.53	0.44
1:A:85:LEU:HD22	1:A:119:ALA:HB2	2.00	0.44
1:A:126:ARG:HH21	1:A:169:LYS:HB3	1.81	0.44
1:A:456:ILE:HD11	1:A:511:PHE:CG	2.52	0.44
1:B:121:LYS:HD3	1:B:121:LYS:HA	1.84	0.44
1:B:124:PHE:CE1	1:B:128:GLN:NE2	2.85	0.44
1:A:412:PRO:O	1:A:413:ALA:HB3	2.18	0.44
1:A:415:PRO:HA	1:A:430:SER:CB	2.47	0.44
1:A:627:LEU:O	1:A:630:ARG:HB3	2.18	0.44
1:B:337:ARG:O	1:B:338:ILE:CB	2.66	0.44
1:A:456:ILE:HD11	1:A:511:PHE:CD2	2.53	0.43
1:A:497:GLU:HA	1:A:499:PRO:HD3	1.99	0.43
1:B:415:PRO:HA	1:B:430:SER:CB	2.49	0.43
1:B:619:ASP:O	1:B:622:THR:HB	2.17	0.43
1:B:377:LEU:HD22	1:B:438:TYR:HB2	2.00	0.43
1:A:96:LYS:HE3	1:A:99:GLU:OE1	2.19	0.43
1:A:529:ILE:HD12	1:B:597:ALA:HA	2.00	0.43
1:B:141:THR:O	1:B:142:GLY:O	2.37	0.43
1:A:530:MET:HB3	1:A:531:PRO:CD	2.48	0.43
1:A:568:GLU:N	1:A:569:PRO:HD2	2.33	0.43
1:B:118:LEU:O	1:B:119:ALA:CB	2.54	0.43
1:A:347:MET:HG2	1:A:360:LEU:HD23	2.01	0.43
1:B:73:ARG:O	1:B:77:LEU:HG	2.19	0.43
1:A:253:GLN:HA	1:A:300:LEU:HD21	2.01	0.42
1:A:283:VAL:C	1:A:295:VAL:HG22	2.44	0.42
1:A:444:VAL:HG21	1:A:457:PHE:CE2	2.53	0.42
1:B:193:ARG:O	1:B:197:PHE:CD1	2.72	0.42
1:A:118:LEU:C	1:A:120:GLN:H	2.27	0.42
1:A:521:ARG:NH2	1:A:542:LYS:O	2.53	0.42
1:B:64:GLN:O	1:B:67:SER:HB2	2.20	0.42
1:B:64:GLN:HB3	1:B:98:THR:HB	2.01	0.42
1:A:310:PRO:O	1:A:313:SER:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLN:OE1	1:A:376:GLN:CA	2.63	0.42
1:B:261:ILE:HD13	1:B:276:ILE:CG2	2.50	0.42
1:A:41:HIS:O	1:A:42:ALA:C	2.61	0.42
1:B:620:ASP:OD2	1:B:642:LEU:HD12	2.20	0.42
1:A:280:ASP:OD1	1:A:321:PRO:HA	2.20	0.41
1:A:531:PRO:HG2	1:A:585:PHE:HD1	1.85	0.41
1:B:47:ARG:NH1	1:B:486:LEU:O	2.51	0.41
1:B:264:MET:HE3	1:B:271:ALA:HA	2.01	0.41
1:A:118:LEU:O	1:A:119:ALA:CB	2.59	0.41
1:B:612:ARG:HD2	1:B:615:GLU:OE1	2.20	0.41
1:A:412:PRO:HA	2:A:701:HOH:O	2.21	0.41
1:B:406:LEU:O	1:B:407:SER:C	2.64	0.41
1:A:333:LEU:HD23	1:A:333:LEU:HA	1.76	0.41
1:A:415:PRO:HA	1:A:430:SER:HB3	2.02	0.41
1:B:116:TYR:HE2	1:B:213:LEU:HD22	1.85	0.41
1:B:421:ASP:OD1	1:B:421:ASP:C	2.63	0.41
1:A:64:GLN:O	1:A:67:SER:HB2	2.21	0.41
1:B:257:ASP:O	1:B:257:ASP:CG	2.64	0.41
1:B:400:LEU:HD22	1:B:511:PHE:CZ	2.56	0.41
1:A:85:LEU:HD21	1:A:119:ALA:HB2	1.98	0.41
1:A:461:MET:HA	1:A:461:MET:CE	2.47	0.41
1:A:403:ALA:HB2	1:A:453:ALA:HB1	2.03	0.40
1:A:406:LEU:O	1:A:407:SER:C	2.63	0.40
1:A:483:TYR:HA	1:A:504:VAL:O	2.21	0.40
1:A:515:ASN:OD1	1:A:515:ASN:C	2.63	0.40
1:B:115:LEU:O	1:B:118:LEU:O	2.39	0.40
1:A:345:VAL:HG23	1:A:362:ILE:CG1	2.51	0.40
1:B:426:VAL:HG21	1:B:553:ILE:HD11	2.03	0.40
1:A:140:PHE:HE2	1:A:178:LYS:CE	2.35	0.40
1:B:199:ILE:O	1:B:202:LEU:HB3	2.22	0.40
1:A:498:TRP:H	1:A:499:PRO:CD	2.26	0.40
1:B:41:HIS:O	1:B:42:ALA:C	2.64	0.40
1:B:284:GLY:HA2	1:B:293:VAL:O	2.22	0.40
1:B:411:ILE:HD12	1:B:464:TYR:CZ	2.57	0.40
1:B:483:TYR:HA	1:B:504:VAL:O	2.22	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	637/688 (93%)	607 (95%)	24 (4%)	6 (1%)	14	41
1	B	632/688 (92%)	588 (93%)	37 (6%)	7 (1%)	11	37
All	All	1269/1376 (92%)	1195 (94%)	61 (5%)	13 (1%)	12	39

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	ASP
1	A	452	ILE
1	B	245	LEU
1	B	452	ILE
1	A	338	ILE
1	A	413	ALA
1	B	142	GLY
1	B	311	LYS
1	B	338	ILE
1	B	433	ASP
1	A	334	THR
1	B	278	VAL
1	A	498	TRP

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	552/590 (94%)	529 (96%)	23 (4%)	26	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	550/590 (93%)	526 (96%)	24 (4%)	25	50
All	All	1102/1180 (93%)	1055 (96%)	47 (4%)	26	50

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	242	SER
1	A	288	THR
1	A	291	PRO
1	A	314	LYS
1	A	381	GLU
1	A	401	THR
1	A	404	VAL
1	A	425	LYS
1	A	448	ARG
1	A	480	VAL
1	A	489	ILE
1	A	495	ARG
1	A	503	SER
1	A	515	ASN
1	A	519	THR
1	A	539	THR
1	A	542	LYS
1	A	598	MET
1	A	600	ASP
1	A	636	LYS
1	A	647	LYS
1	A	648	ASP
1	B	30	ASP
1	B	108	LYS
1	B	205	THR
1	B	227	ASN
1	B	253	GLN
1	B	255	ASP
1	B	256	ASP
1	B	277	SER
1	B	301	ASP
1	B	339	ARG
1	B	378	GLN
1	B	401	THR
1	B	480	VAL

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Mol	Chain	Res	Type
1	B	489	ILE
1	B	531	PRO
1	B	570	GLU
1	B	572	LEU
1	B	573	LYS
1	B	581	LYS
1	B	598	MET
1	B	614	LYS
1	B	620	ASP
1	B	641	LYS
1	B	642	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	650	GLN
1	B	227	ASN
1	B	482	GLN
1	B	505	GLN
1	B	509	GLN
1	B	650	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	639/688 (92%)	0.45	53 (8%) 17 15	16, 59, 139, 196	0
1	B	636/688 (92%)	0.55	54 (8%) 16 14	24, 71, 149, 196	0
All	All	1275/1376 (92%)	0.50	107 (8%) 17 15	16, 65, 146, 196	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	85	LEU	10.3
1	B	66	PHE	5.4
1	A	243	LEU	5.0
1	A	166	TRP	4.9
1	B	449	PHE	4.4
1	B	148	LEU	4.3
1	B	426	VAL	4.1
1	A	649	TYR	4.1
1	A	574	GLU	4.0
1	A	309	GLY	3.8
1	A	194	ARG	3.8
1	B	126	ARG	3.7
1	B	550	TRP	3.7
1	A	490	TYR	3.7
1	B	498	TRP	3.6
1	B	110	ASP	3.6
1	B	293	VAL	3.5
1	A	644	ASP	3.4
1	B	130	ALA	3.3
1	B	318	GLU	3.3
1	A	617	ASN	3.2
1	B	166	TRP	3.1
1	A	650	GLN	3.1
1	B	242	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	84	VAL	3.1
1	B	523	GLY	3.1
1	B	548	LEU	3.0
1	A	90	VAL	3.0
1	A	167	ASP	3.0
1	A	173	ASP	3.0
1	B	436	VAL	3.0
1	B	73	ARG	3.0
1	B	364	GLY	3.0
1	A	572	LEU	3.0
1	B	195	TYR	3.0
1	B	146	TYR	2.9
1	B	168	SER	2.9
1	B	140	PHE	2.9
1	A	327	LYS	2.9
1	B	551	ASP	2.8
1	A	83	ASN	2.8
1	B	437	PHE	2.8
1	A	138	MET	2.7
1	A	119	ALA	2.7
1	A	182	LYS	2.7
1	B	162	LEU	2.7
1	B	262	ASN	2.7
1	B	380	LEU	2.7
1	B	83	ASN	2.6
1	A	670	GLU	2.6
1	A	326	THR	2.6
1	A	118	LEU	2.6
1	A	452	ILE	2.6
1	B	40	GLN	2.6
1	A	143	ASN	2.6
1	A	178	LYS	2.6
1	A	654	PRO	2.6
1	A	597	ALA	2.5
1	B	332	THR	2.5
1	B	154	PRO	2.5
1	A	396	GLY	2.5
1	B	549	PRO	2.5
1	B	654	PRO	2.5
1	B	152	LYS	2.4
1	B	335	ARG	2.4
1	B	597	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	295	VAL	2.4
1	B	274	LYS	2.4
1	A	93	PHE	2.4
1	B	171	LYS	2.4
1	A	624	LEU	2.4
1	B	174	GLU	2.4
1	A	619	ASP	2.3
1	B	492	GLN	2.3
1	B	292	MET	2.3
1	B	450	SER	2.3
1	A	507	THR	2.3
1	B	132	SER	2.3
1	B	300	LEU	2.3
1	A	116	TYR	2.3
1	B	252	TYR	2.3
1	B	472	GLU	2.3
1	B	131	LEU	2.3
1	B	328	THR	2.3
1	A	335	ARG	2.3
1	B	128	GLN	2.3
1	A	142	GLY	2.2
1	B	153	ALA	2.2
1	A	144	ASP	2.2
1	A	317	LEU	2.2
1	A	527	ASP	2.2
1	A	115	LEU	2.2
1	B	489	ILE	2.1
1	A	169	LYS	2.1
1	A	199	ILE	2.1
1	A	124	PHE	2.1
1	B	515	ASN	2.1
1	A	50	SER	2.1
1	A	302	ASP	2.1
1	A	183	THR	2.1
1	A	598	MET	2.1
1	A	174	GLU	2.1
1	A	279	GLY	2.1
1	A	127	TYR	2.0
1	A	186	GLU	2.0
1	A	257	ASP	2.0
1	B	172	PHE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.