



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:55 PM UTC

PDB ID : 1GGU / pdb_00001ggu
Title : HUMAN FACTOR XIII WITH CALCIUM 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 : 1998-07-22
Resolution : 2.10 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

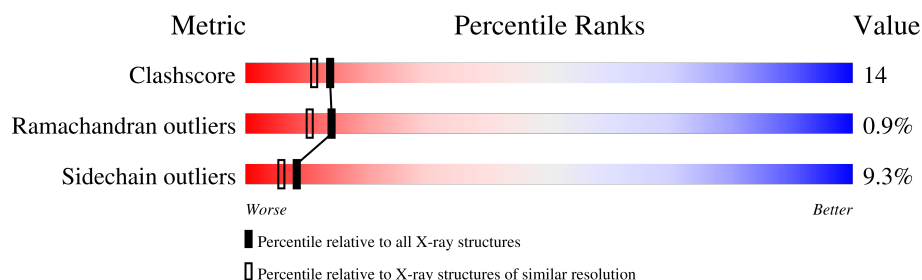
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	731	 58% 30% 7% . .
1	B	731	 62% 28% 5% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12297 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	701	Total	C	N	O	S	0	0	0
			5627	3571	967	1063	26			
1	B	707	Total	C	N	O	S	0	0	0
			5667	3595	975	1071	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	567	GLU	GLN	conflict	UNP P00488
B	567	GLU	GLN	conflict	UNP P00488

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	437	Total	O	0	0
			437	437		
3	B	564	Total	O	0	0
			564	564		



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	100.17Å 70.76Å 133.82Å 90.00° 106.11° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	91.9 (20.00-2.10)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.227 , 0.313	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12297	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.01	9/5760 (0.2%)	1.26	59/7817 (0.8%)
1	B	1.05	8/5800 (0.1%)	1.27	47/7871 (0.6%)
All	All	1.03	17/11560 (0.1%)	1.27	106/15688 (0.7%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	VAL	CA-CB	8.86	1.61	1.54
1	B	387	VAL	CA-CB	7.05	1.61	1.54
1	A	629	ILE	CA-CB	6.89	1.63	1.54
1	B	629	ILE	CA-CB	6.71	1.60	1.53
1	B	47	VAL	CA-CB	6.46	1.62	1.54
1	B	406	MET	SD-CE	6.40	1.95	1.79
1	B	520	MET	SD-CE	-6.27	1.63	1.79
1	B	136	MET	SD-CE	5.93	1.94	1.79
1	A	380	MET	SD-CE	-5.90	1.64	1.79
1	A	334	ILE	CA-CB	-5.88	1.47	1.54
1	B	650	VAL	CA-CB	5.62	1.60	1.54
1	A	265	MET	SD-CE	-5.59	1.65	1.79
1	A	634	ILE	CA-CB	5.42	1.60	1.54
1	B	18	ASN	CA-C	-5.36	1.46	1.52
1	A	555	ALA	CA-CB	-5.31	1.45	1.53
1	A	242	MET	SD-CE	-5.09	1.66	1.79
1	A	211	VAL	CA-CB	5.08	1.61	1.54

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	LEU	N-CA-C	-11.68	91.74	110.32
1	B	382	ARG	CA-C-N	9.47	129.12	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	ARG	C-N-CA	9.47	129.12	119.56
1	B	314	CYS	N-CA-C	9.22	122.17	111.11
1	B	196	ASP	N-CA-C	9.10	126.30	111.37
1	B	280	ASP	N-CA-C	8.30	123.13	112.92
1	B	595	MET	N-CA-C	8.14	120.95	111.02
1	A	504	LYS	CA-C-N	7.70	127.33	119.56
1	A	504	LYS	C-N-CA	7.70	127.33	119.56
1	B	9	GLY	N-CA-C	-7.48	95.45	113.18
1	A	469	ILE	N-CA-C	7.37	117.49	110.42
1	A	54	LYS	N-CA-C	7.25	121.84	112.92
1	B	488	GLU	N-CA-C	7.19	123.24	111.37
1	B	165	THR	N-CA-C	-7.17	97.77	109.82
1	A	683	ILE	N-CA-C	-7.16	98.15	108.17
1	B	597	GLN	N-CA-C	7.11	121.97	112.30
1	A	314	CYS	N-CA-C	7.05	119.57	111.11
1	B	682	GLU	N-CA-C	7.04	119.09	108.46
1	A	274	VAL	N-CA-C	6.92	117.53	110.82
1	B	613	ASN	N-CA-C	6.91	119.40	111.11
1	B	93	ASP	CA-C-N	6.83	128.37	119.84
1	B	93	ASP	C-N-CA	6.83	128.37	119.84
1	A	284	ALA	N-CA-C	6.73	122.41	111.37
1	A	111	GLU	CA-C-N	6.68	129.55	120.54
1	A	111	GLU	C-N-CA	6.68	129.55	120.54
1	B	351	ASP	N-CA-C	6.56	120.98	109.96
1	B	399	PRO	N-CA-C	6.56	121.81	111.38
1	A	559	PHE	N-CA-C	-6.54	101.10	110.59
1	B	54	LYS	N-CA-C	6.54	120.25	112.93
1	A	597	GLN	N-CA-C	6.49	122.28	113.97
1	B	557	ILE	N-CA-C	-6.48	99.25	108.58
1	B	284	ALA	N-CA-C	6.43	121.98	111.37
1	B	631	GLU	N-CA-C	6.38	118.26	110.41
1	A	96	ARG	N-CA-C	6.38	119.05	110.88
1	B	97	ASP	N-CA-C	6.38	119.01	109.25
1	A	86	ILE	CB-CA-C	-6.37	101.34	110.83
1	A	688	THR	N-CA-C	-6.36	99.84	109.95
1	B	465	VAL	N-CA-C	6.33	119.39	108.95
1	A	589	ILE	N-CA-C	-6.29	99.52	108.58
1	A	204	TYR	N-CA-C	6.24	120.15	112.54
1	A	440	ILE	CB-CA-C	-6.22	101.94	110.77
1	B	234	ILE	N-CA-C	6.20	116.94	110.62
1	A	436	ASN	N-CA-C	6.16	120.83	112.88
1	B	52	LEU	CA-C-N	-6.12	113.81	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	LEU	C-N-CA	-6.12	113.81	123.12
1	A	44	PHE	N-CA-C	6.06	120.67	113.28
1	A	557	ILE	N-CA-C	-6.05	99.87	108.58
1	B	674	ARG	N-CA-C	-6.02	101.45	110.24
1	A	128	GLY	N-CA-C	5.98	124.29	115.08
1	B	116	TYR	N-CA-C	-5.97	98.67	108.41
1	B	458	THR	N-CA-C	5.92	120.52	112.88
1	B	672	VAL	N-CA-C	-5.91	106.48	111.56
1	B	34	VAL	N-CA-C	5.89	121.59	109.34
1	A	646	MET	N-CA-C	-5.86	100.14	109.23
1	B	656	LEU	N-CA-C	5.81	118.04	110.43
1	A	52	LEU	N-CA-C	-5.76	99.86	109.24
1	B	487	GLN	N-CA-C	5.70	118.25	110.55
1	B	422	VAL	N-CA-C	5.70	120.11	112.98
1	B	90	ARG	CA-C-N	5.69	126.95	119.84
1	B	90	ARG	C-N-CA	5.69	126.95	119.84
1	A	524	VAL	N-CA-C	-5.65	101.67	109.46
1	B	474	MET	N-CA-C	5.63	119.00	109.76
1	A	500	TYR	N-CA-C	5.62	119.79	111.87
1	A	10	GLY	N-CA-C	5.60	125.19	115.62
1	A	118	PRO	N-CA-C	-5.59	100.96	112.47
1	A	389	PHE	N-CA-C	5.59	119.79	112.92
1	B	632	ILE	N-CA-C	-5.55	100.36	108.97
1	A	301	GLU	N-CA-C	-5.52	105.34	111.36
1	A	595	MET	N-CA-C	5.51	122.53	110.80
1	A	582	PHE	N-CA-C	-5.49	99.48	108.76
1	A	694	VAL	CB-CA-C	-5.48	105.99	111.80
1	A	488	GLU	N-CA-C	5.47	118.75	111.75
1	A	712	ASP	N-CA-C	-5.43	106.67	113.72
1	B	59	THR	N-CA-C	5.42	119.16	112.54
1	B	646	MET	N-CA-C	-5.41	99.86	109.06
1	A	619	LEU	N-CA-C	-5.37	100.15	108.90
1	A	330	ILE	N-CA-C	-5.34	101.79	107.77
1	A	340	SER	N-CA-C	5.34	117.43	108.73
1	A	624	SER	N-CA-C	-5.33	101.66	109.81
1	B	83	TYR	N-CA-C	5.32	118.48	109.76
1	A	656	LEU	N-CA-C	5.30	118.36	110.52
1	A	442	ILE	N-CA-C	5.29	115.73	108.12
1	B	92	TYR	N-CA-C	-5.28	102.57	110.23
1	A	275	LEU	N-CA-C	5.27	117.49	108.90
1	A	407	TYR	N-CA-C	5.27	116.99	109.14
1	A	90	ARG	CA-C-N	-5.26	114.54	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ARG	C-N-CA	-5.26	114.54	119.85
1	B	206	LEU	N-CA-C	5.25	119.74	113.23
1	A	196	ASP	N-CA-C	5.23	121.94	110.80
1	A	465	VAL	N-CA-C	5.23	117.58	108.90
1	A	465	VAL	N-CA-CB	-5.23	102.69	112.36
1	B	626	VAL	N-CA-C	-5.23	100.67	108.46
1	A	505	PRO	N-CA-C	5.22	120.39	113.86
1	A	146	ILE	CB-CA-C	-5.19	104.48	110.91
1	A	287	VAL	CA-C-N	-5.18	115.93	119.66
1	A	287	VAL	C-N-CA	-5.18	115.93	119.66
1	B	614	GLU	N-CA-C	5.18	117.67	111.71
1	A	566	ALA	N-CA-C	5.18	116.94	108.76
1	A	151	LYS	N-CA-C	-5.17	106.29	112.59
1	B	44	PHE	N-CA-C	5.14	119.70	113.38
1	A	520	MET	N-CA-C	-5.10	101.62	109.52
1	A	206	LEU	N-CA-C	5.09	119.65	113.38
1	A	161	VAL	N-CA-C	-5.05	100.85	108.12
1	A	75	ILE	N-CA-C	-5.04	100.27	107.78
1	A	644	SER	N-CA-C	5.04	117.27	108.76
1	B	196	ASP	CB-CA-C	-5.03	102.49	110.84

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	5627	0	5478	170	0
1	B	5667	0	5512	159	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	437	0	0	14	0
3	B	564	0	0	14	0
All	All	12297	0	10990	320	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 14.

All (320) 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:331:PRO:HG2	1:A:379:TRP:HB3	1.26	1.13
1:A:633:ILE:HB	1:A:651:GLU:HB3	1.51	0.89
1:B:44:PHE:O	1:B:45:LEU:HB2	1.74	0.86
1:A:520:MET:HB2	1:A:619:LEU:HD13	1.59	0.83
1:B:137:ARG:HG3	1:B:137:ARG:HH11	1.44	0.82
1:B:31:LEU:HD22	1:B:167:TYR:O	1.82	0.79
1:A:443:THR:HB	1:A:451:VAL:HG13	1.64	0.78
1:A:567:GLU:HG2	1:A:570:LYS:HD2	1.64	0.76
1:A:354:LEU:HD23	1:A:618:VAL:HG11	1.68	0.76
1:A:518:VAL:HG12	1:A:619:LEU:HD11	1.69	0.74
1:B:520:MET:HE1	1:B:621:LYS:HB2	1.70	0.73
1:A:44:PHE:O	1:A:45:LEU:HB2	1.86	0.73
1:B:674:ARG:HD2	1:B:675:PRO:HD2	1.71	0.73
1:A:612:ILE:HG22	1:A:613:ASN:H	1.53	0.73
1:A:136:MET:HB3	1:A:143:ARG:HB3	1.70	0.72
1:B:604:LEU:HB2	1:B:625:THR:HG22	1.69	0.72
1:A:605:HIS:CE1	1:A:622:GLN:HE21	2.08	0.71
1:B:12:ARG:HD3	3:B:6149:HOH:O	1.90	0.71
1:A:185:ASN:ND2	1:A:188:CYS:HB2	2.06	0.70
1:B:548:THR:HG22	1:B:613:ASN:ND2	2.07	0.70
1:B:548:THR:HG22	1:B:613:ASN:HD22	1.59	0.68
1:A:46:ASN:OD1	1:A:89:SER:HB3	1.95	0.67
1:A:666:HIS:O	1:A:707:ALA:HA	1.94	0.67
1:A:660:LEU:O	1:A:682:GLU:HA	1.95	0.67
1:B:704:LYS:HD2	1:B:720:GLU:OE1	1.96	0.65
1:A:211:VAL:HG22	1:A:467:LYS:HB2	1.79	0.65
1:A:634:ILE:HB	1:A:721:LEU:HB2	1.79	0.65
1:B:425:GLN:HG2	3:B:6139:HOH:O	1.95	0.64
1:A:549:ILE:HG22	1:A:550:THR:N	2.11	0.64
1:A:648:VAL:O	1:A:692:GLU:HA	1.98	0.64
1:B:625:THR:HG21	3:B:6217:HOH:O	1.98	0.64
1:B:100:ARG:HB2	1:B:119:VAL:O	1.98	0.64
1:A:528:VAL:HB	1:A:531:LYS:HG3	1.80	0.64
1:A:559:PHE:HD2	1:B:8:PHE:CE2	2.16	0.63
1:A:663:VAL:HA	1:A:711:SER:HA	1.80	0.63
1:A:605:HIS:HE1	1:A:622:GLN:HE21	1.46	0.63
1:A:659:THR:HG22	1:A:685:PRO:HD3	1.80	0.63
1:B:359:ASN:HD21	1:B:570:LYS:HE3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:MET:HE1	1:A:367:ASP:O	1.98	0.62
1:A:518:VAL:CG1	1:A:619:LEU:HD11	2.29	0.62
1:B:546:ARG:NH1	1:B:546:ARG:HG3	2.14	0.62
1:A:569:LYS:CD	1:A:589:ILE:HD12	2.28	0.62
1:A:629:ILE:HG13	1:A:630:PRO:HD2	1.81	0.62
1:A:335:VAL:HG22	1:A:477:ILE:HD11	1.81	0.62
1:B:516:SER:N	3:B:6294:HOH:O	2.32	0.62
1:B:443:THR:HB	1:B:451:VAL:HG13	1.81	0.62
1:A:637:ARG:HG2	1:A:638:GLY:N	2.15	0.62
1:A:516:SER:O	1:A:517:ASN:HB2	1.99	0.62
1:A:721:LEU:HD23	3:A:6314:HOH:O	1.99	0.62
1:B:247:MET:HE3	1:B:257:LYS:HG2	1.81	0.61
1:A:268:ALA:HA	1:A:273:GLY:HA3	1.82	0.61
1:A:682:GLU:CD	1:A:684:ARG:HE	2.08	0.61
1:A:282:ILE:HG13	1:A:283:TYR:N	2.15	0.61
1:A:569:LYS:HD3	1:A:589:ILE:HD12	1.82	0.61
1:A:623:LYS:HD2	3:A:6156:HOH:O	2.00	0.60
1:B:546:ARG:HG3	1:B:546:ARG:HH11	1.67	0.60
1:B:620:ALA:O	1:B:621:LYS:HG2	2.02	0.60
1:B:709:MET:HE1	1:B:714:LEU:HG	1.83	0.60
1:B:424:PHE:HB2	3:B:6348:HOH:O	2.02	0.60
1:A:162:ALA:HB3	1:A:164:TRP:CZ3	2.36	0.59
1:B:437:SER:HB2	1:B:460:ILE:HD13	1.83	0.59
1:B:128:GLY:HA2	1:B:150:PRO:HD3	1.84	0.59
1:A:443:THR:HB	1:A:451:VAL:CG1	2.31	0.59
1:A:559:PHE:CD2	1:B:8:PHE:HE2	2.21	0.59
1:A:174:ARG:NH2	1:A:179:ASP:OD1	2.37	0.58
1:B:538:THR:HB	1:B:584:LYS:HG2	1.84	0.58
1:B:549:ILE:CG2	1:B:610:ALA:HB1	2.33	0.58
1:A:95:ARG:NH1	1:A:96:ARG:NH1	2.52	0.58
1:A:604:LEU:HB2	1:A:625:THR:HG22	1.84	0.58
1:B:494:LEU:HD22	1:B:494:LEU:O	2.04	0.58
1:B:573:PHE:CE2	1:B:585:GLU:HG3	2.39	0.58
1:A:12:ARG:HH22	1:B:406:MET:HE1	1.69	0.57
1:B:193:VAL:HG13	1:B:331:PRO:HD3	1.84	0.57
1:A:529:LEU:HD11	1:A:598:LEU:CD1	2.34	0.57
1:A:664:TRP:CD2	1:A:679:MET:HB2	2.39	0.57
1:B:213:PHE:CE1	1:B:474:MET:HB3	2.39	0.57
1:B:648:VAL:O	1:B:692:GLU:HA	2.04	0.57
1:B:527:ALA:HB2	1:B:533:PHE:HB3	1.85	0.57
1:A:418:LYS:HD2	1:A:480:THR:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ARG:HA	1:A:703:ARG:NE	2.20	0.56
1:A:313:GLN:H	1:A:316:VAL:HB	1.69	0.56
1:B:137:ARG:HH11	1:B:137:ARG:CG	2.16	0.56
1:B:385:LEU:HD22	1:B:424:PHE:HB3	1.88	0.56
1:A:95:ARG:HG2	1:A:96:ARG:HD3	1.87	0.56
1:A:287:VAL:CG1	1:A:291:ALA:HB3	2.35	0.56
1:A:354:LEU:CD2	1:A:618:VAL:HG11	2.36	0.56
1:B:553:LEU:HD23	1:B:608:VAL:CG2	2.36	0.56
1:A:355:GLU:HG3	1:A:359:ASN:O	2.04	0.56
1:A:541:ASN:ND2	1:A:579:PRO:HA	2.21	0.56
1:A:559:PHE:HD2	1:B:8:PHE:HE2	1.54	0.56
1:B:31:LEU:HA	1:B:168:GLY:HA3	1.88	0.56
1:A:382:ARG:NH2	1:A:425:GLN:O	2.39	0.56
1:B:549:ILE:HG22	1:B:550:THR:N	2.21	0.55
1:B:715:ARG:HG2	1:B:716:HIS:N	2.21	0.55
1:B:465:VAL:HG21	1:B:474:MET:SD	2.46	0.55
1:B:382:ARG:NH2	1:B:411:PRO:O	2.39	0.54
1:B:553:LEU:O	1:B:570:LYS:HD2	2.08	0.54
1:B:679:MET:HG2	1:B:680:PHE:N	2.22	0.54
1:B:12:ARG:HD2	1:B:16:PRO:HD3	1.90	0.54
1:A:55:GLU:HG3	1:A:57:TRP:CH2	2.42	0.54
1:A:287:VAL:HG12	1:A:288:PRO:O	2.08	0.54
1:B:139:ASP:O	1:B:140:ARG:HB2	2.06	0.54
1:A:559:PHE:CD2	1:B:8:PHE:CE2	2.95	0.54
1:A:100:ARG:HG2	1:A:164:TRP:CZ3	2.43	0.54
1:A:605:HIS:CE1	1:A:622:GLN:NE2	2.77	0.53
1:B:26:LEU:HD11	1:B:104:VAL:HG11	1.89	0.53
1:B:68:LYS:HE2	1:B:206:LEU:HG	1.91	0.53
1:A:305:SER:O	1:A:306:GLU:HB2	2.06	0.53
1:A:95:ARG:O	1:A:96:ARG:HD2	2.08	0.53
1:A:559:PHE:HB2	1:B:8:PHE:HE2	1.72	0.53
1:B:537:ILE:HD12	1:B:573:PHE:CZ	2.44	0.53
1:A:459:HIS:HA	1:A:462:LYS:HE3	1.90	0.53
1:A:541:ASN:HB2	1:A:577:LEU:HD13	1.90	0.53
1:A:678:LYS:HD2	1:A:691:TRP:CD1	2.44	0.53
1:A:281:ASN:HD21	1:A:600:GLU:HG2	1.74	0.52
1:A:335:VAL:O	1:A:374:CYS:HA	2.09	0.52
1:B:679:MET:HE1	1:B:681:ARG:HD3	1.92	0.52
1:B:664:TRP:O	1:B:709:MET:HA	2.09	0.52
1:A:653:THR:O	1:A:655:PRO:HD3	2.10	0.52
1:B:650:VAL:HG22	1:B:691:TRP:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ASN:H	1:B:72:ASN:HD22	1.55	0.52
1:A:425:GLN:HB2	1:A:426:PHE:CD2	2.45	0.52
1:B:549:ILE:HG12	1:B:612:ILE:HG12	1.92	0.52
1:B:541:ASN:O	1:B:580:LEU:HA	2.09	0.51
1:B:284:ALA:HB3	3:B:6521:HOH:O	2.10	0.51
1:B:528:VAL:HB	1:B:531:LYS:HG3	1.93	0.51
1:A:663:VAL:HG13	1:A:709:MET:SD	2.51	0.51
1:A:720:GLU:HG3	3:A:6312:HOH:O	2.09	0.51
1:B:140:ARG:NH1	3:B:6420:HOH:O	2.42	0.51
1:B:553:LEU:O	1:B:570:LYS:HA	2.11	0.51
1:B:636:VAL:HB	1:B:646:MET:HE3	1.92	0.51
1:A:331:PRO:HG2	1:A:379:TRP:CB	2.19	0.51
1:A:538:THR:CG2	1:A:582:PHE:CZ	2.93	0.51
1:A:612:ILE:HG22	1:A:613:ASN:N	2.24	0.51
1:B:558:THR:HG22	1:B:564:PRO:HA	1.92	0.51
1:B:662:ASN:N	1:B:662:ASN:HD22	2.07	0.51
1:B:533:PHE:CE1	1:B:589:ILE:HG13	2.46	0.51
1:A:12:ARG:HH22	1:B:406:MET:CE	2.24	0.51
1:A:154:VAL:HG21	1:A:184:PHE:CE2	2.46	0.51
1:A:158:ARG:HG2	1:A:174:ARG:CZ	2.41	0.51
1:A:189:GLU:HA	1:A:194:TYR:CD1	2.46	0.50
1:A:353:PHE:CD2	1:A:364:LEU:HB3	2.46	0.50
1:A:356:GLU:O	1:A:611:ARG:NE	2.44	0.50
1:B:652:PHE:CZ	1:B:709:MET:HE2	2.46	0.50
1:A:189:GLU:HA	1:A:194:TYR:CG	2.46	0.50
1:B:56:ARG:HD3	3:B:6081:HOH:O	2.10	0.50
1:A:14:VAL:HG12	3:A:6244:HOH:O	2.11	0.50
1:B:452:VAL:HG13	1:B:452:VAL:O	2.11	0.50
1:A:112:ASN:HB2	3:A:6073:HOH:O	2.11	0.50
1:A:296:VAL:HG21	3:A:6212:HOH:O	2.12	0.49
1:B:136:MET:HB3	1:B:143:ARG:HB3	1.94	0.49
1:A:198:GLU:OE1	1:A:201:ARG:NH1	2.45	0.49
1:B:86:ILE:HD12	1:B:144:LEU:HD11	1.93	0.49
1:B:18:ASN:C	1:B:18:ASN:HD22	2.21	0.49
1:A:128:GLY:HA2	1:A:150:PRO:CD	2.42	0.49
1:A:683:ILE:HG12	1:A:689:VAL:HG11	1.94	0.49
1:A:516:SER:N	3:A:6284:HOH:O	2.45	0.49
1:A:209:ILE:HG12	1:A:670:PRO:CG	2.42	0.49
1:A:44:PHE:O	1:A:45:LEU:CB	2.58	0.49
1:A:51:HIS:HB2	1:A:85:GLN:HB3	1.94	0.49
1:B:526:ASN:HB3	3:B:6198:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ASP:O	1:B:95:ARG:N	2.46	0.49
1:A:552:TYR:O	1:A:608:VAL:HA	2.13	0.49
1:B:331:PRO:HB2	1:B:379:TRP:HB3	1.94	0.49
1:A:568:PHE:HB2	1:A:593:GLU:O	2.13	0.48
1:A:573:PHE:HE1	3:A:6168:HOH:O	1.96	0.48
1:B:454:ASN:ND2	3:B:6060:HOH:O	2.46	0.48
1:B:716:HIS:CE1	3:B:6556:HOH:O	2.66	0.48
1:A:337:ASN:OD1	1:A:461:GLY:HA2	2.13	0.48
1:B:26:LEU:HD12	1:B:160:TYR:CE2	2.48	0.48
1:A:102:GLU:HA	1:A:117:ILE:O	2.13	0.48
1:A:196:ASP:HB2	3:A:6125:HOH:O	2.13	0.48
1:B:137:ARG:HG2	1:B:142:VAL:HG12	1.95	0.48
1:B:537:ILE:HD12	1:B:573:PHE:HZ	1.78	0.48
1:A:313:GLN:OE1	1:A:315:TRP:CH2	2.66	0.48
1:A:68:LYS:HG3	3:A:6049:HOH:O	2.13	0.48
1:B:490:GLU:O	1:B:490:GLU:HG2	2.14	0.48
1:B:551:ALA:HA	1:B:610:ALA:HA	1.96	0.48
1:A:535:LEU:HD23	1:A:536:SER:N	2.29	0.48
1:B:397:SER:HA	1:B:408:ARG:HB3	1.94	0.48
1:A:634:ILE:HD12	1:A:720:GLU:HA	1.96	0.48
1:A:297:ASP:N	1:A:297:ASP:OD1	2.46	0.47
1:B:117:ILE:HG21	1:B:130:TRP:CE2	2.49	0.47
1:A:640:GLN:HG2	1:A:646:MET:SD	2.54	0.47
1:B:350:MET:HE2	1:B:350:MET:HB2	1.83	0.47
1:A:81:SER:HA	1:A:146:ILE:O	2.13	0.47
1:B:418:LYS:NZ	1:B:479:ASP:O	2.39	0.47
1:A:339:PHE:HA	1:A:370:TRP:O	2.15	0.47
1:B:213:PHE:CD1	1:B:222:THR:HG22	2.48	0.47
1:A:224:SER:HB3	1:A:706:ILE:HD11	1.96	0.47
1:A:520:MET:HE2	1:A:520:MET:HB3	1.69	0.47
1:B:81:SER:HA	1:B:146:ILE:O	2.14	0.47
1:A:652:PHE:O	1:A:688:THR:HA	2.15	0.47
1:A:90:ARG:HH11	1:A:90:ARG:HG3	1.79	0.47
1:B:268:ALA:HA	1:B:273:GLY:HA3	1.96	0.47
1:B:402:ASN:HD21	1:B:407:TYR:HB2	1.80	0.46
1:B:633:ILE:HB	1:B:651:GLU:HG3	1.97	0.46
1:B:553:LEU:HD23	1:B:608:VAL:HG22	1.96	0.46
1:A:358:GLY:O	1:A:609:THR:HB	2.15	0.46
1:B:703:ARG:HB2	1:B:723:VAL:HG23	1.97	0.46
1:A:683:ILE:HD11	1:A:689:VAL:HG21	1.98	0.46
1:B:128:GLY:HA2	1:B:150:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:VAL:N	1:A:170:LEU:O	2.42	0.46
1:A:45:LEU:HD22	1:A:97:ASP:CG	2.40	0.46
1:A:354:LEU:O	1:A:443:THR:HA	2.15	0.46
1:A:538:THR:HG21	1:A:582:PHE:CZ	2.49	0.46
1:B:705:LEU:O	1:B:720:GLU:HA	2.15	0.46
1:A:153:ILE:HD11	1:A:250:SER:HA	1.98	0.46
1:B:339:PHE:HA	1:B:370:TRP:O	2.16	0.46
1:B:706:ILE:HG21	3:B:6430:HOH:O	2.16	0.46
1:A:8:PHE:CE2	1:B:559:PHE:CD1	3.04	0.46
1:B:559:PHE:HD1	1:B:599:LEU:HD13	1.79	0.46
1:A:128:GLY:HA2	1:A:150:PRO:HD3	1.98	0.46
1:B:660:LEU:O	1:B:682:GLU:HA	2.15	0.46
1:A:667:LEU:HA	1:A:706:ILE:O	2.16	0.45
1:A:418:LYS:HE3	1:A:479:ASP:O	2.16	0.45
1:B:541:ASN:HB2	1:B:577:LEU:HD13	1.98	0.45
1:B:709:MET:HE3	1:B:717:VAL:HB	1.99	0.45
1:B:715:ARG:HG2	1:B:716:HIS:H	1.81	0.45
1:A:296:VAL:HB	3:A:6019:HOH:O	2.15	0.45
1:B:591:ALA:HA	1:B:594:TYR:CE2	2.52	0.45
1:B:297:ASP:OD1	1:B:297:ASP:N	2.49	0.45
1:A:162:ALA:HB3	1:A:164:TRP:HZ3	1.79	0.45
1:A:726:GLN:O	1:A:727:ARG:HB3	2.17	0.45
1:B:197:ASN:ND2	1:B:200:GLU:OE1	2.42	0.45
1:B:496:THR:O	1:B:499:MET:HG2	2.17	0.45
1:A:213:PHE:CE1	1:A:474:MET:HB2	2.52	0.44
1:A:355:GLU:O	1:A:611:ARG:NH2	2.49	0.44
1:A:520:MET:SD	1:A:608:VAL:HG12	2.57	0.44
1:B:153:ILE:HD11	1:B:250:SER:HA	2.00	0.44
1:B:444:ALA:HA	1:B:450:HIS:HD2	1.82	0.44
1:A:703:ARG:HA	1:A:703:ARG:HE	1.81	0.44
1:A:98:LEU:HG	1:A:164:TRP:HB2	1.99	0.44
1:A:247:MET:HE3	1:A:257:LYS:HG2	1.99	0.44
1:A:591:ALA:O	1:A:595:MET:HG2	2.17	0.44
1:A:629:ILE:HG13	1:A:717:VAL:HG22	2.00	0.44
1:A:709:MET:SD	1:A:709:MET:C	3.00	0.44
1:A:642:VAL:HG21	1:A:700:SER:HB3	1.99	0.44
1:B:213:PHE:CZ	1:B:474:MET:HB3	2.53	0.44
1:B:568:PHE:CE2	1:B:604:LEU:HG	2.52	0.44
1:B:679:MET:HB3	1:B:679:MET:HE2	1.82	0.44
1:B:213:PHE:CE1	1:B:222:THR:HG22	2.51	0.44
1:B:706:ILE:CG2	3:B:6430:HOH:O	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PRO:HB3	1:A:139:ASP:O	2.18	0.44
1:B:363:LYS:O	1:B:366:LYS:HD3	2.18	0.43
1:B:377:GLU:HB3	1:B:392:TRP:CE3	2.53	0.43
1:B:557:ILE:CD1	1:B:568:PHE:HB3	2.48	0.43
1:A:123:SER:O	1:A:133:LYS:HG3	2.18	0.43
1:A:162:ALA:HB1	1:A:169:VAL:CG1	2.48	0.43
1:B:342:HIS:ND1	1:B:434:GLU:OE2	2.50	0.43
1:B:90:ARG:NH1	1:B:97:ASP:OD2	2.52	0.43
1:B:93:ASP:C	1:B:95:ARG:H	2.25	0.43
1:A:664:TRP:CE3	1:A:679:MET:HB2	2.53	0.43
1:B:104:VAL:HG12	1:B:116:TYR:HD1	1.84	0.43
1:A:549:ILE:CG2	1:A:550:THR:N	2.78	0.43
1:B:516:SER:N	1:B:617:ASP:OD2	2.52	0.43
1:B:544:HIS:C	1:B:579:PRO:HB3	2.44	0.43
1:A:221:LYS:HA	1:A:221:LYS:HD2	1.73	0.43
1:A:697:PRO:HG3	1:A:725:ILE:HD12	2.00	0.43
1:B:557:ILE:HD12	1:B:568:PHE:HD2	1.83	0.43
1:A:681:ARG:HG3	1:A:681:ARG:HH11	1.84	0.42
1:B:44:PHE:O	1:B:45:LEU:CB	2.54	0.42
1:A:51:HIS:HB3	3:A:6432:HOH:O	2.18	0.42
1:B:197:ASN:ND2	1:B:197:ASN:H	2.17	0.42
1:B:518:VAL:HB	1:B:612:ILE:HD11	2.01	0.42
1:B:519:ASP:HB3	1:B:540:ARG:HD2	2.01	0.42
1:B:652:PHE:CE2	1:B:709:MET:HE2	2.55	0.42
1:A:204:TYR:O	1:A:326:ARG:HG2	2.18	0.42
1:A:490:GLU:O	1:A:490:GLU:HG2	2.19	0.42
1:B:642:VAL:CG2	1:B:700:SER:HB3	2.49	0.42
1:B:700:SER:HA	1:B:725:ILE:HG22	2.00	0.42
1:A:95:ARG:CG	1:A:96:ARG:HH11	2.32	0.42
1:B:650:VAL:HG11	1:B:667:LEU:HD13	2.01	0.42
1:A:636:VAL:HG12	1:A:648:VAL:HG22	2.01	0.42
1:B:353:PHE:CD2	1:B:364:LEU:HB3	2.54	0.42
1:B:557:ILE:HD12	1:B:568:PHE:CD2	2.54	0.42
1:A:589:ILE:HD13	1:A:589:ILE:N	2.35	0.42
1:A:639:THR:O	1:A:646:MET:HB3	2.19	0.42
1:B:642:VAL:HG11	1:B:727:ARG:HH22	1.85	0.42
1:A:555:ALA:HA	1:A:605:HIS:O	2.20	0.42
1:A:662:ASN:HB2	1:A:712:ASP:OD1	2.20	0.42
1:B:310:ARG:HA	1:B:311:TYR:HA	1.81	0.42
1:B:565:LYS:HB3	1:B:565:LYS:HE2	1.71	0.42
1:B:641:VAL:HG22	1:B:726:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:THR:HG21	1:B:299:LEU:HB3	2.01	0.42
1:A:187:TRP:NE1	1:A:201:ARG:HD2	2.34	0.42
1:A:310:ARG:HA	1:A:311:TYR:HA	1.91	0.42
1:A:350:MET:HE3	1:A:350:MET:HB3	1.58	0.42
1:B:440:ILE:HG23	1:B:440:ILE:HD12	1.71	0.42
1:B:549:ILE:CG2	1:B:550:THR:N	2.82	0.42
1:A:678:LYS:HD2	1:A:691:TRP:NE1	2.35	0.41
1:B:187:TRP:CE2	1:B:201:ARG:HD3	2.55	0.41
1:B:472:ASP:OD2	1:B:704:LYS:NZ	2.53	0.41
1:B:556:ASN:HD22	1:B:567:GLU:HA	1.85	0.41
1:B:642:VAL:HG11	1:B:727:ARG:NH2	2.35	0.41
1:B:468:GLN:HG2	1:B:473:GLY:C	2.45	0.41
1:A:235:LEU:HA	1:A:327:CYS:SG	2.60	0.41
1:A:193:VAL:HG13	1:A:331:PRO:HD3	2.01	0.41
1:A:303:ARG:HG2	3:A:6281:HOH:O	2.21	0.41
1:A:548:THR:HG22	1:A:576:THR:HG23	2.03	0.41
1:B:393:GLN:HB3	1:B:411:PRO:HB2	2.01	0.41
1:A:559:PHE:HB2	1:B:8:PHE:CE2	2.54	0.41
1:A:77:ARG:HB3	1:A:185:ASN:HB2	2.02	0.41
1:A:194:TYR:HB3	3:A:6320:HOH:O	2.20	0.41
1:A:269:LYS:O	1:A:270:ASP:HB2	2.21	0.41
1:B:93:ASP:C	1:B:95:ARG:N	2.79	0.41
1:B:679:MET:CE	1:B:681:ARG:HD3	2.51	0.41
1:B:45:LEU:HG	1:B:88:PHE:CD1	2.56	0.41
1:A:313:GLN:OE1	1:A:315:TRP:HH2	2.04	0.40
1:B:611:ARG:HE	1:B:611:ARG:HB3	1.46	0.40
1:A:185:ASN:HD22	1:A:188:CYS:HB2	1.82	0.40
1:A:600:GLU:O	1:A:601:GLN:HB2	2.22	0.40
1:A:636:VAL:HG11	1:A:646:MET:CE	2.52	0.40
1:B:197:ASN:H	1:B:197:ASN:HD22	1.68	0.40
1:B:293:THR:HA	3:B:6430:HOH:O	2.20	0.40
1:B:341:ALA:HB2	1:B:460:ILE:HD13	2.03	0.40
1:B:137:ARG:CG	1:B:137:ARG:NH1	2.82	0.40
1:A:186:PRO:HG2	1:A:205:VAL:HG21	2.03	0.40
1:A:353:PHE:HA	1:A:442:ILE:O	2.22	0.40
1:B:30:GLU:O	1:B:168:GLY:HA3	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	695/731 (95%)	644 (93%)	44 (6%)	7 (1%)	12	9
1	B	701/731 (96%)	662 (94%)	34 (5%)	5 (1%)	18	15
All	All	1396/1462 (96%)	1306 (94%)	78 (6%)	12 (1%)	14	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	B	45	LEU
1	A	281	ASN
1	A	270	ASP
1	A	196	ASP
1	A	681	ARG
1	A	711	SER
1	A	612	ILE
1	B	34	VAL
1	B	686	ASN
1	B	470	GLY
1	B	94	PRO

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	618/644 (96%)	563 (91%)	55 (9%)	9	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	621/644 (96%)	561 (90%)	60 (10%)	8	5
All	All	1239/1288 (96%)	1124 (91%)	115 (9%)	8	6

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	47	VAL
1	A	86	ILE
1	A	104	VAL
1	A	112	ASN
1	A	124	GLU
1	A	135	VAL
1	A	136	MET
1	A	174	ARG
1	A	193	VAL
1	A	195	LEU
1	A	206	LEU
1	A	211	VAL
1	A	221	LYS
1	A	223	ARG
1	A	271	ASP
1	A	281	ASN
1	A	282	ILE
1	A	289	PRO
1	A	297	ASP
1	A	301	GLU
1	A	335	VAL
1	A	347	ASN
1	A	350	MET
1	A	354	LEU
1	A	364	LEU
1	A	368	SER
1	A	369	VAL
1	A	386	PRO
1	A	415	GLN
1	A	455	VAL
1	A	460	ILE
1	A	463	LEU
1	A	465	VAL
1	A	491	ARG
1	A	498	LEU

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Mol	Chain	Res	Type
1	A	516	SER
1	A	523	GLU
1	A	525	GLU
1	A	534	LYS
1	A	553	LEU
1	A	570	LYS
1	A	572	THR
1	A	587	VAL
1	A	597	GLN
1	A	604	LEU
1	A	618	VAL
1	A	625	THR
1	A	629	ILE
1	A	637	ARG
1	A	661	ARG
1	A	681	ARG
1	A	684	ARG
1	A	694	VAL
1	A	721	LEU
1	B	12	ARG
1	B	14	VAL
1	B	18	ASN
1	B	42	GLN
1	B	47	VAL
1	B	72	ASN
1	B	76	VAL
1	B	98	LEU
1	B	112	ASN
1	B	137	ARG
1	B	138	GLU
1	B	151	LYS
1	B	167	TYR
1	B	169	VAL
1	B	172	THR
1	B	174	ARG
1	B	176	PRO
1	B	193	VAL
1	B	195	LEU
1	B	206	LEU
1	B	212	ILE
1	B	223	ARG
1	B	235	LEU

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Mol	Chain	Res	Type
1	B	239	LEU
1	B	304	SER
1	B	359	ASN
1	B	408	ARG
1	B	451	VAL
1	B	455	VAL
1	B	463	LEU
1	B	465	VAL
1	B	468	GLN
1	B	482	LYS
1	B	484	GLN
1	B	488	GLU
1	B	489	GLU
1	B	494	LEU
1	B	498	LEU
1	B	507	ASN
1	B	519	ASP
1	B	520	MET
1	B	531	LYS
1	B	538	THR
1	B	546	ARG
1	B	557	ILE
1	B	571	GLU
1	B	578	GLU
1	B	588	LEU
1	B	589	ILE
1	B	604	LEU
1	B	611	ARG
1	B	625	THR
1	B	626	VAL
1	B	637	ARG
1	B	639	THR
1	B	650	VAL
1	B	656	LEU
1	B	661	ARG
1	B	721	LEU
1	B	727	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS

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Mol	Chain	Res	Type
1	A	112	ASN
1	A	185	ASN
1	A	267	ASN
1	A	281	ASN
1	A	421	HIS
1	A	526	ASN
1	A	544	HIS
1	A	597	GLN
1	A	605	HIS
1	A	622	GLN
1	A	640	GLN
1	A	666	HIS
1	B	18	ASN
1	B	42	GLN
1	B	72	ASN
1	B	112	ASN
1	B	126	GLN
1	B	267	ASN
1	B	359	ASN
1	B	415	GLN
1	B	450	HIS
1	B	454	ASN
1	B	468	GLN
1	B	484	GLN
1	B	545	ASN
1	B	556	ASN
1	B	613	ASN
1	B	662	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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.