



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:31 pm BST

PDB ID : 1GGY
Title : HUMAN FACTOR XIII WITH YTTERBIUM BOUND IN THE ION SITE
Authors : Fox, B.A.; Yee, V.C.; Pederson, L.C.; Trong, I.L.; Bishop, P.D.; Stenkamp, R.E.; Teller, D.C.
Deposited on : 1998-07-23
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

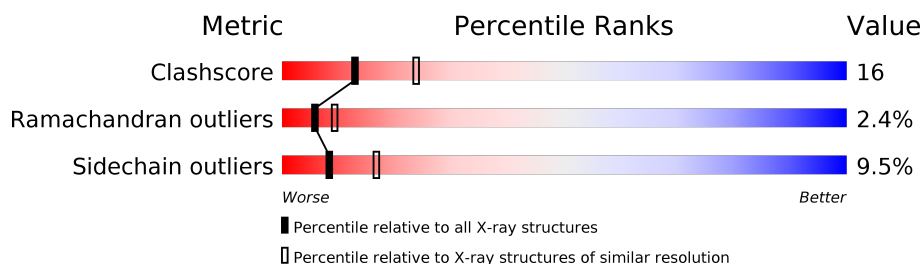
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	731	
1	B	731	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11569 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 PROTEIN (COAGULATION FACTOR XIII).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	702	Total	C	N	O	S	0	0	0
			5637	3577	968	1066	26			
1	B	705	Total	C	N	O	S	0	0	0
			5659	3589	973	1071	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	651	GLU	GLN	conflict	UNP P00488
B	651	GLU	GLN	conflict	UNP P00488

- Molecule 2 is YTTERBIUM (III) ION (three-letter code: Yb) (formula: Yb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Yb	0	0
			3	3		
2	A	5	Total	Yb	0	0
			5	5		

- Molecule 3 is water.

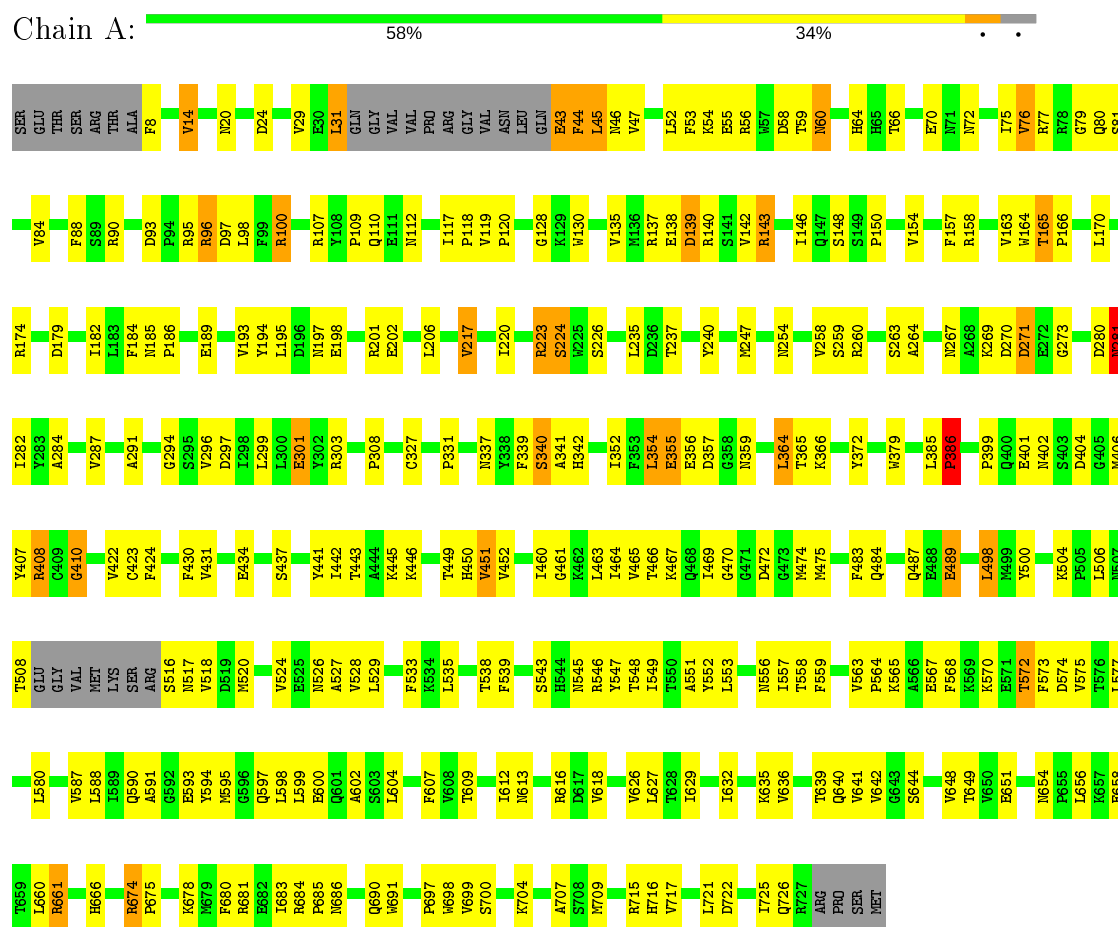
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	139	Total	O	0	0
			139	139		
3	B	126	Total	O	0	0
			126	126		

3 Residue-property plots

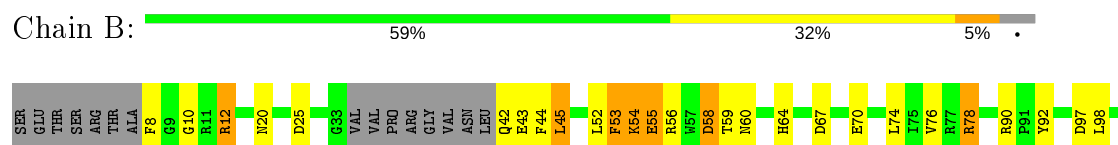
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: PROTEIN (COAGULATION FACTOR XIII)



• Molecule 1: PROTEIN (COAGULATION FACTOR XIII)



V101	A192	N307	Y467	GLY	E578	V672
E102	V193	F308	R408	VAL	F579	T673
Y103	D196	V309	P411	MET	L580	R674
V104	E200	R310	Q415	LYS	S581	P675
I105	L206	Y311	H419	ARG	F582	M676
N112	L212	C314	G420	S516	K583	K677
K113	F213	F327	H421	D519	K584	K678
T115	V217	L328	F426	M520	L588	M679
P118	N218	P331	F430	D521	I589	P684
I121	R223	A332	V431	F522	Q590	P685
E124	Q229	R333	F436	E525	A591	P697
L125	L235	I334	S437	M526	Y594	S700
Q126	D236	V335	T443	A527	Q597	G701
S127	T237	L336	K446	V528	L598	H702
G128	Y240	T337	H450	L529	L599	R703
K129	R252	N337	V451	E530	E600	K704
V135	P255	Y338	V452	K531	L604	L705
M136	R260	F339	T458	D532	H605	L706
R137	A268	S340	K462	F533	F606	A707
E138	G273	A341	L463	K534	F607	S713
D139	V274	H342	K467	S536	V608	I714
R140	L275	D343	Q468	I537	T609	L715
S141	N281	N344	I469	T538	A610	R716
V142	I282	D345	G470	F539	R611	H721
R143	Y283	A346	M474	R540	I612	D722
S148	A284	N347	I477	M541	R613	V723
I153	V287	L348	E485	S542	R616	Q724
V154	S290	Q349	G486	E543	A620	I725
F157	A291	M350	Q487	B544	K623	Q726
R158	W292	E356	E490	M545	S624	R727
M159	D297	N359	R491	T548	I633	ARG
Y160	E301	K363	L492	I549	I634	PRO
P166	R303	K366	L498	T550	K635	SER
Y167	E306	V369	K503	A551	V636	MET
T172	G405	Y372	K504	M554	R637	I638
S173	M406	E377	T508	A555	T638	T639
R174		Q379	GLU	M556	V640	V641
T178		M379		I557	V642	V642
D179		M380		F559	M646	M646
T180		T381		V563	T647	T647
Y181		R382		P664	V648	V648
I182		K392		K565	T649	T649
L183		E401		F568	V650	E651
F184		M402		K569	E651	L656
N185		E401		R573	L656	T659
C188		M406		D574		

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.06 Å 72.39 Å 135.99 Å 90.00° 106.09° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	75.9 (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.188 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11569	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.56	0/5770	0.78	2/7830 (0.0%)
1	B	0.55	0/5792	0.80	2/7859 (0.0%)
All	All	0.56	0/11562	0.79	4/15689 (0.0%)

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	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	269	LYS	N-CA-C	-5.48	96.20	111.00
1	B	405	GLY	N-CA-C	5.20	126.09	113.10
1	A	518	VAL	N-CA-C	-5.18	97.00	111.00
1	B	604	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	181	TYR	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	5637	0	5489	189	0
1	B	5659	0	5508	183	0
2	A	5	0	0	0	0
2	B	3	0	0	0	0
3	A	139	0	0	7	0
3	B	126	0	0	9	0
All	All	11569	0	10997	368	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 16.

All (368) 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:220:ILE:HD13	1:B:474:MET:HE1	1.37	1.04
1:B:575:VAL:HG13	1:B:583:LYS:HD3	1.43	1.01
1:B:356:GLU:HG3	1:B:446:LYS:HD2	1.48	0.96
1:A:331:PRO:HG2	1:A:379:TRP:HB3	1.46	0.96
1:B:211:VAL:HG22	1:B:467:LYS:HD2	1.49	0.93
1:A:356:GLU:HG3	1:A:446:LYS:HG2	1.52	0.92
1:A:437:SER:HB2	1:A:460:ILE:HD12	1.55	0.87
1:B:659:THR:HG22	1:B:684:ARG:HA	1.60	0.84
1:B:44:PHE:O	1:B:45:LEU:HB2	1.78	0.83
1:A:651:GLU:HB3	1:A:690:GLN:HG3	1.60	0.81
1:B:548:THR:HB	1:B:613:ASN:HD21	1.44	0.81
1:A:95:ARG:HG2	1:A:96:ARG:HG3	1.63	0.80
1:A:8:PHE:O	1:B:563:VAL:HG11	1.85	0.77
1:A:341:ALA:HB2	1:A:460:ILE:HD13	1.64	0.76
1:B:331:PRO:HB2	1:B:379:TRP:HB3	1.68	0.75
1:A:100:ARG:HG2	1:A:164:TRP:HE1	1.50	0.75
1:A:100:ARG:HG2	1:A:164:TRP:NE1	2.01	0.75
1:B:281:ASN:OD1	1:B:600:GLU:HG3	1.88	0.73
1:A:635:LYS:HG3	1:A:649:THR:HB	1.69	0.73
1:A:64:HIS:HE1	1:A:80:GLN:HB3	1.53	0.73
1:B:345:ASP:O	1:B:503:LYS:HE2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:HIS:HA	1:B:579:PRO:HB3	1.71	0.72
1:A:443:THR:HB	1:A:451:VAL:HG13	1.70	0.72
1:A:483:PHE:HB3	1:A:487:GLN:HE21	1.55	0.72
1:A:44:PHE:HD2	1:A:90:ARG:HE	1.39	0.71
1:A:527:ALA:HB2	1:A:533:PHE:HB3	1.73	0.71
1:A:549:ILE:HB	1:A:575:VAL:HB	1.73	0.71
1:B:213:PHE:CD1	1:B:222:THR:HG22	2.25	0.71
1:A:29:VAL:HG22	1:A:31:LEU:HD22	1.73	0.70
1:B:537:ILE:HD12	1:B:573:PHE:HZ	1.54	0.69
1:B:678:LYS:HD3	1:B:679:MET:H	1.57	0.69
1:A:467:LYS:HE2	1:A:472:ASP:HA	1.73	0.69
1:A:337:ASN:HD21	1:A:461:GLY:HA2	1.57	0.69
1:A:198:GLU:O	1:A:202:GLU:HG3	1.92	0.68
1:A:559:PHE:HZ	1:B:8:PHE:CD1	2.11	0.68
1:A:98:LEU:HD23	1:A:164:TRP:HB2	1.74	0.68
1:B:290:SER:OG	1:B:716:HIS:HD2	1.76	0.68
1:B:633:ILE:HB	1:B:651:GLU:HG3	1.76	0.68
1:B:541:ASN:HB2	1:B:577:LEU:HB3	1.75	0.67
1:A:44:PHE:O	1:A:45:LEU:HB2	1.94	0.67
1:B:126:GLN:HG3	1:B:127:SER:N	2.09	0.67
1:A:636:VAL:HG12	1:A:648:VAL:HA	1.77	0.66
1:A:64:HIS:CE1	1:A:80:GLN:HB3	2.30	0.66
1:A:90:ARG:HG3	1:A:90:ARG:HH11	1.60	0.66
1:B:527:ALA:HB2	1:B:533:PHE:HB3	1.77	0.66
1:B:172:THR:HB	3:B:3044:HOH:O	1.95	0.66
1:B:642:VAL:HG21	1:B:700:SER:HB3	1.77	0.66
1:A:557:ILE:HG21	1:A:597:GLN:O	1.96	0.66
1:B:565:LYS:HE2	1:B:597:GLN:HB2	1.79	0.65
1:A:235:LEU:HA	1:A:327:CYS:SG	2.37	0.65
1:A:157:PHE:CD1	1:A:182:ILE:HD12	2.31	0.65
1:B:78:ARG:HG2	1:B:183:LEU:O	1.97	0.65
1:B:591:ALA:HA	1:B:594:TYR:CE2	2.33	0.64
1:B:522:PHE:O	1:B:623:LYS:HE3	1.98	0.63
1:B:280:ASP:OD2	1:B:282:ILE:HB	1.99	0.63
1:A:465:VAL:HG13	1:A:474:MET:HG3	1.79	0.63
1:B:638:GLY:HA3	1:B:646:MET:HA	1.81	0.63
1:A:237:THR:HG22	1:A:303:ARG:HD2	1.81	0.62
1:A:524:VAL:HG22	1:A:535:LEU:HG	1.80	0.62
1:B:528:VAL:HB	1:B:531:LYS:HG2	1.79	0.62
1:A:465:VAL:CG1	1:A:474:MET:HG3	2.30	0.62
1:B:557:ILE:HG21	1:B:597:GLN:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:O	1:B:54:LYS:HG3	2.00	0.62
1:A:263:SER:OG	1:A:408:ARG:HD3	1.98	0.62
1:A:135:VAL:HG12	1:A:143:ARG:O	1.99	0.62
1:B:127:SER:O	1:B:129:LYS:HG3	2.01	0.61
1:A:356:GLU:HB2	1:A:446:LYS:HE2	1.83	0.61
1:B:678:LYS:HD3	1:B:679:MET:N	2.16	0.60
1:B:535:LEU:HD11	1:B:606:PHE:CD1	2.37	0.60
1:A:139:ASP:O	1:A:140:ARG:HG2	2.02	0.59
1:A:280:ASP:O	1:A:282:ILE:N	2.36	0.59
1:B:105:ILE:HD11	1:B:157:PHE:CE2	2.38	0.59
1:B:136:MET:HB3	1:B:143:ARG:HB3	1.84	0.59
1:A:254:ASN:O	1:A:258:VAL:HG23	2.03	0.58
1:B:335:VAL:HG13	1:B:477:ILE:HD11	1.85	0.57
1:B:468:GLN:HG2	1:B:473:GLY:O	2.04	0.57
1:A:547:TYR:HB3	1:A:612:ILE:HG23	1.87	0.57
1:B:193:VAL:HG13	1:B:193:VAL:O	2.04	0.57
1:B:349:GLN:HE21	1:B:504:LYS:HG3	1.69	0.57
1:B:558:THR:HG22	1:B:564:PRO:HA	1.86	0.57
1:A:90:ARG:HG3	1:A:90:ARG:NH1	2.18	0.57
1:B:656:LEU:HA	3:B:6075:HOH:O	2.04	0.56
1:A:112:ASN:HB2	3:A:3003:HOH:O	2.05	0.56
1:A:237:THR:HG22	1:A:303:ARG:CD	2.35	0.56
1:A:24:ASP:O	1:A:158:ARG:NH2	2.38	0.56
1:A:422:VAL:HG23	1:A:500:TYR:HB2	1.87	0.56
1:B:611:ARG:HD2	1:B:616:ARG:NH1	2.20	0.56
1:A:117:ILE:HG21	1:A:130:TRP:CD2	2.41	0.55
1:B:684:ARG:HB3	1:B:685:PRO:HD2	1.87	0.55
1:A:698:TRP:CD1	1:A:699:VAL:HG23	2.41	0.55
1:B:105:ILE:CD1	1:B:115:THR:HA	2.35	0.55
1:B:356:GLU:HB2	1:B:446:LYS:NZ	2.21	0.55
1:B:52:LEU:HD21	1:B:159:MET:SD	2.46	0.55
1:B:401:GLU:HA	1:B:406:MET:H	1.72	0.55
1:B:575:VAL:HG12	1:B:577:LEU:HD12	1.89	0.55
1:B:382:ARG:NH2	1:B:411:PRO:O	2.39	0.54
1:A:163:VAL:HB	1:A:170:LEU:HB2	1.89	0.54
1:B:273:GLY:O	1:B:308:PRO:HG3	2.07	0.54
1:B:549:ILE:HG22	1:B:550:THR:N	2.23	0.54
1:B:90:ARG:HH11	1:B:90:ARG:HG3	1.71	0.54
1:A:539:PHE:HB3	1:A:577:LEU:HD11	1.90	0.54
1:B:297:ASP:O	1:B:301:GLU:HB2	2.07	0.54
1:A:271:ASP:HA	1:A:308:PRO:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ILE:HD12	1:B:115:THR:HA	1.88	0.54
1:B:485:GLU:HA	1:B:490:GLU:HG2	1.90	0.53
1:B:634:ILE:HG22	1:B:721:LEU:HD12	1.90	0.53
1:A:565:LYS:HB2	1:A:599:LEU:HD11	1.90	0.53
1:A:70:GLU:HB3	3:A:6058:HOH:O	2.07	0.53
1:B:126:GLN:HG3	1:B:127:SER:H	1.71	0.53
1:B:143:ARG:HB2	1:B:143:ARG:NH1	2.23	0.53
1:B:634:ILE:HD11	1:B:707:ALA:HB2	1.90	0.53
1:B:52:LEU:HD11	1:B:178:THR:HA	1.90	0.53
1:B:136:MET:HG2	1:B:137:ARG:N	2.24	0.53
1:B:223:ARG:NH2	3:B:6078:HOH:O	2.42	0.53
1:B:555:ALA:HB3	1:B:569:LYS:HB3	1.90	0.53
1:A:402:ASN:HA	1:A:430:PHE:CZ	2.45	0.52
1:A:385:LEU:HD22	1:A:424:PHE:HB3	1.91	0.52
1:A:354:LEU:HD23	1:A:618:VAL:HG11	1.92	0.52
1:B:458:THR:O	1:B:462:LYS:HE3	2.09	0.52
1:B:52:LEU:O	1:B:54:LYS:N	2.42	0.52
1:B:535:LEU:HD12	1:B:589:ILE:HD11	1.92	0.52
1:B:642:VAL:CG2	1:B:700:SER:HB3	2.40	0.52
1:B:217:VAL:HG22	1:B:338:TYR:HB3	1.92	0.51
1:A:14:VAL:HG21	1:A:110:GLN:NE2	2.26	0.51
1:A:551:ALA:HB3	1:A:573:PHE:HB2	1.92	0.51
1:A:629:ILE:HG21	1:A:717:VAL:HG22	1.92	0.51
1:B:575:VAL:CG1	1:B:583:LYS:HD3	2.30	0.51
1:A:117:ILE:HG21	1:A:130:TRP:CE2	2.46	0.51
1:A:158:ARG:HG2	1:A:174:ARG:NH2	2.26	0.51
1:A:704:LYS:HE2	1:A:722:ASP:OD1	2.11	0.51
1:B:103:TYR:HA	1:B:158:ARG:O	2.11	0.50
1:B:220:ILE:HG21	1:B:474:MET:CE	2.41	0.50
1:B:540:ARG:HA	1:B:582:PHE:HA	1.93	0.50
1:B:101:VAL:O	1:B:118:PRO:O	2.30	0.50
1:B:554:SER:HB3	1:B:607:PHE:HB2	1.92	0.50
1:A:128:GLY:HA2	1:A:150:PRO:CD	2.41	0.50
1:A:632:ILE:HD11	1:A:709:MET:HB2	1.92	0.50
1:A:224:SER:HB2	3:A:3058:HOH:O	2.11	0.50
1:B:715:ARG:HG2	1:B:716:HIS:N	2.25	0.50
1:B:402:ASN:HA	1:B:430:PHE:CE2	2.46	0.50
1:A:53:PHE:O	1:A:60:ASN:HB2	2.12	0.50
1:A:247:MET:HA	3:B:3004:HOH:O	2.11	0.50
1:B:211:VAL:HG23	1:B:467:LYS:HB2	1.93	0.50
1:B:255:PRO:HD2	3:B:3022:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ARG:NH1	1:B:408:ARG:CZ	2.74	0.50
1:B:53:PHE:O	1:B:60:ASN:HB2	2.11	0.50
1:A:165:THR:HB	1:A:166:PRO:HD2	1.93	0.49
1:B:211:VAL:CG2	1:B:467:LYS:HB2	2.42	0.49
1:B:609:THR:HG22	1:B:620:ALA:CB	2.41	0.49
1:A:237:THR:O	1:A:240:TYR:HB3	2.12	0.49
1:A:678:LYS:HD2	1:A:691:TRP:CD1	2.47	0.49
1:B:640:GLN:O	1:B:725:ILE:HA	2.12	0.49
1:A:260:ARG:HH11	1:A:410:GLY:HA3	1.78	0.49
1:B:443:THR:O	1:B:450:HIS:HA	2.12	0.49
1:B:672:VAL:HG11	1:B:705:LEU:HD21	1.92	0.49
1:B:260:ARG:HH12	1:B:408:ARG:CZ	2.24	0.49
1:B:342:HIS:ND1	1:B:434:GLU:OE2	2.44	0.49
1:A:364:LEU:O	1:A:366:LYS:HG2	2.13	0.49
1:A:684:ARG:H	1:A:684:ARG:HD2	1.77	0.49
1:B:200:GLU:HG2	1:B:469:ILE:HD11	1.93	0.49
1:B:54:LYS:O	1:B:55:GLU:O	2.30	0.49
1:A:548:THR:HB	1:A:613:ASN:HB2	1.94	0.49
1:A:641:VAL:HG12	1:A:642:VAL:O	2.13	0.49
1:A:700:SER:HA	1:A:725:ILE:HB	1.93	0.49
1:B:90:ARG:NH1	1:B:90:ARG:HG3	2.28	0.49
1:A:164:TRP:N	1:A:164:TRP:CD1	2.81	0.49
1:A:437:SER:HB2	1:A:460:ILE:CD1	2.36	0.49
1:B:211:VAL:HG22	1:B:467:LYS:CD	2.34	0.49
1:A:629:ILE:CG2	1:A:717:VAL:HG22	2.43	0.48
1:B:545:ASN:C	1:B:579:PRO:HG3	2.33	0.48
1:B:541:ASN:HB3	1:B:578:GLU:O	2.14	0.48
1:A:632:ILE:HG13	1:A:717:VAL:HG12	1.95	0.48
1:A:654:ASN:HB2	1:A:683:ILE:CG2	2.43	0.48
1:A:66:THR:HG21	1:A:75:ILE:HG22	1.96	0.48
1:B:185:ASN:ND2	1:B:188:CYS:HB2	2.28	0.48
1:A:517:ASN:HA	3:A:5040:HOH:O	2.13	0.48
1:A:93:ASP:O	1:A:97:ASP:HB2	2.14	0.48
1:B:705:LEU:O	1:B:706:ILE:HG13	2.14	0.48
1:A:339:PHE:O	1:A:460:ILE:HG23	2.14	0.47
1:A:186:PRO:HA	1:A:194:TYR:HA	1.96	0.47
1:A:220:ILE:HG21	1:A:474:MET:CE	2.44	0.47
1:B:539:PHE:N	1:B:539:PHE:CD1	2.82	0.47
1:A:498:LEU:HA	1:A:498:LEU:HD13	1.75	0.47
1:B:153:ILE:HG23	1:B:252:ARG:HB2	1.96	0.47
1:A:100:ARG:HB2	1:A:119:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ASP:O	1:B:346:ALA:HB3	2.14	0.47
1:B:402:ASN:HA	1:B:430:PHE:CZ	2.50	0.47
1:B:192:ALA:O	1:B:381:THR:HG23	2.13	0.47
1:B:356:GLU:HB2	1:B:446:LYS:HZ2	1.78	0.47
1:A:516:SER:O	1:A:517:ASN:HB2	2.15	0.47
1:A:81:SER:HA	1:A:146:ILE:O	2.15	0.47
1:A:567:GLU:OE2	1:A:570:LYS:HD3	2.14	0.47
1:A:642:VAL:HA	1:A:697:PRO:O	2.14	0.47
1:A:128:GLY:HA2	1:A:150:PRO:HD2	1.97	0.47
1:A:549:ILE:HG13	1:A:612:ILE:HD13	1.96	0.47
1:A:117:ILE:N	1:A:117:ILE:HD12	2.29	0.47
1:A:197:ASN:O	1:A:201:ARG:HG3	2.15	0.47
1:A:598:LEU:HD11	1:A:627:LEU:HD12	1.96	0.47
1:A:549:ILE:HG13	1:A:612:ILE:CD1	2.45	0.47
1:B:342:HIS:O	1:B:343:ASP:HB2	2.15	0.47
1:B:55:GLU:HB2	1:B:58:ASP:HB2	1.97	0.47
1:B:124:GLU:HB2	3:B:5056:HOH:O	2.14	0.47
1:B:64:HIS:CG	1:B:76:VAL:HG22	2.50	0.47
1:A:52:LEU:HD23	1:A:84:VAL:HG12	1.97	0.46
1:B:102:GLU:HB2	1:B:160:TYR:HB2	1.97	0.46
1:B:349:GLN:NE2	1:B:504:LYS:HG3	2.30	0.46
1:B:56:ARG:NH1	1:B:67:ASP:O	2.43	0.46
1:A:354:LEU:CD2	1:A:618:VAL:HG11	2.45	0.46
1:B:533:PHE:CE2	1:B:589:ILE:HG13	2.50	0.46
1:A:385:LEU:HB3	1:A:386:PRO:HD2	1.96	0.46
1:A:654:ASN:HB2	1:A:683:ILE:HG21	1.97	0.46
1:B:158:ARG:HG2	1:B:174:ARG:NH2	2.31	0.46
1:B:348:LEU:HA	1:B:437:SER:HB2	1.97	0.46
1:B:535:LEU:HD11	1:B:606:PHE:CE1	2.50	0.46
1:B:237:THR:O	1:B:240:TYR:HB3	2.15	0.46
1:B:380:MET:HG3	1:B:381:THR:O	2.14	0.46
1:B:549:ILE:HG21	1:B:610:ALA:HB1	1.96	0.46
1:A:297:ASP:O	1:A:301:GLU:HB2	2.15	0.46
1:B:240:TYR:OH	1:B:306:GLU:HG2	2.15	0.46
1:B:701:GLY:N	1:B:725:ILE:O	2.47	0.46
1:B:703:ARG:NE	1:B:703:ARG:HA	2.30	0.46
1:A:423:CYS:HB3	1:A:500:TYR:CD1	2.51	0.46
1:A:602:ALA:HB1	1:A:627:LEU:HB2	1.97	0.46
1:A:138:GLU:O	1:A:140:ARG:N	2.49	0.46
1:A:506:LEU:HD23	1:A:506:LEU:HA	1.64	0.46
1:B:44:PHE:CD1	1:B:44:PHE:N	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ARG:NH2	1:A:681:ARG:O	2.49	0.45
1:A:558:THR:HG22	1:A:564:PRO:HA	1.98	0.45
1:A:220:ILE:HD13	1:A:474:MET:HE1	1.98	0.45
1:B:333:ARG:HG2	1:B:392:TRP:CZ3	2.51	0.45
1:A:100:ARG:HE	1:A:100:ARG:HB3	1.63	0.45
1:A:107:ARG:HG2	1:A:107:ARG:O	2.15	0.45
1:A:590:GLN:HB3	1:A:593:GLU:HG3	1.98	0.45
1:A:29:VAL:O	1:A:29:VAL:HG13	2.16	0.45
1:A:580:LEU:N	1:A:580:LEU:HD12	2.32	0.45
1:A:43:GLU:HA	1:A:165:THR:CG2	2.47	0.45
1:B:542:ASN:O	1:B:580:LEU:HD23	2.15	0.45
1:B:419:HIS:HB2	1:B:421:HIS:HD2	1.82	0.45
1:B:623:LYS:HD3	3:B:6029:HOH:O	2.15	0.45
1:B:674:ARG:HG2	1:B:674:ARG:HH11	1.82	0.45
1:A:76:VAL:O	1:A:182:ILE:HA	2.17	0.45
1:A:352:ILE:HG21	1:A:441:TYR:CE1	2.52	0.45
1:B:549:ILE:CG2	1:B:610:ALA:HB1	2.46	0.45
1:B:54:LYS:HG2	1:B:74:LEU:HB2	1.98	0.45
1:B:575:VAL:HG12	1:B:577:LEU:CD1	2.47	0.45
1:A:483:PHE:CE2	1:A:489:GLU:HB2	2.52	0.44
1:B:174:ARG:NH2	1:B:179:ASP:OD1	2.50	0.44
1:A:337:ASN:ND2	1:A:464:ILE:HG12	2.32	0.44
1:A:573:PHE:HZ	1:A:587:VAL:CG2	2.30	0.44
1:B:310:ARG:HB3	1:B:311:TYR:CD1	2.51	0.44
1:B:532:ASP:OD2	1:B:590:GLN:HA	2.17	0.44
1:A:98:LEU:CD2	1:A:164:TRP:HB2	2.46	0.44
1:B:498:LEU:HD12	1:B:498:LEU:HA	1.84	0.44
1:B:153:ILE:HG22	1:B:154:VAL:N	2.32	0.44
1:B:635:LYS:HG3	1:B:649:THR:HB	1.99	0.44
1:A:674:ARG:HA	1:A:674:ARG:HD2	1.82	0.44
1:B:538:THR:HG22	1:B:584:LYS:HG3	2.00	0.44
1:A:77:ARG:HB3	1:A:185:ASN:HB2	1.99	0.44
1:A:602:ALA:O	1:A:626:VAL:HA	2.18	0.44
1:B:112:ASN:C	1:B:113:LYS:HG2	2.38	0.44
1:B:674:ARG:HG3	1:B:675:PRO:HD2	1.99	0.44
1:A:43:GLU:HA	1:A:165:THR:HG21	2.00	0.44
1:A:401:GLU:HA	1:A:406:MET:H	1.83	0.44
1:A:552:TYR:CD1	1:A:572:THR:HB	2.53	0.44
1:B:287:VAL:HB	1:B:292:TRP:CZ2	2.53	0.44
1:B:337:ASN:O	1:B:372:TYR:HA	2.17	0.44
1:A:154:VAL:HG21	1:A:184:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:VAL:HG12	1:A:529:LEU:N	2.33	0.43
1:B:235:LEU:HA	1:B:327:CYS:SG	2.58	0.43
1:A:639:THR:OG1	1:A:644:SER:HB3	2.18	0.43
1:A:79:GLY:HA2	1:A:148:SER:O	2.18	0.43
1:A:287:VAL:CG1	1:A:291:ALA:HB3	2.49	0.43
1:A:354:LEU:HD22	1:A:441:TYR:HB3	1.99	0.43
1:A:546:ARG:HA	1:A:577:LEU:O	2.18	0.43
1:A:559:PHE:CD2	1:B:10:GLY:HA2	2.53	0.43
1:B:193:VAL:HG22	1:B:331:PRO:HD2	2.00	0.43
1:B:275:LEU:HA	1:B:309:VAL:O	2.19	0.43
1:B:559:PHE:CD1	1:B:599:LEU:HD13	2.54	0.43
1:A:337:ASN:OD1	1:A:340:SER:HB2	2.18	0.43
1:A:44:PHE:HD2	1:A:90:ARG:NE	2.13	0.43
1:A:678:LYS:HD3	1:A:680:PHE:CZ	2.53	0.43
1:A:220:ILE:HG21	1:A:474:MET:HE1	2.00	0.43
1:A:355:GLU:N	1:A:359:ASN:O	2.52	0.43
1:B:229:GLN:HB2	1:B:327:CYS:HB2	2.01	0.43
1:B:333:ARG:HG2	1:B:392:TRP:CH2	2.54	0.43
1:A:587:VAL:HG12	1:A:588:LEU:N	2.34	0.43
1:B:637:ARG:NH2	1:B:647:THR:HG21	2.33	0.43
1:B:703:ARG:HB2	1:B:723:VAL:HG23	2.00	0.43
1:A:189:GLU:HA	1:A:194:TYR:CG	2.54	0.43
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.91	0.43
1:A:337:ASN:ND2	1:A:461:GLY:HA2	2.30	0.43
1:A:466:THR:O	1:A:475:MET:N	2.52	0.43
1:A:666:HIS:O	1:A:707:ALA:HA	2.19	0.43
1:B:126:GLN:HG2	1:B:129:LYS:HD3	2.01	0.43
1:A:107:ARG:C	1:A:109:PRO:HD3	2.39	0.42
1:A:43:GLU:HA	1:A:165:THR:HB	2.01	0.42
1:A:559:PHE:HD1	1:A:563:VAL:O	2.02	0.42
1:B:703:ARG:HE	1:B:703:ARG:HA	1.83	0.42
1:A:354:LEU:HA	1:A:354:LEU:HD12	1.74	0.42
1:A:709:MET:CE	1:A:717:VAL:HG21	2.49	0.42
1:B:166:PRO:HG2	1:B:167:TYR:CZ	2.53	0.42
1:A:342:HIS:ND1	1:A:434:GLU:OE2	2.52	0.42
1:A:559:PHE:HZ	1:B:8:PHE:CE1	2.36	0.42
1:B:143:ARG:HB2	1:B:143:ARG:HH11	1.83	0.42
1:A:684:ARG:N	1:A:684:ARG:HD2	2.35	0.42
1:A:399:PRO:HA	1:A:407:TYR:O	2.20	0.42
1:A:331:PRO:CG	1:A:379:TRP:HB3	2.34	0.42
1:A:543:SER:O	1:A:580:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:ARG:O	1:B:676:MET:HG3	2.20	0.42
1:A:193:VAL:HG13	1:A:331:PRO:HD2	2.01	0.42
1:A:445:LYS:HB2	1:A:449:THR:HB	2.00	0.42
1:A:449:THR:HG22	1:A:450:HIS:N	2.35	0.42
1:A:281:ASN:ND2	1:A:715:ARG:NH1	2.67	0.42
1:A:88:PHE:HE2	1:A:142:VAL:CG2	2.32	0.42
1:B:126:GLN:HE21	1:B:126:GLN:HA	1.84	0.42
1:B:310:ARG:HA	1:B:311:TYR:HA	1.87	0.42
1:B:45:LEU:HA	1:B:45:LEU:HD12	1.75	0.42
1:B:705:LEU:C	1:B:706:ILE:HG13	2.40	0.42
1:A:44:PHE:O	1:A:45:LEU:CB	2.66	0.42
1:A:654:ASN:O	1:A:686:ASN:HA	2.20	0.42
1:B:715:ARG:CG	1:B:716:HIS:N	2.82	0.42
1:A:424:PHE:HA	3:A:4006:HOH:O	2.20	0.42
1:B:350:MET:HE3	3:B:3025:HOH:O	2.19	0.42
1:A:64:HIS:CD2	1:A:76:VAL:HG12	2.55	0.42
1:B:158:ARG:HG2	1:B:174:ARG:CZ	2.50	0.42
1:B:401:GLU:HA	1:B:406:MET:N	2.35	0.42
1:B:363:LYS:O	1:B:366:LYS:HE2	2.20	0.41
1:A:174:ARG:NH2	1:A:179:ASP:OD1	2.53	0.41
1:A:264:ALA:HA	1:A:408:ARG:HG2	2.02	0.41
1:A:469:ILE:HD11	3:A:3080:HOH:O	2.19	0.41
1:A:558:THR:C	1:A:599:LEU:HD12	2.41	0.41
1:A:674:ARG:HG3	1:A:675:PRO:HD2	2.03	0.41
1:A:726:GLN:HE21	1:A:726:GLN:HA	1.85	0.41
1:B:325:LEU:HA	1:B:325:LEU:HD23	1.83	0.41
1:A:118:PRO:O	1:A:120:PRO:HD3	2.20	0.41
1:A:193:VAL:HG13	1:A:331:PRO:CD	2.51	0.41
1:A:557:ILE:HG13	1:A:568:PHE:CD1	2.56	0.41
1:B:12:ARG:HH11	1:B:12:ARG:CB	2.32	0.41
1:B:555:ALA:HB1	1:B:568:PHE:CZ	2.55	0.41
1:A:337:ASN:HD22	1:A:464:ILE:HG12	1.86	0.41
1:B:605:HIS:HD2	1:B:624:SER:OG	2.03	0.41
1:A:504:LYS:HB3	1:A:504:LYS:HE2	1.96	0.41
1:A:591:ALA:HA	1:A:594:TYR:CE2	2.56	0.41
1:A:656:LEU:HD12	1:A:660:LEU:HD21	2.03	0.41
1:B:335:VAL:HG21	1:B:377:GLU:HG3	2.03	0.41
1:B:42:GLN:OE1	1:B:44:PHE:HE1	2.04	0.41
1:B:600:GLU:OE2	1:B:715:ARG:HD2	2.21	0.41
1:A:223:ARG:NH2	3:A:5021:HOH:O	2.53	0.41
1:A:658:GLU:C	1:A:685:PRO:HG3	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:PRO:CB	1:B:725:ILE:HD13	2.51	0.41
1:B:425:GLN:HA	1:B:426:PHE:HA	1.79	0.41
1:A:226:SER:HB3	1:A:294:GLY:HA3	2.01	0.41
1:A:337:ASN:O	1:A:372:TYR:HA	2.21	0.41
1:A:217:VAL:HG11	1:A:339:PHE:CE2	2.56	0.41
1:B:307:ASN:HA	1:B:308:PRO:HD3	1.93	0.40
1:A:280:ASP:CG	1:A:280:ASP:O	2.60	0.40
1:A:442:ILE:HG12	1:A:452:VAL:HG12	2.03	0.40
1:A:563:VAL:HA	1:A:564:PRO:HD3	1.85	0.40
1:B:121:ILE:H	1:B:121:ILE:HD13	1.86	0.40
1:B:519:ASP:HB2	3:B:4008:HOH:O	2.19	0.40
1:B:137:ARG:HG3	1:B:137:ARG:HH11	1.86	0.40
1:B:45:LEU:HD22	1:B:97:ASP:HB3	2.02	0.40
1:A:709:MET:HE3	1:A:717:VAL:HG21	2.03	0.40
1:B:105:ILE:HG13	1:B:157:PHE:CD2	2.57	0.40
1:B:184:PHE:HD2	1:B:328:LEU:O	2.05	0.40
1:B:486:GLY:O	1:B:487:GLN:HG3	2.22	0.40
1:B:551:ALA:HA	1:B:610:ALA:HA	2.03	0.40
1:B:92:TYR:HD2	1:B:137:ARG:HD3	1.85	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	696/731 (95%)	617 (89%)	60 (9%)	19 (3%)	5 7
1	B	699/731 (96%)	620 (89%)	65 (9%)	14 (2%)	7 12
All	All	1395/1462 (95%)	1237 (89%)	125 (9%)	33 (2%)	6 9

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	139	ASP
1	B	45	LEU
1	B	55	GLU
1	B	600	GLU
1	A	54	LYS
1	A	55	GLU
1	A	56	ARG
1	A	270	ASP
1	A	273	GLY
1	A	281	ASN
1	A	296	VAL
1	A	410	GLY
1	B	53	PHE
1	B	219	ASP
1	B	284	ALA
1	B	314	CYS
1	B	406	MET
1	A	595	MET
1	A	600	GLU
1	B	54	LYS
1	B	268	ALA
1	A	217	VAL
1	A	284	ALA
1	A	365	THR
1	A	716	HIS
1	B	581	SER
1	B	613	ASN
1	A	60	ASN
1	A	386	PRO
1	B	172	THR
1	B	470	GLY
1	A	470	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	619/644 (96%)	563 (91%)	56 (9%)	9	19
1	B	621/644 (96%)	559 (90%)	62 (10%)	7	15
All	All	1240/1288 (96%)	1122 (90%)	118 (10%)	8	17

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	20	ASN
1	A	31	LEU
1	A	43	GLU
1	A	44	PHE
1	A	46	ASN
1	A	47	VAL
1	A	58	ASP
1	A	59	THR
1	A	72	ASN
1	A	76	VAL
1	A	96	ARG
1	A	100	ARG
1	A	137	ARG
1	A	143	ARG
1	A	165	THR
1	A	195	LEU
1	A	206	LEU
1	A	223	ARG
1	A	224	SER
1	A	259	SER
1	A	267	ASN
1	A	271	ASP
1	A	281	ASN
1	A	301	GLU
1	A	340	SER
1	A	354	LEU
1	A	355	GLU
1	A	357	ASP
1	A	364	LEU
1	A	386	PRO
1	A	404	ASP
1	A	408	ARG
1	A	431	VAL
1	A	451	VAL

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Mol	Chain	Res	Type
1	A	463	LEU
1	A	484	GLN
1	A	489	GLU
1	A	498	LEU
1	A	508	THR
1	A	520	MET
1	A	526	ASN
1	A	538	THR
1	A	545	ASN
1	A	553	LEU
1	A	556	ASN
1	A	572	THR
1	A	574	ASP
1	A	604	LEU
1	A	607	PHE
1	A	609	THR
1	A	616	ARG
1	A	640	GLN
1	A	661	ARG
1	A	674	ARG
1	A	721	LEU
1	B	12	ARG
1	B	20	ASN
1	B	25	ASP
1	B	43	GLU
1	B	58	ASP
1	B	59	THR
1	B	70	GLU
1	B	78	ARG
1	B	98	LEU
1	B	104	VAL
1	B	105	ILE
1	B	112	ASN
1	B	121	ILE
1	B	126	GLN
1	B	135	VAL
1	B	139	ASP
1	B	140	ARG
1	B	142	VAL
1	B	143	ARG
1	B	148	SER
1	B	172	THR

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Mol	Chain	Res	Type
1	B	174	ARG
1	B	193	VAL
1	B	196	ASP
1	B	206	LEU
1	B	217	VAL
1	B	223	ARG
1	B	235	LEU
1	B	301	GLU
1	B	303	ARG
1	B	340	SER
1	B	359	ASN
1	B	363	LYS
1	B	369	VAL
1	B	408	ARG
1	B	415	GLN
1	B	431	VAL
1	B	435	VAL
1	B	452	VAL
1	B	463	LEU
1	B	490	GLU
1	B	492	LEU
1	B	498	LEU
1	B	519	ASP
1	B	520	MET
1	B	525	GLU
1	B	526	ASN
1	B	529	LEU
1	B	535	LEU
1	B	540	ARG
1	B	542	ASN
1	B	553	LEU
1	B	573	PHE
1	B	576	THR
1	B	588	LEU
1	B	604	LEU
1	B	613	ASN
1	B	639	THR
1	B	640	GLN
1	B	674	ARG
1	B	713	SER
1	B	721	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	72	ASN
1	A	337	ASN
1	A	373	HIS
1	A	556	ASN
1	A	726	GLN
1	B	72	ASN
1	B	112	ASN
1	B	126	GLN
1	B	421	HIS
1	B	545	ASN
1	B	605	HIS
1	B	613	ASN
1	B	686	ASN
1	B	716	HIS

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 ⓘ

Of 8 ligands modelled in this entry, 8 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

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.