Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 10:10 PM JST

PDB ID	:	6IQR
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:

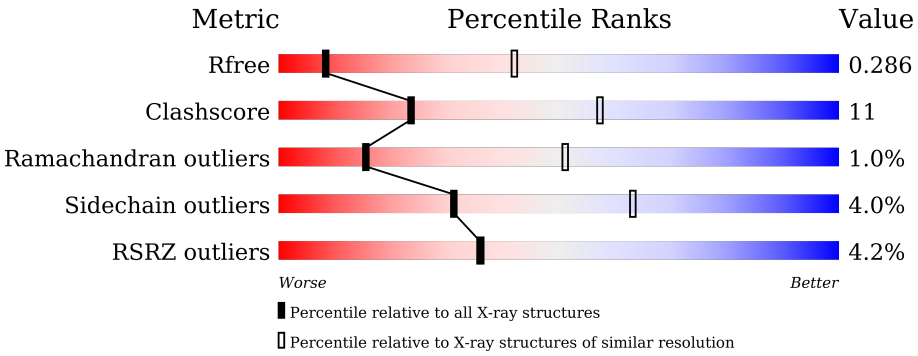
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 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}	130704	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	4% 67% 23% • 7%
1	B	688	4% 69% 21% • 8%

2 Entry composition (i)

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

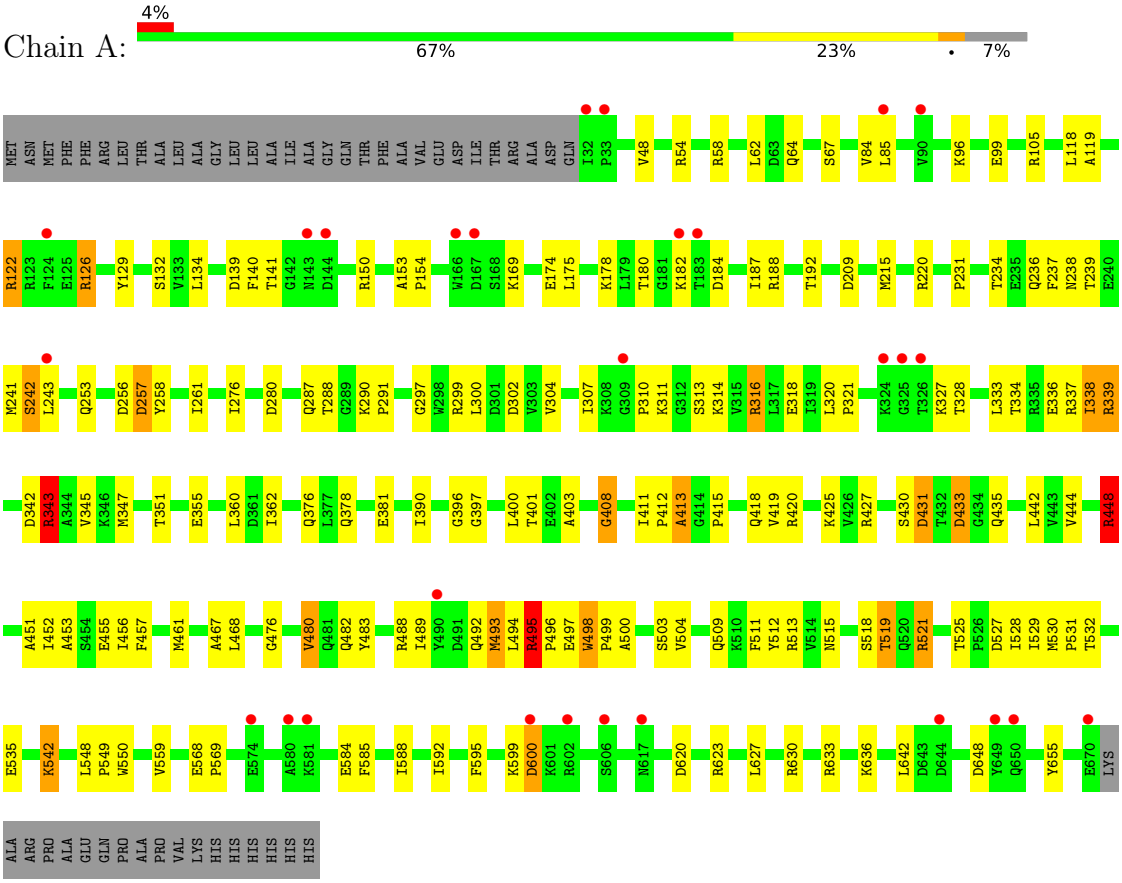
- Molecule 2 is water.

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

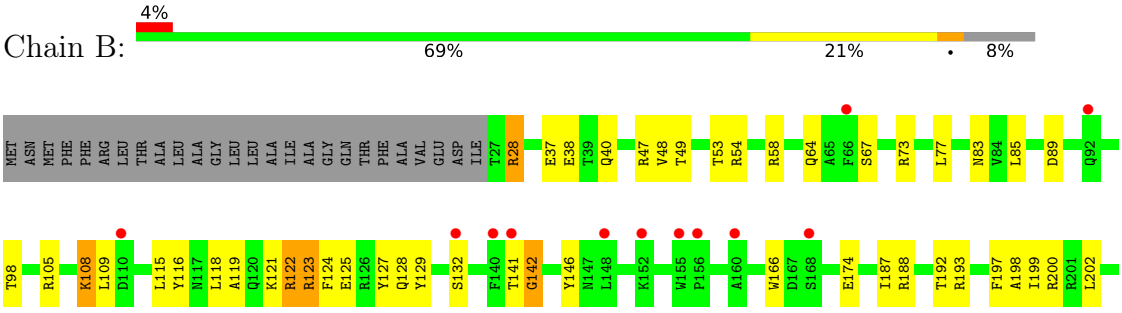
3 Residue-property plots (i)

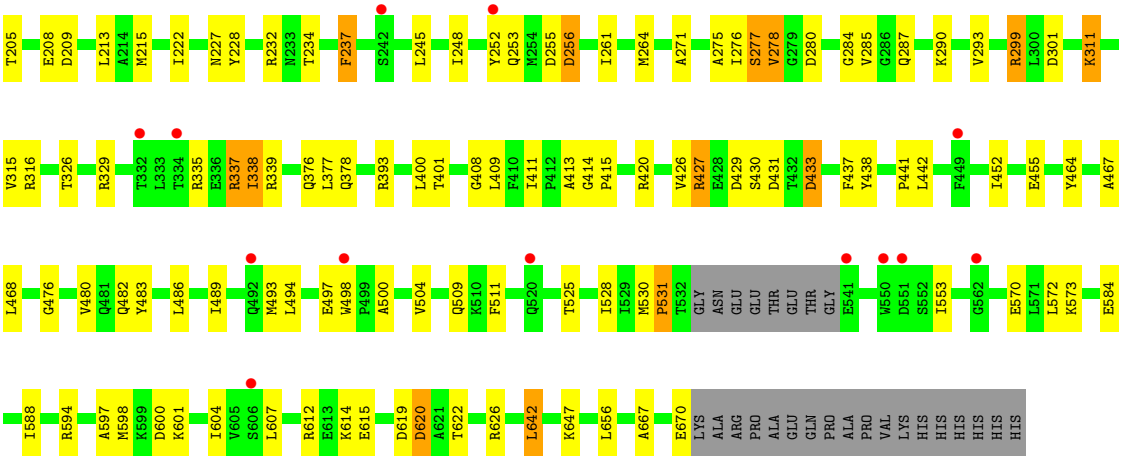
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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




T205 E208 D209 L213 A214 M215 I222 N227 Y228 R232 N233 T234 F237 S242 L245 I248 Y252 Q253 M254 D255 D256 I261 M264 A271 A275 I276 S277 V278 G279 D280 G284 V285 G286 Q287 K290 V293 R299 L300 D301 K311
V315 R316 T326 R329 T332 L333 T334 R335 E336 R337 I338 R339 Q376 L377 Q378 R393 L400 T401 G408 L409 F410 I411 P412 A413 G414 P415 R420 V426 R427 E428 D429 S430 D431 T432 D433 F437 Y438 P441 L442 F449 I452 E455 Y464 A467
L468 G476 V480 Q481 Q482 Y483 L486 I489 Q492 M493 L494 E497 W498 P499 A500 V504 Q509 K510 F511 Q520 T525 I528 I529 M530 P531 T532 GLY ASN GLU GLU THR GLU THR GLY E541 W550 D551 S552 I553 G562 E570 L571 L572 K573 E584
I588 R594 A597 M598 K599 D600 K601 I604 V605 S606 L607 R612 E613 K614 E615 D619 D620 A621 T622 R626 L642 K647 L656 A667 E670 LYS ALA ARG PRO ALA GLU GLN PRO ALA PRO VAL LYS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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 29.95 – 3.42	Depositor EDS
% Data completeness (in resolution range)	90.9 (29.97-3.42) 91.1 (29.95-3.42)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.27%)	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)	0.27 , 59.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.099 for -h,-k,l	Xtriage
F_o,F_c correlation	0.84	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.73	3/5168 (0.1%)	0.98	10/6979 (0.1%)
1	B	0.68	4/5150 (0.1%)	0.91	2/6953 (0.0%)
All	All	0.71	7/10318 (0.1%)	0.95	12/13932 (0.1%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	GLU	CD-OE1	8.30	1.34	1.25
1	A	435	GLN	C-O	-7.09	1.09	1.23
1	B	414	GLY	N-CA	5.53	1.54	1.46
1	B	38	GLU	CD-OE2	5.42	1.31	1.25
1	A	408	GLY	C-O	-5.29	1.15	1.23
1	A	519	THR	C-O	-5.22	1.13	1.23
1	B	670	GLU	CD-OE2	-5.07	1.20	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	513	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	A	337	ARG	CB-CA-C	7.65	125.69	110.40
1	B	123	ARG	NE-CZ-NH1	-6.91	116.85	120.30
1	A	342	ASP	CB-CA-C	6.79	123.99	110.40
1	A	433	ASP	CB-CA-C	-6.72	96.97	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	521	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	431	ASP	CB-CG-OD1	-5.71	113.16	118.30
1	B	311	LYS	CB-CA-C	-5.60	99.21	110.40
1	A	493	MET	CG-SD-CE	5.57	109.11	100.20
1	A	343	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	527	ASP	CB-CG-OD1	-5.19	113.62	118.30
1	A	234	THR	CB-CA-C	-5.01	98.08	111.60

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
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 (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	5080	0	5093	135	0
1	B	5063	0	5085	96	0
2	A	1	0	0	4	0
2	B	1	0	0	2	0
All	All	10145	0	10178	227	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 11.

All (227) 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
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: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:B:28:ARG:HH11	1:B:128:GLN:CD	1.80	0.85
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:376:GLN:OE1	1:A:376:GLN:HA	1.91	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: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:408:GLY:HA3	1:B:431:ASP:CG	2.17	0.65
1:B:275:ALA:O	1:B:329:ARG:NH2	2.29	0.64
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: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:B:28:ARG:NH1	1:B:128:GLN:CD	2.51	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:B:376:GLN:HA	1:B:376:GLN:OE1	2.00	0.59
1:A:62:LEU:O	1:A:105:ARG:NH2	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:A:408:GLY:HA3	1:A:431:ASP:CG	2.28	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: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: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:A:498:TRP:C	1:A:500:ALA:N	2.63	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:237:PHE:C	1:A:237:PHE:CD2	2.83	0.51
1:A:498:TRP:C	1:A:500:ALA:H	2.14	0.51
1:A:532:THR:OG1	1:A:655:TYR:OH	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:209:ASP:CG	1:A:299:ARG:HH11	2.10	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
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:A:290:LYS:O	1:A:316:ARG:NH2	2.42	0.48
1:B:420:ARG:O	1:B:509:GLN:HA	2.14	0.48
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: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:B:620:ASP:CG	1:B:642:LEU:HD12	2.36	0.46
1:A:180:THR:HG21	1:A:182:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:620:ASP:CG	1:A:642:LEU:HD23	2.36	0.46
1:B:261:ILE:HD13	1:B:276:ILE:HG23	1.97	0.46
1:A:261:ILE:HD12	1:A:276:ILE:CG2	2.47	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
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:600:ASP:CG	1:B:525:THR:HG21	2.37	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:B:493:MET:CE	1:B:494:LEU:HD21	2.48	0.44
1:A:461:MET:CE	1:A:461:MET:HA	2.47	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:B:277:SER:O	1:B:278:VAL:C	2.56	0.43
1:A:96:LYS:HE3	1:A:99:GLU:OE1	2.19	0.43
1:A:236:GLN:O	1:A:237:PHE:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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:498:TRP:C	1:B:500:ALA:N	2.74	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:264:MET:HE3	1:B:271:ALA:HA	2.02	0.41
1:A:64:GLN:O	1:A:67:SER:HB2	2.21	0.41
1:A:497:GLU:C	1:A:499:PRO:CD	2.88	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:403:ALA:HB2	1:A:453:ALA:HB1	2.03	0.40
1:A:483:TYR:HA	1:A:504:VAL:O	2.21	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: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%)	17 53
1	B	632/688 (92%)	588 (93%)	37 (6%)	7 (1%)	14 49
All	All	1269/1376 (92%)	1195 (94%)	61 (5%)	13 (1%)	15 51

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%)	531 (96%)	21 (4%)	33 64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	550/590 (93%)	527 (96%)	23 (4%)	30 62
All	All	1102/1180 (93%)	1058 (96%)	44 (4%)	31 63

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	SER
1	A	288	THR
1	A	291	PRO
1	A	302	ASP
1	A	339	ARG
1	A	378	GLN
1	A	381	GLU
1	A	401	THR
1	A	425	LYS
1	A	448	ARG
1	A	480	VAL
1	A	482	GLN
1	A	489	ILE
1	A	495	ARG
1	A	503	SER
1	A	515	ASN
1	A	519	THR
1	A	542	LYS
1	A	600	ASP
1	A	636	LYS
1	A	648	ASP
1	B	108	LYS
1	B	205	THR
1	B	227	ASN
1	B	237	PHE
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	482	GLN
1	B	489	ILE
1	B	531	PRO

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Mol	Chain	Res	Type
1	B	570	GLU
1	B	572	LEU
1	B	573	LYS
1	B	598	MET
1	B	614	LYS
1	B	620	ASP
1	B	642	LEU
1	B	647	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	482	GLN
1	B	509	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	639/688 (92%)	-0.05	28 (4%)	34	34	16, 59, 139, 196	0
1	B	636/688 (92%)	0.00	25 (3%)	39	39	24, 71, 149, 196	0
All	All	1275/1376 (92%)	-0.03	53 (4%)	36	36	16, 65, 146, 196	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	650	GLN	7.1
1	A	617	ASN	6.3
1	A	649	TYR	6.1
1	A	167	ASP	5.3
1	A	85	LEU	4.5
1	A	143	ASN	3.9
1	B	541	GLU	3.6
1	B	110	ASP	3.4
1	A	326	THR	3.4
1	B	141	THR	3.2
1	A	644	ASP	3.1
1	B	92	GLN	3.0
1	A	166	TRP	3.0
1	A	182	LYS	2.9
1	B	242	SER	2.9
1	A	90	VAL	2.8
1	A	32	ILE	2.8
1	A	581	LYS	2.8
1	B	155	TRP	2.7
1	B	492	GLN	2.7
1	B	550	TRP	2.7
1	B	606	SER	2.6
1	A	670	GLU	2.6
1	B	551	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	574	GLU	2.6
1	A	606	SER	2.5
1	B	449	PHE	2.5
1	B	156	PRO	2.5
1	B	132	SER	2.5
1	B	160	ALA	2.4
1	B	168	SER	2.4
1	A	325	GLY	2.4
1	A	33	PRO	2.4
1	A	183	THR	2.4
1	A	324	LYS	2.3
1	A	144	ASP	2.3
1	B	334	THR	2.3
1	B	252	TYR	2.3
1	A	490	TYR	2.3
1	B	520	GLN	2.3
1	B	152	LYS	2.3
1	B	562	GLY	2.3
1	A	124	PHE	2.3
1	B	148	LEU	2.2
1	A	580	ALA	2.2
1	A	309	GLY	2.2
1	A	600	ASP	2.2
1	B	498	TRP	2.2
1	A	602	ARG	2.1
1	B	332	THR	2.1
1	A	243	LEU	2.0
1	B	140	PHE	2.0
1	B	66	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 monosaccharides 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.