



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:14 PM GMT

PDB ID : 1JEQ
Title : Crystal Structure of the Ku Heterodimer
Authors : Walker, J.R.; Corpina, R.A.; Goldberg, J.
Deposited on : 2001-06-18
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

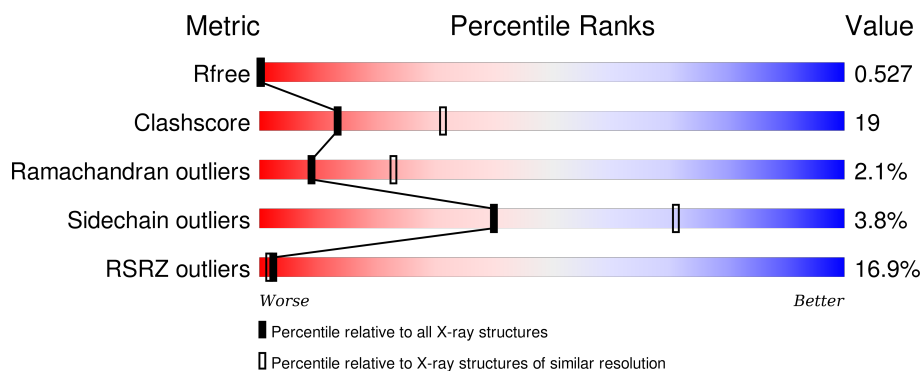
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	609	
2	B	565	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8633 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 KU70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4419	2830	748	821	20			

- Molecule 2 is a protein called KU80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	520	Total	C	N	O	S	0	0	0
			4172	2673	700	776	23			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	21	Total	O	0	0
			21	21		

LYS LYS ASP VAL THR ALA GLN GLU ILE PHE GLN ASP ASN HIS GLU ASP GLY PRO THR ALA LYS	P446	S335	I267	GLU	ASP	L133	LYS
	Q450	E336	L268	ASP	GLY	M84	VAL
	L451	G337	Q269	SER	GLY	L85	ARG
	M452	S341	V272	GLY	GLY	P86	SER
	A453	G346	K274	ASP	ARG	L90	GLY
	V454	K347	T275	GLY	ASP	N6	K7
	D455	Q350	W276	ASP	GLY	I94	L12
	A456	Q350	V279	GLY	P182	E95	C13
	L457	R354	D280	F183	I198	S96	T19
	I458	K363	T283	G186	N22	K97	
LYS	M461	S362	L284	G189	A105	I98	
	S462	V364	K285	PRO	D106	Q104	S23
	L463	F365	K286	SER	F107	I108	P25
	D467	A366	E287	F192	D109	L108	G26
	E468	A367	D288	F193	I112	E28	I27
	K469	E371	I289	L194	V113	S29	S29
	T470	S378	K291	K195	M115	P30	
	D471	S379	E292	G196	I118	F30	
	F477	L380	T293	I197	K35	K35	
	T479	I381	V294	T198	K36		
LYS	T480	E382	Y295				
		C296	L297	Q201			
	M484	D385	L297	K202	I126		
	P485	D386	E298	E203	K126		
	F487	M389	D299	G204	F127		
	Q488	M300	D300	E207	E128		
		R394	E302	V208	K129		
	Q492	K399	T303	V211	R130		
	L495	Q404	V305	E223	H131		
	R497	L306	E304	E223	E133		
LYS	A498	K307	E308	S226	I134		
	L499	V407	D309	E229	F135		
		K413	I310	E229	L138		
	Q509	E417	Q312	R232	S143		
	M517	C418	G313	R232	Q146		
	P518	F314	R315	F237	L147		
	F519	Q423	R315	H243	D148		
		L424	P425	S244	I149		
	V522	F426	M427	I245	I151		
	Q527	M427	VAL	H246	H152		
LYS	I528	F435	D327	P248	Q73		
	P529	L438	E329	L251	Y74		
		K439	E329	L251	S160		
	I533	M440	Q330	S255	L161		
	P537	N440	Q330	S255	Q162		
	P538	K443	K332	Y264	I169		
	I539	Y444	R334	K265	GLY		
		A445	K334	S266	LYS		
	A542				H82		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.21Å 86.19Å 203.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.70 74.61 – 1.22	Depositor EDS
% Data completeness (in resolution range)	80.8 (19.89-2.70) 11.8 (74.61-1.22)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	21.45 (at 1.22Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.222 , 0.283 0.522 , 0.527	Depositor DCC
R_{free} test set	927 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	7.1	Xtriage
Anisotropy	1.902	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 12.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 49462 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.56	EDS
Total number of atoms	8633	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.42	0/4504	0.65	0/6061
2	B	0.43	0/4256	0.66	0/5739
All	All	0.42	0/8760	0.66	0/11800

There are no bond length outliers.

There are no bond angle outliers.

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	4419	0	4512	222	0
2	B	4172	0	4209	142	0
3	A	21	0	0	1	0
3	B	21	0	0	2	0
All	All	8633	0	8721	326	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 19.

All (326) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:MET:HE1	2:B:363:LYS:HD2	1.40	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:TYR:O	1:A:536:PRO:HD3	1.65	0.96
1:A:178:ASN:HD22	1:A:178:ASN:H	1.13	0.94
1:A:588:TYR:HB2	1:A:590:LEU:HD22	1.57	0.87
1:A:326:GLN:NE2	1:A:328:ILE:HD11	1.91	0.86
1:A:485:GLN:HE21	1:A:489:ASN:HD21	1.26	0.83
2:B:404:GLN:HG2	2:B:423:GLN:NE2	1.94	0.82
2:B:313:GLY:HA2	2:B:323:PHE:H	1.45	0.81
1:A:403:ARG:HE	1:A:406:ILE:HD11	1.48	0.77
1:A:446:MET:CE	2:B:363:LYS:HD2	2.15	0.76
2:B:112:ILE:HA	2:B:115:MET:HE3	1.68	0.76
1:A:520:SER:O	1:A:524:GLU:HG3	1.86	0.76
1:A:500:PRO:HG2	1:A:502:GLN:HE22	1.51	0.75
2:B:226:SER:OG	2:B:229:GLU:HG2	1.87	0.74
1:A:485:GLN:NE2	1:A:489:ASN:HD21	1.87	0.73
2:B:273:LYS:HG3	2:B:274:LYS:N	2.05	0.71
2:B:77:ILE:HG21	2:B:113:VAL:HG21	1.72	0.71
1:A:178:ASN:HD22	1:A:178:ASN:N	1.84	0.71
2:B:28:GLU:OE2	2:B:36:LYS:HE3	1.91	0.71
1:A:296:VAL:HG11	2:B:295:TYR:HB3	1.73	0.71
1:A:500:PRO:HG2	1:A:502:GLN:NE2	2.06	0.70
1:A:178:ASN:H	1:A:178:ASN:ND2	1.88	0.69
2:B:469:LYS:O	2:B:471:ASP:N	2.25	0.69
2:B:457:LEU:HD22	2:B:533:ILE:HD12	1.74	0.69
1:A:328:ILE:O	1:A:329:LEU:HD23	1.93	0.69
1:A:157:VAL:HG11	1:A:161:MET:SD	2.33	0.68
2:B:467:ASP:CG	2:B:468:GLU:H	1.97	0.68
1:A:592:SER:HB2	1:A:599:LEU:HD21	1.75	0.68
2:B:273:LYS:HG3	2:B:274:LYS:H	1.58	0.67
1:A:348:MET:CE	2:B:518:PRO:HD3	2.25	0.67
1:A:585:CYS:HA	1:A:590:LEU:HD21	1.76	0.67
1:A:142:SER:OG	1:A:145:GLU:HG3	1.94	0.67
1:A:488:ARG:HG2	1:A:501:GLU:O	1.95	0.67
1:A:593:GLY:HA3	1:A:598:GLU:OE1	1.96	0.66
1:A:534:TYR:HD2	1:A:536:PRO:HG3	1.61	0.66
1:A:143:LEU:H	1:A:176:HIS:HE1	1.43	0.65
1:A:454:ALA:HB2	2:B:378:SER:HB3	1.79	0.65
2:B:35:LYS:HE3	2:B:94:ILE:O	1.96	0.65
1:A:242:LEU:O	1:A:246:VAL:HG23	1.97	0.64
1:A:451:LYS:HE2	1:A:453:MET:SD	2.36	0.64
2:B:152:HIS:CE1	2:B:156:LYS:HE3	2.32	0.64
1:A:320:GLN:HG3	2:B:276:TRP:CE3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:LYS:HE3	2:B:455:ASP:HB2	1.79	0.64
2:B:207:ILE:O	2:B:211:VAL:HG23	1.97	0.64
1:A:251:THR:HG22	1:A:252:ARG:N	2.11	0.63
2:B:115:MET:HE2	2:B:150:ILE:HG23	1.80	0.63
1:A:490:LEU:HD21	2:B:314:PHE:HB2	1.81	0.63
1:A:592:SER:HB2	1:A:599:LEU:CD2	2.28	0.63
1:A:574:GLY:HA2	1:A:600:LEU:HD21	1.80	0.63
1:A:151:ALA:HB2	1:A:193:LEU:HD21	1.79	0.63
2:B:528:ILE:HB	2:B:529:PRO:HD3	1.81	0.62
2:B:24:ILE:HG23	2:B:25:PRO:HD2	1.80	0.62
1:A:444:ARG:NH1	2:B:268:LEU:O	2.32	0.62
2:B:27:ILE:HG23	2:B:183:PHE:CD2	2.34	0.62
2:B:54:ILE:HD12	2:B:86:PRO:HB3	1.82	0.62
1:A:52:GLN:O	1:A:54:GLU:HG3	2.00	0.62
2:B:115:MET:CE	2:B:150:ILE:HG23	2.30	0.61
1:A:534:TYR:CD2	1:A:536:PRO:HG3	2.35	0.61
1:A:142:SER:HA	1:A:176:HIS:CE1	2.35	0.61
1:A:157:VAL:HG11	1:A:161:MET:CE	2.31	0.61
1:A:252:ARG:HD2	1:A:252:ARG:N	2.16	0.61
1:A:326:GLN:HE21	1:A:328:ILE:HD11	1.64	0.60
1:A:302:THR:OG1	2:B:291:LYS:HG2	2.02	0.60
1:A:597:GLN:O	1:A:601:GLU:HG3	2.01	0.60
1:A:461:LYS:HG3	1:A:528:LEU:HD12	1.83	0.60
1:A:522:VAL:HG12	1:A:523:ASP:N	2.15	0.59
1:A:522:VAL:HB	3:A:630:HOH:O	2.02	0.59
1:A:590:LEU:H	1:A:590:LEU:HD23	1.67	0.59
2:B:364:VAL:O	2:B:418:CYS:HB2	2.03	0.59
2:B:131:HIS:ND1	2:B:160:SER:OG	2.33	0.58
1:A:578:VAL:HG22	1:A:579:PRO:HD3	1.85	0.58
1:A:302:THR:HG22	1:A:311:LEU:HD12	1.85	0.58
1:A:367:PHE:HZ	1:A:430:PRO:O	1.87	0.58
1:A:348:MET:HE1	2:B:518:PRO:HD3	1.86	0.57
2:B:313:GLY:CA	2:B:323:PHE:H	2.17	0.57
1:A:68:GLN:O	1:A:72:ILE:HG13	2.03	0.57
2:B:468:GLU:O	2:B:470:THR:N	2.36	0.57
1:A:72:ILE:O	1:A:76:ILE:HG12	2.05	0.57
1:A:102:ILE:HG12	1:A:146:VAL:HG22	1.86	0.57
1:A:534:TYR:C	1:A:536:PRO:HD3	2.24	0.57
1:A:363:ARG:NH1	1:A:364:PRO:O	2.37	0.57
1:A:72:ILE:HG12	1:A:116:ILE:HD13	1.87	0.57
2:B:65:ASP:HB3	2:B:78:THR:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LYS:HG3	1:A:528:LEU:CD1	2.34	0.56
1:A:585:CYS:HA	1:A:590:LEU:CD2	2.35	0.56
2:B:7:LYS:HD2	2:B:127:PHE:CE2	2.40	0.56
1:A:400:TYR:CE2	1:A:402:PRO:HG3	2.40	0.56
2:B:194:LEU:O	2:B:202:LYS:HE2	2.04	0.56
1:A:182:LYS:HG2	1:A:185:ARG:NH2	2.20	0.56
1:A:44:ALA:O	1:A:137:HIS:HB2	2.07	0.55
2:B:246:HIS:CD2	2:B:248:PRO:HG3	2.42	0.55
1:A:54:GLU:C	1:A:56:GLU:H	2.09	0.55
2:B:39:THR:O	2:B:43:GLN:HG3	2.05	0.55
1:A:145:GLU:O	1:A:149:VAL:HG23	2.06	0.55
1:A:578:VAL:CG2	1:A:579:PRO:HD3	2.37	0.55
1:A:302:THR:O	1:A:310:LEU:HD12	2.06	0.55
1:A:363:ARG:HB2	1:A:364:PRO:HD2	1.89	0.54
1:A:420:LEU:HD23	1:A:426:GLN:HA	1.88	0.54
1:A:363:ARG:NH1	1:A:436:PHE:CE1	2.75	0.54
1:A:584:ALA:HB3	1:A:603:LEU:HD11	1.88	0.54
1:A:333:GLU:OE2	2:B:497:ARG:NH2	2.39	0.54
1:A:212:ASP:HB3	1:A:215:LEU:HG	1.89	0.54
2:B:112:ILE:HD11	2:B:146:GLN:HB3	1.88	0.54
1:A:46:LYS:HA	1:A:137:HIS:HD2	1.73	0.54
1:A:445:LYS:HG2	1:A:446:MET:N	2.23	0.54
1:A:43:ASP:O	1:A:48:MET:HG3	2.07	0.54
2:B:266:SER:HB2	2:B:363:LYS:HG3	1.88	0.54
2:B:280:ASP:HB2	2:B:289:ILE:HD11	1.89	0.54
2:B:323:PHE:CE2	2:B:328:GLU:HB3	2.43	0.54
2:B:294:VAL:HG12	2:B:295:TYR:N	2.23	0.54
2:B:59:PHE:HB2	2:B:105:ALA:HB3	1.88	0.53
1:A:113:ALA:HB1	1:A:495:LEU:HG	1.90	0.53
1:A:294:GLU:OE1	2:B:297:LEU:HD22	2.07	0.53
1:A:216:PHE:CZ	1:A:220:ILE:HD11	2.43	0.53
2:B:44:ARG:HG2	2:B:237:PHE:CE2	2.44	0.53
1:A:232:HIS:ND1	1:A:233:PHE:N	2.56	0.53
2:B:232:ARG:HG3	2:B:232:ARG:HH11	1.73	0.53
2:B:12:LEU:O	2:B:56:LEU:HD12	2.08	0.53
2:B:131:HIS:CE1	2:B:162:GLN:HG3	2.44	0.53
1:A:352:PRO:HA	1:A:394:VAL:HG23	1.91	0.53
1:A:42:VAL:HB	1:A:87:PHE:CD2	2.43	0.53
1:A:452:ILE:HD13	2:B:371:GLU:HG3	1.91	0.53
1:A:251:THR:CG2	1:A:252:ARG:N	2.72	0.53
2:B:223:GLU:OE1	2:B:223:GLU:HA	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:484:ASN:HB3	2:B:487:PHE:CE1	2.44	0.52
1:A:66:CYS:O	1:A:70:VAL:HG23	2.09	0.52
2:B:193:PRO:C	2:B:195:LYS:H	2.12	0.52
1:A:488:ARG:NE	1:A:488:ARG:HA	2.24	0.52
1:A:128:GLN:O	1:A:132:GLN:HG2	2.10	0.52
1:A:351:LYS:C	1:A:394:VAL:HG22	2.30	0.52
1:A:199:PHE:CD1	1:A:199:PHE:N	2.77	0.52
1:A:200:LEU:HD23	1:A:200:LEU:C	2.30	0.51
1:A:171:ASN:HB3	1:A:205:LEU:HB2	1.92	0.51
1:A:348:MET:HE3	2:B:518:PRO:HD3	1.92	0.51
1:A:38:LEU:HB2	1:A:252:ARG:HH22	1.75	0.51
2:B:72:ASP:HA	2:B:75:GLN:NE2	2.24	0.51
2:B:27:ILE:HG23	2:B:183:PHE:CE2	2.46	0.51
2:B:134:ILE:HD11	2:B:161:LEU:HD11	1.91	0.51
1:A:447:PRO:HG3	2:B:243:HIS:CD2	2.45	0.51
2:B:450:GLN:HB3	2:B:537:PHE:CZ	2.46	0.51
1:A:588:TYR:HB2	1:A:590:LEU:CD2	2.38	0.50
1:A:59:PRO:HA	1:A:62:MET:HE2	1.93	0.50
1:A:296:VAL:HG13	2:B:296:CYS:O	2.11	0.50
1:A:296:VAL:CG1	2:B:295:TYR:HB3	2.40	0.50
1:A:488:ARG:HD3	1:A:501:GLU:OE2	2.12	0.50
1:A:157:VAL:HG11	1:A:161:MET:HE2	1.93	0.50
2:B:49:GLU:O	2:B:51:LYS:HE2	2.12	0.50
1:A:76:ILE:HD12	1:A:487:PHE:CD1	2.47	0.50
2:B:478:PRO:O	2:B:480:THR:N	2.45	0.50
1:A:261:LEU:C	1:A:261:LEU:HD23	2.32	0.49
1:A:199:PHE:HD1	1:A:199:PHE:N	2.10	0.49
2:B:251:LEU:C	2:B:251:LEU:HD23	2.32	0.49
1:A:369:TYR:CG	1:A:370:PRO:HD2	2.47	0.49
1:A:348:MET:HE1	2:B:517:ASN:HA	1.94	0.49
2:B:118:ILE:HD13	2:B:130:ARG:HB3	1.94	0.49
1:A:438:PRO:HB2	1:A:442:ASP:HB2	1.93	0.49
1:A:266:ASP:O	1:A:268:VAL:HG23	2.13	0.49
1:A:328:ILE:C	1:A:329:LEU:HD23	2.34	0.49
1:A:35:ARG:O	1:A:161:MET:HA	2.13	0.49
1:A:178:ASN:N	1:A:178:ASN:ND2	2.55	0.48
1:A:240:GLU:O	1:A:244:ARG:HG3	2.13	0.48
2:B:192:PHE:N	2:B:192:PHE:CD1	2.81	0.48
1:A:397:LEU:HD12	1:A:411:VAL:O	2.13	0.48
1:A:428:THR:HG23	2:B:354:ARG:CZ	2.44	0.48
1:A:499:GLU:HB2	1:A:500:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:VAL:HG23	1:A:97:VAL:O	2.14	0.48
2:B:19:THR:HG23	2:B:104:GLN:NE2	2.28	0.47
1:A:48:MET:HA	1:A:59:PRO:HG2	1.95	0.47
1:A:362:LEU:O	1:A:362:LEU:HG	2.14	0.47
2:B:49:GLU:OE2	2:B:274:LYS:NZ	2.47	0.47
2:B:467:ASP:CG	2:B:468:GLU:N	2.67	0.47
2:B:232:ARG:HG3	2:B:232:ARG:NH1	2.30	0.47
2:B:295:TYR:N	2:B:295:TYR:CD1	2.81	0.47
2:B:463:LEU:HD23	2:B:522:VAL:HG21	1.95	0.47
2:B:299:ASP:O	2:B:300:ASP:O	2.32	0.47
2:B:488:GLN:HG2	3:B:573:HOH:O	2.15	0.47
1:A:434:LEU:HD23	1:A:434:LEU:C	2.34	0.47
1:A:165:ARG:HA	1:A:199:PHE:O	2.15	0.47
1:A:264:ASN:C	1:A:264:ASN:OD1	2.52	0.47
1:A:403:ARG:CG	1:A:406:ILE:HD12	2.45	0.47
2:B:186:GLY:O	2:B:232:ARG:HD3	2.15	0.47
1:A:347:LEU:CD2	2:B:461:MET:HE3	2.45	0.47
1:A:357:LYS:O	1:A:360:HIS:HB2	2.14	0.47
1:A:362:LEU:HD11	2:B:269:GLN:HB2	1.97	0.46
1:A:371:GLU:HA	1:A:371:GLU:OE1	2.16	0.46
1:A:171:ASN:O	1:A:207:LYS:HD2	2.15	0.46
1:A:132:GLN:OE1	1:A:137:HIS:CE1	2.69	0.46
2:B:42:VAL:HG12	2:B:91:LEU:HD21	1.98	0.46
1:A:605:LYS:HG3	1:A:609:ASP:HB3	1.95	0.46
2:B:288:ASP:N	2:B:288:ASP:OD1	2.49	0.46
1:A:179:ASP:O	1:A:181:ALA:N	2.48	0.46
1:A:36:ASP:OD2	1:A:252:ARG:HD3	2.16	0.46
2:B:329:GLU:C	2:B:331:MET:H	2.18	0.46
1:A:441:ASP:O	1:A:444:ARG:NH1	2.49	0.46
2:B:484:ASN:C	2:B:486:ARG:H	2.19	0.46
1:A:383:SER:O	1:A:387:ILE:HG13	2.16	0.46
1:A:253:LYS:HD3	2:B:435:PHE:CE2	2.51	0.46
1:A:234:GLU:HG2	1:A:424:LYS:HG2	1.98	0.46
1:A:135:MET:O	1:A:136:GLY:C	2.52	0.45
2:B:323:PHE:CD2	2:B:328:GLU:HB3	2.52	0.45
2:B:106:ASP:HB3	2:B:109:ASP:HB2	1.98	0.45
2:B:77:ILE:HD11	2:B:109:ASP:HB3	1.98	0.45
1:A:217:TYR:HA	1:A:220:ILE:HB	1.99	0.45
2:B:424:LEU:HB3	2:B:425:PRO:HD2	1.98	0.45
1:A:318:ARG:O	1:A:328:ILE:HA	2.17	0.45
1:A:179:ASP:C	1:A:181:ALA:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ILE:C	1:A:199:PHE:HD1	2.20	0.45
2:B:283:THR:O	2:B:284:LEU:HB2	2.17	0.45
2:B:109:ASP:O	2:B:113:VAL:HG23	2.16	0.45
1:A:121:GLN:OE1	1:A:130:ARG:NH1	2.49	0.45
1:A:252:ARG:O	1:A:254:ARG:HG3	2.17	0.45
1:A:196:THR:HG22	1:A:196:THR:O	2.16	0.45
2:B:477:PHE:N	2:B:478:PRO:HD3	2.32	0.45
1:A:303:PHE:HA	1:A:311:LEU:HG	1.98	0.45
1:A:458:GLN:NE2	1:A:528:LEU:O	2.43	0.45
2:B:83:LEU:O	2:B:84:MET:HB3	2.17	0.45
2:B:90:LEU:O	2:B:94:ILE:HG12	2.17	0.45
1:A:56:GLU:HG2	1:A:237:SER:O	2.16	0.45
1:A:264:ASN:OD1	1:A:266:ASP:N	2.49	0.45
1:A:573:LEU:O	1:A:576:PHE:HB2	2.17	0.44
1:A:91:GLU:N	1:A:136:GLY:O	2.51	0.44
1:A:71:TYR:OH	1:A:85:VAL:HG23	2.18	0.44
2:B:138:LEU:O	2:B:201:GLN:HA	2.17	0.44
2:B:7:LYS:HE3	2:B:126:LYS:O	2.16	0.44
1:A:448:PHE:N	1:A:448:PHE:CD2	2.86	0.44
1:A:302:THR:HA	2:B:291:LYS:HA	2.00	0.44
1:A:578:VAL:N	1:A:579:PRO:CD	2.81	0.44
1:A:262:LYS:HG2	1:A:268:VAL:HG22	2.00	0.44
1:A:59:PRO:HA	1:A:62:MET:CE	2.48	0.44
1:A:470:ARG:O	1:A:471:PHE:HB3	2.18	0.44
1:A:595:LYS:HB2	1:A:598:GLU:HG3	2.00	0.44
1:A:584:ALA:CB	1:A:603:LEU:HD11	2.48	0.44
2:B:66:ASN:HA	2:B:67:PRO:HD3	1.88	0.44
1:A:465:ILE:HG23	1:A:518:LEU:CD2	2.47	0.44
2:B:337:GLY:HA2	2:B:399:LYS:HA	2.00	0.44
1:A:363:ARG:HG3	1:A:363:ARG:HH11	1.83	0.43
1:A:154:PHE:CD1	1:A:198:ILE:HD13	2.53	0.43
1:A:445:LYS:CG	1:A:446:MET:N	2.81	0.43
2:B:332:LYS:HG2	2:B:333:TYR:N	2.33	0.43
1:A:256:LEU:N	1:A:273:ILE:O	2.41	0.43
1:A:379:SER:HB2	2:B:444:TYR:CD2	2.53	0.43
1:A:347:LEU:HD21	2:B:461:MET:HE3	2.00	0.43
1:A:388:LYS:HB3	2:B:458:ILE:HD12	2.01	0.43
1:A:151:ALA:CB	1:A:193:LEU:HD21	2.48	0.43
2:B:131:HIS:HE1	2:B:162:GLN:HG3	1.82	0.43
1:A:473:TYR:CZ	2:B:424:LEU:HD13	2.53	0.43
1:A:289:TYR:O	1:A:291:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ARG:CZ	2:B:389:MET:HE3	2.49	0.43
1:A:149:VAL:O	1:A:153:LEU:HG	2.19	0.43
2:B:6:ASN:N	2:B:128:GLU:OE1	2.51	0.43
1:A:437:LEU:HD23	3:B:579:HOH:O	2.19	0.43
1:A:353:LEU:CD2	1:A:395:ALA:HB2	2.49	0.43
1:A:338:LYS:O	1:A:340:PHE:HD1	2.02	0.43
1:A:108:LEU:HD11	1:A:154:PHE:CD2	2.53	0.42
1:A:158:GLN:N	1:A:158:GLN:OE1	2.52	0.42
1:A:511:VAL:HG11	2:B:255:SER:HB3	2.00	0.42
1:A:216:PHE:CZ	1:A:220:ILE:CD1	3.02	0.42
2:B:134:ILE:N	2:B:134:ILE:HD12	2.35	0.42
1:A:399:ARG:HG2	1:A:408:PRO:HB2	2.01	0.42
2:B:73:GLN:O	2:B:74:TYR:C	2.55	0.42
1:A:142:SER:HB3	1:A:182:LYS:HD3	2.02	0.42
1:A:420:LEU:CD2	1:A:426:GLN:HA	2.49	0.42
2:B:347:LYS:HB2	2:B:350:GLN:HG3	2.01	0.42
1:A:447:PRO:HD3	2:B:243:HIS:CD2	2.54	0.42
1:A:366:LEU:HB2	1:A:434:LEU:HB3	2.02	0.42
1:A:508:LEU:HD23	2:B:394:ARG:NE	2.34	0.42
2:B:193:PRO:C	2:B:195:LYS:N	2.72	0.42
1:A:263:LEU:HD22	1:A:347:LEU:HD22	2.02	0.42
1:A:418:GLU:CG	1:A:419:GLU:N	2.82	0.42
1:A:403:ARG:HG3	1:A:406:ILE:HD12	2.01	0.42
1:A:577:THR:OG1	1:A:580:MET:HG3	2.19	0.42
2:B:147:LEU:HA	2:B:150:ILE:HD12	2.00	0.42
1:A:196:THR:CG2	1:A:196:THR:O	2.67	0.42
2:B:135:PHE:CD1	2:B:135:PHE:N	2.87	0.42
2:B:413:LYS:HD3	2:B:413:LYS:HA	1.82	0.42
1:A:340:PHE:HB2	1:A:408:PRO:HD3	2.02	0.42
1:A:204:HIS:N	1:A:204:HIS:ND1	2.66	0.41
1:A:251:THR:CG2	1:A:252:ARG:H	2.33	0.41
1:A:67:ILE:HG22	1:A:119:LEU:HD13	2.02	0.41
1:A:141:TYR:C	1:A:141:TYR:CD1	2.93	0.41
2:B:146:GLN:HB2	2:B:150:ILE:HD11	2.02	0.41
1:A:568:ILE:HG12	1:A:573:LEU:HD22	2.02	0.41
2:B:335:SER:C	2:B:337:GLY:H	2.23	0.41
2:B:204:GLY:O	2:B:208:VAL:HG23	2.20	0.41
1:A:406:ILE:HA	1:A:407:PRO:HD3	1.96	0.41
2:B:381:ILE:HD11	2:B:418:CYS:HA	2.03	0.41
1:A:236:SER:OG	1:A:245:LYS:HD2	2.20	0.41
1:A:233:PHE:CD2	1:A:245:LYS:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:GLU:C	2:B:129:LYS:HG3	2.40	0.41
1:A:99:PHE:HD2	1:A:99:PHE:HA	1.72	0.41
1:A:422:ASP:OD1	1:A:423:GLN:HG2	2.20	0.41
1:A:329:LEU:HD22	2:B:497:ARG:HE	1.85	0.41
2:B:19:THR:H	2:B:104:GLN:HE22	1.66	0.41
2:B:283:THR:HB	2:B:285:LYS:HG2	2.00	0.41
2:B:71:GLY:O	2:B:73:GLN:HG3	2.21	0.41
1:A:490:LEU:HA	1:A:490:LEU:HD12	1.74	0.41
2:B:197:ILE:HD11	2:B:202:LYS:HG2	2.02	0.41
1:A:63:SER:HG	1:A:169:PHE:HD2	1.68	0.41
1:A:451:LYS:HE3	2:B:417:GLU:CD	2.41	0.41
1:A:451:LYS:HE3	2:B:417:GLU:CG	2.51	0.41
2:B:382:HIS:NE2	2:B:417:GLU:OE2	2.49	0.41
1:A:511:VAL:CG1	2:B:255:SER:HB3	2.51	0.41
1:A:423:GLN:HB2	1:A:425:ILE:HG13	2.03	0.41
1:A:585:CYS:O	1:A:590:LEU:HD23	2.21	0.41
2:B:528:ILE:O	2:B:529:PRO:C	2.58	0.41
2:B:245:ILE:HG22	2:B:246:HIS:N	2.36	0.41
1:A:465:ILE:HG23	1:A:518:LEU:HD21	2.02	0.41
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.81	0.41
1:A:491:GLU:HG3	2:B:316:TYR:CE2	2.56	0.41
2:B:492:GLN:NE2	2:B:509:GLN:HG3	2.36	0.41
2:B:294:VAL:HG12	2:B:295:TYR:H	1.85	0.41
2:B:132:ILE:HB	2:B:161:LEU:CD1	2.51	0.41
1:A:142:SER:HA	1:A:176:HIS:NE2	2.36	0.40
1:A:447:PRO:CD	2:B:243:HIS:CD2	3.04	0.40
2:B:246:HIS:HB3	2:B:264:TYR:CE2	2.57	0.40
1:A:474:ARG:HG2	1:A:476:ASP:OD1	2.21	0.40
1:A:318:ARG:HG3	1:A:334:THR:HG21	2.04	0.40
1:A:166:ILE:O	1:A:200:LEU:HA	2.22	0.40
2:B:366:ALA:O	2:B:367:ALA:C	2.60	0.40
1:A:101:ASN:ND2	1:A:139:SER:HB3	2.36	0.40
1:A:582:LYS:O	1:A:586:ARG:HG3	2.21	0.40
1:A:530:TYR:O	1:A:531:PRO:C	2.59	0.40
1:A:326:GLN:HE21	1:A:328:ILE:CD1	2.33	0.40
1:A:442:ASP:HA	1:A:444:ARG:NH1	2.37	0.40
1:A:495:LEU:O	1:A:496:ASP:C	2.60	0.40
1:A:286:ILE:HG22	1:A:287:LYS:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	542/609 (89%)	473 (87%)	56 (10%)	13 (2%)	7	19
2	B	512/565 (91%)	454 (89%)	49 (10%)	9 (2%)	11	27
All	All	1054/1174 (90%)	927 (88%)	105 (10%)	22 (2%)	9	23

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	180	SER
1	A	290	ARG
2	B	96	SER
2	B	97	LYS
2	B	300	ASP
2	B	470	THR
1	A	136	GLY
1	A	267	ILE
1	A	402	PRO
2	B	468	GLU
2	B	479	THR
2	B	527	GLN
2	B	469	LYS
1	A	137	HIS
1	A	138	GLY
1	A	522	VAL
1	A	98	ASN
1	A	535	ASN
1	A	602	ALA
2	B	95	GLU
1	A	589	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	495/548 (90%)	473 (96%)	22 (4%)	35	65
2	B	469/505 (93%)	454 (97%)	15 (3%)	46	77
All	All	964/1053 (92%)	927 (96%)	37 (4%)	40	71

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	SER
1	A	78	SER
1	A	99	PHE
1	A	144	SER
1	A	178	ASN
1	A	184	SER
1	A	243	LEU
1	A	266	ASP
1	A	303	PHE
1	A	360	HIS
1	A	381	LEU
1	A	394	VAL
1	A	409	TYR
1	A	441	ASP
1	A	449	THR
1	A	453	MET
1	A	471	PHE
1	A	474	ARG
1	A	488	ARG
1	A	496	ASP
1	A	517	ARG
1	A	609	ASP
2	B	28	GLU
2	B	30	PRO
2	B	72	ASP
2	B	107	PHE
2	B	130	ARG

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Mol	Chain	Res	Type
2	B	288	ASP
2	B	300	ASP
2	B	323	PHE
2	B	329	GLU
2	B	330	GLN
2	B	341	SER
2	B	380	LEU
2	B	386	ASP
2	B	427	MET
2	B	471	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	176	HIS
1	A	178	ASN
1	A	326	GLN
1	A	433	GLN
1	A	485	GLN
1	A	502	GLN
2	B	43	GLN
2	B	75	GLN
2	B	104	GLN
2	B	152	HIS
2	B	423	GLN
2	B	452	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [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	548/609 (89%)	1.12	104 (18%) 2 1	16, 45, 86, 99	0
2	B	520/565 (92%)	0.98	77 (14%) 3 2	15, 39, 91, 101	0
All	All	1068/1174 (90%)	1.05	181 (16%) 2 2	15, 42, 88, 101	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	538	GLY	10.7
1	A	592	SER	9.9
1	A	181	ALA	8.3
1	A	200	LEU	7.6
1	A	608	GLN	7.0
1	A	294	GLU	7.0
2	B	308	GLU	6.7
1	A	451	LYS	6.7
1	A	292	THR	6.5
2	B	440	ASN	6.1
2	B	302	GLU	6.0
1	A	293	ASN	5.9
2	B	6	ASN	5.9
1	A	310	LEU	5.8
2	B	290	GLN	5.8
2	B	285	LYS	5.5
2	B	294	VAL	5.4
1	A	55	ASP	5.3
1	A	609	ASP	5.2
2	B	333	TYR	5.2
1	A	191	GLY	5.1
2	B	303	THR	5.0
2	B	156	LYS	4.9
2	B	312	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
2	B	192	PHE	4.8
2	B	105	ALA	4.8
1	A	534	TYR	4.6
2	B	287	GLU	4.6
1	A	251	THR	4.5
1	A	535	ASN	4.4
1	A	492	ALA	4.3
1	A	223	ILE	4.3
1	A	452	ILE	4.2
2	B	311	ILE	4.2
2	B	453	ALA	4.2
1	A	515	ASN	4.2
2	B	499	LEU	4.1
2	B	150	ILE	4.1
2	B	22	ASN	4.1
1	A	602	ALA	4.1
1	A	302	THR	4.0
2	B	143	SER	4.0
1	A	300	THR	3.9
2	B	189	GLY	3.9
1	A	387	ILE	3.8
1	A	58	THR	3.8
2	B	273	LYS	3.8
2	B	305	VAL	3.8
1	A	503	ALA	3.5
1	A	314	SER	3.5
2	B	246	HIS	3.5
1	A	459	VAL	3.5
2	B	334	LYS	3.4
1	A	248	ALA	3.4
1	A	257	SER	3.4
1	A	448	PHE	3.4
2	B	306	LEU	3.4
1	A	537	GLU	3.3
2	B	527	GLN	3.3
2	B	310	ILE	3.3
1	A	165	ARG	3.3
1	A	297	LYS	3.3
1	A	499	GLU	3.3
1	A	291	GLU	3.2
2	B	385	ASP	3.2
2	B	423	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	137	HIS	3.2
2	B	364	VAL	3.2
1	A	246	VAL	3.2
1	A	123	LYS	3.2
2	B	160	SER	3.1
2	B	292	GLU	3.1
1	A	516	LYS	3.1
2	B	386	ASP	3.1
2	B	528	ILE	3.1
2	B	301	ASP	3.1
2	B	186	GLY	3.0
1	A	520	SER	3.0
2	B	78	THR	3.0
1	A	355	LEU	3.0
2	B	293	THR	3.0
1	A	218	ARG	3.0
1	A	595	LYS	3.0
1	A	427	VAL	3.0
2	B	365	PHE	2.9
2	B	13	CYS	2.9
1	A	139	SER	2.9
1	A	221	ILE	2.9
1	A	385	LEU	2.8
2	B	335	SER	2.8
2	B	438	LEU	2.8
1	A	313	PRO	2.8
1	A	495	LEU	2.8
1	A	271	VAL	2.8
1	A	252	ARG	2.8
2	B	297	LEU	2.7
2	B	68	LEU	2.7
2	B	195	LYS	2.7
2	B	452	ASN	2.7
2	B	323	PHE	2.7
2	B	194	LEU	2.7
2	B	327	ASP	2.6
1	A	295	PRO	2.6
1	A	47	ALA	2.6
1	A	36	ASP	2.6
1	A	466	VAL	2.6
2	B	98	ILE	2.6
1	A	245	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	48	ALA	2.6
1	A	536	PRO	2.6
1	A	502	GLN	2.5
1	A	272	GLY	2.5
1	A	315	ASP	2.5
2	B	72	ASP	2.5
1	A	177	GLY	2.5
2	B	300	ASP	2.5
2	B	304	GLU	2.5
1	A	573	LEU	2.5
1	A	158	GLN	2.5
1	A	375	VAL	2.4
2	B	279	VAL	2.4
1	A	565	LYS	2.4
1	A	301	ARG	2.4
2	B	346	CYS	2.4
2	B	379	SER	2.4
2	B	81	ARG	2.4
2	B	147	LEU	2.4
1	A	513	ALA	2.4
2	B	149	ILE	2.4
1	A	156	ASP	2.4
1	A	52	GLN	2.4
2	B	298	ASN	2.3
1	A	370	PRO	2.3
1	A	453	MET	2.3
2	B	529	PRO	2.3
1	A	339	ARG	2.3
2	B	446	PRO	2.3
1	A	45	SER	2.3
1	A	101	ASN	2.3
1	A	178	ASN	2.3
1	A	50	GLU	2.3
2	B	519	PRO	2.3
1	A	286	ILE	2.3
2	B	495	LEU	2.2
1	A	560	SER	2.2
1	A	338	LYS	2.2
2	B	469	LYS	2.2
2	B	198	THR	2.2
1	A	201	ASP	2.2
1	A	180	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	272	VAL	2.2
2	B	70	GLY	2.2
1	A	289	TYR	2.2
1	A	304	ASN	2.2
1	A	53	SER	2.2
1	A	464	ALA	2.2
1	A	449	THR	2.2
1	A	77	SER	2.1
1	A	417	GLU	2.1
2	B	443	LYS	2.1
1	A	135	MET	2.1
2	B	27	ILE	2.1
1	A	175	PRO	2.1
1	A	75	ILE	2.1
1	A	585	CYS	2.1
1	A	219	ASP	2.1
2	B	407	VAL	2.1
1	A	51	SER	2.1
2	B	471	ASP	2.1
1	A	586	ARG	2.1
1	A	373	SER	2.1
1	A	497	LEU	2.1
1	A	296	VAL	2.0
1	A	500	PRO	2.0
2	B	539	LEU	2.0
1	A	198	ILE	2.0
1	A	454	ALA	2.0
2	B	50	ASN	2.0
1	A	80	ARG	2.0
2	B	329	GLU	2.0
1	A	579	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.