



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:39 AM UTC

PDB ID : 1QRK / pdb_00001qrk
Title : HUMAN FACTOR XIII WITH STRONTIUM BOUND IN THE ION SITE
Authors : Fox, B.A.; Yee, V.C.; Pederson, L.C.; Le Trong, I.; Bishop, P.D.; Stenkamp, R.E.; Teller, D.C.
Deposited on : 1999-06-14
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

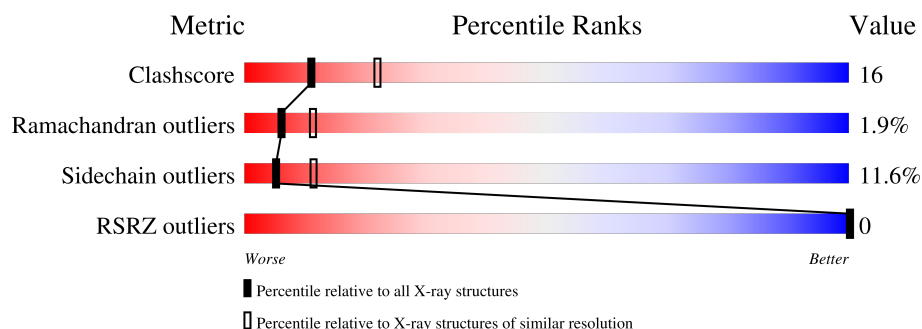
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11492 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	700	Total	C	N	O	S	0	0	0
			5610	3557	966	1061	26			
1	B	705	Total	C	N	O	S	0	0	0
			5650	3583	973	1068	26			

There are 2 discrepancies between the modelled and reference sequences:

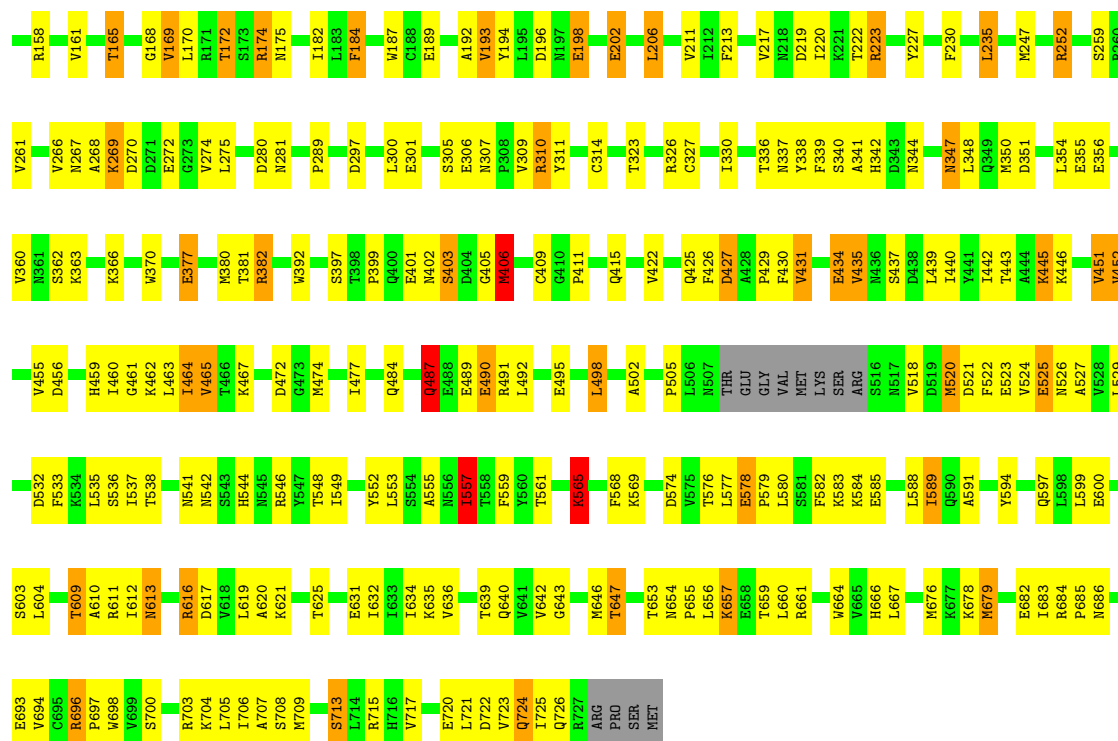
Chain	Residue	Modelled	Actual	Comment	Reference
A	651	GLU	GLN	conflict	UNP P00488
B	651	GLU	GLN	conflict	UNP P00488

- Molecule 2 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	B	115	Total	O	0	0
			115	115		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.90Å 72.32Å 135.03Å 90.00° 105.90° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 10.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	78.5 (10.00-2.50) 77.2 (10.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.183 , 0.275 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 74.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11492	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.72	2/5741 (0.0%)	1.10	37/7792 (0.5%)
1	B	0.73	0/5782	1.13	39/7847 (0.5%)
All	All	0.72	2/11523 (0.0%)	1.11	76/15639 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	380	MET	SD-CE	-7.35	1.61	1.79
1	A	309	VAL	CA-CB	5.12	1.61	1.54

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	ARG	CA-C-N	10.58	131.47	120.04
1	B	382	ARG	C-N-CA	10.58	131.47	120.04
1	A	175	ASN	CA-C-N	9.54	129.64	119.05
1	A	175	ASN	C-N-CA	9.54	129.64	119.05
1	A	285	TYR	N-CA-C	8.60	121.88	110.88
1	B	196	ASP	N-CA-C	8.23	122.99	113.19
1	B	170	LEU	N-CA-C	-8.21	95.53	108.90
1	A	458	THR	N-CA-C	8.00	121.83	112.72
1	A	674	ARG	N-CA-C	-7.69	98.84	110.07
1	B	117	ILE	CA-C-N	7.63	126.90	118.97
1	B	117	ILE	C-N-CA	7.63	126.90	118.97
1	B	43	GLU	N-CA-C	-7.55	101.14	110.65
1	B	194	TYR	N-CA-C	7.50	121.20	109.96
1	B	464	ILE	N-CA-C	-7.32	97.87	108.11
1	B	121	ILE	N-CA-C	-7.04	100.50	109.58
1	A	170	LEU	N-CA-C	-6.97	97.85	109.07
1	A	565	LYS	N-CA-C	-6.94	104.81	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	ASN	CA-C-N	6.84	126.86	119.89
1	B	307	ASN	C-N-CA	6.84	126.86	119.89
1	A	52	LEU	N-CA-C	-6.62	99.88	110.14
1	B	44	PHE	N-CA-C	6.51	121.35	113.41
1	A	353	PHE	N-CA-C	6.50	119.43	107.99
1	B	78	ARG	N-CA-C	6.40	119.06	110.35
1	A	672	VAL	N-CA-C	-6.34	106.61	111.62
1	A	559	PHE	N-CA-C	-6.32	102.38	110.53
1	B	274	VAL	N-CA-C	6.31	116.46	110.53
1	B	434	GLU	N-CA-C	-6.27	104.33	112.23
1	B	597	GLN	N-CA-C	6.27	117.80	110.41
1	B	175	ASN	CA-C-N	6.21	126.11	119.28
1	B	175	ASN	C-N-CA	6.21	126.11	119.28
1	B	266	VAL	N-CA-C	6.14	116.92	110.72
1	B	565	LYS	N-CA-C	-6.05	105.81	113.43
1	B	559	PHE	N-CA-C	-6.01	101.88	110.59
1	A	600	GLU	N-CA-C	5.97	123.52	110.80
1	B	314	CYS	N-CA-C	5.93	123.42	110.80
1	B	198	GLU	N-CA-C	5.92	118.50	111.33
1	B	487	GLN	N-CA-C	5.91	123.38	110.80
1	A	266	VAL	N-CA-C	5.82	116.01	110.42
1	A	553	LEU	N-CA-C	-5.77	100.00	109.40
1	B	532	ASP	N-CA-C	-5.77	102.76	110.55
1	A	638	GLY	N-CA-C	5.72	117.33	111.56
1	A	282	ILE	CB-CA-C	-5.69	105.09	111.80
1	B	165	THR	N-CA-C	-5.66	101.90	110.50
1	A	722	ASP	N-CA-C	5.63	118.50	110.68
1	A	436	ASN	N-CA-C	5.62	121.02	113.72
1	B	355	GLU	N-CA-C	-5.58	103.33	110.53
1	A	442	ILE	CB-CA-C	-5.58	102.85	110.77
1	B	631	GLU	N-CA-C	5.54	118.62	110.59
1	A	503	LYS	N-CA-C	5.53	117.91	108.90
1	A	417	ILE	CB-CA-C	-5.51	104.82	111.88
1	B	557	ILE	N-CA-C	-5.50	101.62	108.89
1	B	351	ASP	N-CA-C	5.47	117.65	108.73
1	A	204	TYR	N-CA-C	5.47	119.57	113.01
1	A	465	VAL	N-CA-C	5.42	116.84	108.44
1	B	452	VAL	N-CA-C	5.42	115.06	107.37
1	B	377	GLU	N-CA-C	-5.41	100.08	108.90
1	B	269	LYS	N-CA-C	-5.39	101.01	109.25
1	A	578	GLU	N-CA-C	-5.38	102.21	110.07
1	A	631	GLU	N-CA-C	5.34	116.81	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	718	TYR	N-CA-C	5.31	117.46	109.23
1	B	280	ASP	N-CA-C	5.26	119.54	113.18
1	B	184	PHE	N-CA-C	-5.23	103.58	110.43
1	A	314	CYS	N-CA-C	5.22	119.93	111.37
1	B	146	ILE	CB-CA-C	-5.21	104.44	110.91
1	A	107	ARG	N-CA-C	5.17	119.86	113.50
1	A	663	VAL	N-CA-C	5.15	116.16	108.54
1	B	472	ASP	N-CA-C	5.11	119.23	113.15
1	A	152	CYS	N-CA-C	5.09	117.61	110.23
1	B	323	THR	N-CA-C	-5.09	105.63	111.07
1	A	24	ASP	CA-C-N	-5.07	116.03	122.77
1	A	24	ASP	C-N-CA	-5.07	116.03	122.77
1	A	563	VAL	N-CA-C	5.05	112.98	108.63
1	A	408	ARG	N-CA-C	-5.04	103.87	110.53
1	A	118	PRO	N-CA-C	-5.03	102.35	110.55
1	A	464	ILE	N-CA-C	-5.02	101.25	108.53
1	A	105	ILE	N-CA-C	5.00	115.92	108.46

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	5610	0	5467	168	0
1	B	5650	0	5495	199	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	115	0	0	1	0
3	B	115	0	0	4	0
All	All	11492	0	10962	365	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 (365) 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	1.46	0.97
1:B:544:HIS:HA	1:B:579:PRO:HB3	1.52	0.90
1:B:44:PHE:O	1:B:45:LEU:HB2	1.73	0.87
1:A:709:MET:HB3	1:A:717:VAL:HB	1.58	0.85
1:B:591:ALA:HA	1:B:594:TYR:CE2	2.15	0.82
1:A:128:GLY:HA2	1:A:150:PRO:HD2	1.61	0.81
1:A:198:GLU:O	1:A:202:GLU:HG3	1.80	0.81
1:A:632:ILE:HD11	1:A:709:MET:HB2	1.64	0.79
1:B:90:ARG:HG3	1:B:90:ARG:HH11	1.50	0.76
1:B:527:ALA:HB2	1:B:533:PHE:HB3	1.66	0.76
1:A:100:ARG:HG2	1:A:164:TRP:HE1	1.51	0.75
1:B:435:VAL:HG21	1:B:464:ILE:HD11	1.69	0.75
1:A:128:GLY:HA2	1:A:150:PRO:CD	2.16	0.75
1:B:647:THR:HG23	1:B:694:VAL:HG22	1.69	0.74
1:A:443:THR:HG23	1:A:451:VAL:HG13	1.70	0.74
1:B:697:PRO:CB	1:B:725:ILE:HD13	2.19	0.73
1:B:443:THR:HB	1:B:451:VAL:HG13	1.70	0.73
1:B:632:ILE:HD11	1:B:709:MET:HB2	1.71	0.73
1:B:657:LYS:HE2	1:B:686:ASN:HD21	1.55	0.72
1:A:442:ILE:HG12	1:A:452:VAL:HG12	1.72	0.72
1:A:290:SER:HB3	1:A:716:HIS:HD2	1.56	0.70
1:B:52:LEU:O	1:B:54:LYS:N	2.25	0.70
1:B:440:ILE:HD12	1:B:455:VAL:HG12	1.74	0.70
1:B:642:VAL:HG21	1:B:700:SER:HB3	1.73	0.69
1:B:128:GLY:HA2	1:B:150:PRO:HD3	1.74	0.69
1:A:220:ILE:HG21	1:A:474:MET:HE2	1.74	0.69
1:A:193:VAL:HG13	1:A:331:PRO:HD2	1.74	0.68
1:A:656:LEU:HD12	1:A:660:LEU:HD21	1.75	0.67
1:A:635:LYS:HG3	1:A:649:THR:HB	1.75	0.67
1:B:703:ARG:NE	1:B:703:ARG:HA	2.09	0.67
1:A:402:ASN:HA	1:A:430:PHE:CZ	2.29	0.66
1:A:551:ALA:HB3	1:A:573:PHE:HB2	1.78	0.66
1:B:542:ASN:O	1:B:580:LEU:HD23	1.96	0.66
1:B:97:ASP:O	1:B:98:LEU:HD12	1.96	0.65
1:B:656:LEU:HD12	1:B:660:LEU:HD21	1.79	0.65
1:A:541:ASN:HB2	1:A:577:LEU:HD13	1.79	0.64
1:A:206:LEU:O	1:A:230:PHE:HE2	1.78	0.64
1:A:636:VAL:HG12	1:A:648:VAL:HG22	1.78	0.64
1:A:498:LEU:HA	1:A:502:ALA:HB3	1.79	0.64
1:B:213:PHE:CD2	1:B:222:THR:HG22	2.33	0.64
1:B:642:VAL:CG2	1:B:700:SER:HB3	2.28	0.63
1:A:653:THR:HG23	1:A:688:THR:OG1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:LYS:NZ	1:B:445:LYS:HB3	2.13	0.63
1:A:154:VAL:HG21	1:A:184:PHE:CE2	2.33	0.62
1:B:68:LYS:HG3	1:B:230:PHE:CE1	2.34	0.62
1:B:544:HIS:CA	1:B:579:PRO:HB3	2.25	0.62
1:A:290:SER:HB3	1:A:716:HIS:CD2	2.35	0.62
1:A:653:THR:O	1:A:655:PRO:HD3	1.99	0.62
1:B:549:ILE:HG23	1:B:610:ALA:HB1	1.82	0.62
1:B:247:MET:HA	3:B:1032:HOH:O	2.00	0.61
1:B:235:LEU:HA	1:B:327:CYS:SG	2.40	0.61
1:B:337:ASN:HD21	1:B:461:GLY:HA2	1.65	0.61
1:B:524:VAL:HG11	1:B:625:THR:HG21	1.83	0.61
1:A:98:LEU:HD23	1:A:164:TRP:HB2	1.83	0.60
1:A:521:ASP:OD1	1:A:621:LYS:HE2	2.01	0.60
1:B:90:ARG:HG3	1:B:90:ARG:NH1	2.16	0.60
1:A:630:PRO:HG3	1:A:655:PRO:HG3	1.82	0.60
1:B:223:ARG:NH2	3:B:6078:HOH:O	2.33	0.60
1:A:377:GLU:HA	1:A:393:GLN:O	2.02	0.60
1:A:487:GLN:HB3	1:A:489:GLU:HG2	1.84	0.59
1:B:139:ASP:HB2	3:B:2023:HOH:O	2.03	0.59
1:B:213:PHE:O	1:B:336:THR:HG21	2.01	0.59
1:B:439:LEU:HB2	1:B:456:ASP:HB3	1.85	0.59
1:B:54:LYS:HG3	1:B:55:GLU:H	1.67	0.59
1:B:697:PRO:HB2	1:B:725:ILE:HD13	1.82	0.59
1:B:522:PHE:CD2	1:B:535:LEU:HD21	2.38	0.59
1:A:64:HIS:CD2	1:A:76:VAL:HG12	2.37	0.59
1:B:487:GLN:OE1	1:B:487:GLN:HA	2.02	0.58
1:A:484:GLN:H	1:A:487:GLN:NE2	1.99	0.58
1:A:280:ASP:O	1:A:282:ILE:N	2.36	0.58
1:A:468:GLN:CD	1:A:473:GLY:HA3	2.29	0.58
1:A:529:LEU:HD21	1:A:598:LEU:CD1	2.33	0.57
1:B:676:MET:HE1	1:B:693:GLU:HG3	1.87	0.57
1:B:17:ASN:ND2	1:B:115:THR:HG21	2.18	0.57
1:B:342:HIS:ND1	1:B:434:GLU:OE2	2.36	0.57
1:B:281:ASN:OD1	1:B:600:GLU:HG3	2.04	0.57
1:B:636:VAL:HG11	1:B:723:VAL:HG11	1.86	0.57
1:A:100:ARG:HG2	1:A:164:TRP:NE1	2.19	0.57
1:B:154:VAL:HG21	1:B:184:PHE:CD2	2.40	0.57
1:B:616:ARG:HD2	1:B:616:ARG:O	2.05	0.57
1:A:353:PHE:O	1:A:361:ASN:HB3	2.05	0.57
1:A:385:LEU:HD22	1:A:424:PHE:HB3	1.86	0.56
1:B:30:GLU:HB3	1:B:169:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:667:LEU:HD23	1:B:676:MET:HE2	1.86	0.56
1:A:107:ARG:O	1:A:107:ARG:HG2	2.04	0.56
1:A:634:ILE:HD12	1:A:720:GLU:HA	1.88	0.56
1:B:490:GLU:HG3	1:B:491:ARG:N	2.18	0.56
1:B:522:PHE:HB3	1:B:537:ILE:HG23	1.87	0.56
1:A:281:ASN:ND2	1:A:715:ARG:NH1	2.53	0.56
1:B:47:VAL:HG12	1:B:88:PHE:CE1	2.41	0.55
1:B:65:HIS:O	1:B:68:LYS:HD2	2.06	0.55
1:B:101:VAL:O	1:B:118:PRO:O	2.25	0.55
1:B:685:PRO:O	1:B:686:ASN:HB2	2.06	0.55
1:A:484:GLN:HG2	1:A:487:GLN:HG3	1.88	0.55
1:A:658:GLU:C	1:A:685:PRO:HG3	2.32	0.55
1:A:189:GLU:HA	1:A:194:TYR:CG	2.42	0.55
1:B:442:ILE:HG12	1:B:452:VAL:HG12	1.88	0.55
1:A:154:VAL:HG21	1:A:184:PHE:CD2	2.42	0.55
1:B:705:LEU:O	1:B:720:GLU:HA	2.07	0.55
1:A:399:PRO:HA	1:A:407:TYR:O	2.06	0.55
1:A:508:THR:HB	1:A:511:VAL:HG21	1.87	0.54
1:B:350:MET:HB2	1:B:439:LEU:HD23	1.89	0.54
1:A:257:LYS:HG3	1:B:403:SER:O	2.07	0.54
1:B:600:GLU:HG2	1:B:715:ARG:HH11	1.72	0.54
1:B:659:THR:HG22	1:B:685:PRO:HD3	1.88	0.54
1:A:578:GLU:HB3	1:A:579:PRO:HD2	1.88	0.54
1:B:122:VAL:HG12	1:B:132:ALA:O	2.08	0.54
1:B:17:ASN:HD22	1:B:115:THR:HG21	1.73	0.53
1:A:103:TYR:OH	1:A:159:MET:HE2	2.08	0.53
1:A:530:GLY:HA2	1:A:595:MET:SD	2.48	0.53
1:A:591:ALA:HA	1:A:594:TYR:CE2	2.43	0.53
1:B:275:LEU:HD23	1:B:309:VAL:O	2.09	0.53
1:A:26:LEU:HD11	1:A:104:VAL:HG11	1.89	0.53
1:B:484:GLN:OE1	1:B:484:GLN:N	2.41	0.53
1:A:546:ARG:HB2	1:A:577:LEU:O	2.07	0.53
1:A:520:MET:HG2	1:A:521:ASP:N	2.24	0.53
1:A:633:ILE:HG22	1:A:651:GLU:HG2	1.91	0.53
1:B:211:VAL:HG22	1:B:467:LYS:HB2	1.91	0.53
1:B:704:LYS:HG3	1:B:705:LEU:H	1.74	0.53
1:B:338:TYR:O	1:B:339:PHE:HB2	2.09	0.52
1:A:64:HIS:HE1	1:A:80:GLN:HB3	1.74	0.52
1:B:657:LYS:HE2	1:B:686:ASN:ND2	2.23	0.52
1:A:361:ASN:ND2	1:A:364:LEU:HD22	2.25	0.52
1:A:116:TYR:CE2	1:A:118:PRO:HG3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:VAL:CG1	1:A:648:VAL:HG22	2.39	0.52
1:B:76:VAL:O	1:B:182:ILE:HA	2.10	0.52
1:A:24:ASP:O	1:A:158:ARG:NH2	2.42	0.52
1:B:724:GLN:N	1:B:724:GLN:CD	2.67	0.52
1:A:93:ASP:O	1:A:97:ASP:HB2	2.10	0.51
1:B:634:ILE:HD11	1:B:707:ALA:HB2	1.91	0.51
1:B:269:LYS:O	1:B:270:ASP:HB3	2.11	0.51
1:B:667:LEU:HD23	1:B:676:MET:CE	2.40	0.51
1:A:615:THR:O	1:A:616:ARG:HB2	2.11	0.51
1:A:666:HIS:HB2	1:A:708:SER:OG	2.09	0.51
1:B:445:LYS:HB3	1:B:445:LYS:HZ3	1.74	0.51
1:B:71:ASN:HB3	1:B:75:ILE:HD11	1.92	0.51
1:A:342:HIS:ND1	1:A:434:GLU:OE2	2.44	0.51
1:A:20:ASN:ND2	1:A:20:ASN:O	2.44	0.51
1:B:135:VAL:HG12	1:B:143:ARG:O	2.10	0.51
1:B:348:LEU:HD12	1:B:498:LEU:HD11	1.93	0.51
1:A:64:HIS:HE1	1:A:80:GLN:CB	2.25	0.51
1:A:280:ASP:C	1:A:282:ILE:H	2.20	0.50
1:A:401:GLU:HA	1:A:406:MET:H	1.75	0.50
1:A:528:VAL:HB	1:A:531:LYS:HD2	1.91	0.50
1:B:401:GLU:HA	1:B:406:MET:H	1.76	0.50
1:B:555:ALA:HB1	1:B:568:PHE:CZ	2.47	0.50
1:B:382:ARG:NH2	1:B:411:PRO:O	2.45	0.50
1:A:449:THR:HG22	1:A:450:HIS:H	1.77	0.50
1:B:697:PRO:HB3	1:B:725:ILE:HD13	1.92	0.50
1:B:54:LYS:O	1:B:55:GLU:O	2.29	0.50
1:A:197:ASN:O	1:A:201:ARG:HG3	2.12	0.50
1:A:674:ARG:HG3	1:A:675:PRO:HD2	1.94	0.50
1:A:64:HIS:CE1	1:A:80:GLN:HB3	2.47	0.49
1:A:442:ILE:HA	1:A:452:VAL:HA	1.94	0.49
1:B:541:ASN:HB2	1:B:577:LEU:HD23	1.93	0.49
1:B:704:LYS:HD3	1:B:722:ASP:OD1	2.12	0.49
1:A:602:ALA:O	1:A:626:VAL:HA	2.11	0.49
1:B:377:GLU:HB3	1:B:392:TRP:CE3	2.46	0.49
1:B:518:VAL:HG11	1:B:549:ILE:HD11	1.94	0.49
1:A:90:ARG:NH2	1:A:97:ASP:OD1	2.46	0.49
1:B:12:ARG:HG2	1:B:12:ARG:HH11	1.77	0.49
1:A:594:TYR:CD1	1:A:595:MET:N	2.81	0.49
1:B:435:VAL:CG2	1:B:464:ILE:HD11	2.40	0.49
1:B:139:ASP:O	1:B:140:ARG:HB2	2.12	0.49
1:B:64:HIS:O	1:B:77:ARG:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ASN:HB3	1:B:113:LYS:HG2	1.94	0.48
1:B:47:VAL:HG12	1:B:88:PHE:HE1	1.78	0.48
1:A:281:ASN:HD21	1:A:715:ARG:NH1	2.11	0.48
1:A:565:LYS:HB2	1:A:599:LEU:HD11	1.95	0.48
1:B:524:VAL:CG1	1:B:625:THR:HG21	2.42	0.48
1:A:162:ALA:HB1	1:A:169:VAL:CG1	2.43	0.48
1:B:213:PHE:CE2	1:B:222:THR:HG22	2.48	0.48
1:B:582:PHE:HD1	1:B:583:LYS:N	2.11	0.48
1:A:156:LYS:HD2	1:A:181:TYR:CZ	2.49	0.48
1:A:651:GLU:HB3	1:A:690:GLN:HG3	1.96	0.48
1:B:305:SER:O	1:B:306:GLU:HB2	2.13	0.48
1:B:348:LEU:HD11	1:B:502:ALA:HB1	1.95	0.48
1:A:122:VAL:CG2	1:A:125:LEU:HD23	2.44	0.48
1:B:247:MET:HE2	1:B:261:VAL:HG11	1.96	0.48
1:A:206:LEU:O	1:A:230:PHE:CE2	2.65	0.48
1:B:310:ARG:HB3	1:B:311:TYR:CD1	2.49	0.48
1:B:549:ILE:HA	1:B:611:ARG:O	2.14	0.48
1:A:703:ARG:HA	1:A:703:ARG:NE	2.29	0.47
1:A:213:PHE:CD2	1:A:222:THR:HG22	2.49	0.47
1:B:11:ARG:HG3	1:B:11:ARG:HH11	1.79	0.47
1:A:121:ILE:HG21	1:A:134:ILE:HD11	1.95	0.47
1:A:338:TYR:O	1:A:339:PHE:HB2	2.15	0.47
1:A:468:GLN:HA	1:A:475:MET:HE2	1.96	0.47
1:A:553:LEU:HD23	1:A:553:LEU:C	2.38	0.47
1:A:100:ARG:CG	1:A:164:TRP:HE1	2.24	0.47
1:B:706:ILE:HD12	1:B:706:ILE:N	2.29	0.47
1:A:663:VAL:O	1:A:679:MET:HA	2.14	0.47
1:A:702:HIS:ND1	1:A:702:HIS:C	2.72	0.47
1:B:703:ARG:HA	1:B:703:ARG:HE	1.78	0.47
1:B:704:LYS:HG3	1:B:705:LEU:N	2.30	0.47
1:A:186:PRO:HG3	1:A:205:VAL:HG21	1.97	0.47
1:B:664:TRP:CE2	1:B:679:MET:HG3	2.50	0.47
1:B:709:MET:HB3	1:B:717:VAL:HB	1.96	0.47
1:B:30:GLU:O	1:B:168:GLY:HA3	2.15	0.46
1:B:81:SER:HA	1:B:146:ILE:O	2.15	0.46
1:A:352:ILE:HG21	1:A:441:TYR:CE1	2.51	0.46
1:B:536:SER:HB3	1:B:584:LYS:HE3	1.97	0.46
1:B:696:ARG:NH2	1:B:698:TRP:HA	2.30	0.46
1:A:726:GLN:O	1:A:727:ARG:HB2	2.14	0.46
1:A:281:ASN:HD21	1:A:715:ARG:HH11	1.64	0.46
1:A:698:TRP:CD1	1:A:699:VAL:HG23	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:VAL:HG11	1:B:125:LEU:HD23	1.97	0.46
1:B:153:ILE:HG23	1:B:252:ARG:HB2	1.98	0.46
1:A:519:ASP:HB2	1:A:540:ARG:HB3	1.97	0.46
1:B:569:LYS:HE2	1:B:589:ILE:HD13	1.98	0.46
1:B:161:VAL:H	1:B:172:THR:HG1	1.62	0.46
1:B:267:ASN:OD1	1:B:399:PRO:HG3	2.15	0.46
1:B:529:LEU:HD11	1:B:656:LEU:CD2	2.45	0.46
1:B:636:VAL:HB	1:B:646:MET:CE	2.46	0.46
1:A:134:ILE:HG23	1:A:142:VAL:CG1	2.45	0.46
1:B:552:TYR:N	1:B:609:THR:O	2.47	0.46
1:B:54:LYS:O	1:B:55:GLU:C	2.60	0.45
1:B:71:ASN:CB	1:B:75:ILE:HD11	2.46	0.45
1:B:380:MET:HE2	1:B:380:MET:HB3	1.81	0.45
1:B:684:ARG:HB3	1:B:685:PRO:HD2	1.97	0.45
1:A:484:GLN:O	1:A:487:GLN:HB2	2.16	0.45
1:B:64:HIS:O	1:B:65:HIS:HB2	2.17	0.45
1:B:193:VAL:HG21	1:B:330:ILE:HG23	1.99	0.45
1:A:678:LYS:HD2	1:A:691:TRP:CD1	2.51	0.45
1:B:537:ILE:O	1:B:585:GLU:N	2.46	0.45
1:A:193:VAL:HG13	1:A:331:PRO:CD	2.44	0.45
1:B:122:VAL:N	1:B:132:ALA:O	2.45	0.45
1:B:603:SER:HA	1:B:625:THR:O	2.17	0.45
1:A:107:ARG:HD2	1:A:108:TYR:CZ	2.52	0.45
1:A:235:LEU:HA	1:A:327:CYS:SG	2.57	0.45
1:A:296:VAL:HB	3:A:6039:HOH:O	2.16	0.45
1:B:193:VAL:CG2	1:B:330:ILE:HG23	2.47	0.45
1:B:211:VAL:CG2	1:B:467:LYS:HB2	2.46	0.45
1:A:443:THR:HG22	1:A:453:GLU:HG2	1.99	0.45
1:B:348:LEU:HD12	1:B:498:LEU:CD1	2.46	0.45
1:B:525:GLU:O	1:B:525:GLU:HG3	2.17	0.45
1:B:600:GLU:HG2	1:B:715:ARG:NH1	2.32	0.45
1:A:556:ASN:N	1:A:556:ASN:ND2	2.65	0.44
1:B:422:VAL:HB	1:B:429:PRO:HG3	1.99	0.44
1:A:51:HIS:CE1	1:A:53:PHE:CD1	3.05	0.44
1:A:504:LYS:HE2	1:A:504:LYS:HB3	1.52	0.44
1:B:341:ALA:HB2	1:B:460:ILE:HD13	1.98	0.44
1:B:310:ARG:HB3	1:B:311:TYR:CE1	2.52	0.44
1:B:431:VAL:O	1:B:434:GLU:HB2	2.16	0.44
1:B:661:ARG:HA	1:B:682:GLU:HA	1.99	0.44
1:A:352:ILE:HG21	1:A:441:TYR:HE1	1.81	0.44
1:B:97:ASP:C	1:B:98:LEU:HD12	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:MET:HG3	1:B:381:THR:O	2.17	0.44
1:B:455:VAL:O	1:B:455:VAL:HG23	2.17	0.44
1:A:629:ILE:HG21	1:A:717:VAL:HG22	1.99	0.44
1:A:122:VAL:HG21	1:A:125:LEU:HD23	1.99	0.44
1:B:643:GLY:HA2	1:B:696:ARG:NE	2.32	0.44
1:A:354:LEU:CD2	1:A:618:VAL:HG11	2.47	0.44
1:B:666:HIS:HB2	1:B:708:SER:OG	2.18	0.44
1:B:14:VAL:HG22	1:B:15:PRO:O	2.18	0.44
1:B:520:MET:O	1:B:521:ASP:HB2	2.17	0.44
1:A:460:ILE:HD12	1:A:460:ILE:H	1.82	0.43
1:B:105:ILE:CG2	1:B:115:THR:HG22	2.48	0.43
1:B:548:THR:O	1:B:612:ILE:HA	2.17	0.43
1:B:42:GLN:HA	1:B:44:PHE:CE2	2.52	0.43
1:B:440:ILE:CD1	1:B:455:VAL:HG12	2.46	0.43
1:B:459:HIS:O	1:B:462:LYS:HG2	2.18	0.43
1:B:654:ASN:HB3	1:B:686:ASN:H	1.83	0.43
1:A:555:ALA:HB1	1:A:568:PHE:CE1	2.53	0.43
1:B:107:ARG:C	1:B:109:PRO:HD3	2.43	0.43
1:B:356:GLU:H	1:B:446:LYS:HZ2	1.67	0.43
1:A:422:VAL:HB	1:A:429:PRO:HG3	2.01	0.43
1:B:52:LEU:O	1:B:53:PHE:C	2.61	0.43
1:B:402:ASN:HA	1:B:430:PHE:CZ	2.53	0.43
1:A:158:ARG:HG2	1:A:174:ARG:NH2	2.34	0.43
1:A:666:HIS:O	1:A:707:ALA:HA	2.17	0.43
1:B:676:MET:HE3	1:B:676:MET:HB2	1.86	0.43
1:A:467:LYS:HE2	1:A:472:ASP:HA	2.01	0.43
1:B:646:MET:HB2	1:B:646:MET:HE3	1.72	0.43
1:A:90:ARG:HH22	1:A:97:ASP:CG	2.26	0.43
1:A:223:ARG:NH1	1:A:224:SER:O	2.52	0.43
1:B:193:VAL:O	1:B:193:VAL:HG13	2.17	0.43
1:B:653:THR:O	1:B:655:PRO:HD3	2.19	0.43
1:A:363:LYS:O	1:A:366:LYS:HE2	2.19	0.43
1:A:610:ALA:O	1:A:618:VAL:HA	2.18	0.43
1:B:158:ARG:HG2	1:B:174:ARG:NH2	2.33	0.43
1:A:418:LYS:HD2	1:A:480:THR:O	2.19	0.42
1:A:509:GLU:HB2	1:A:510:GLY:H	1.65	0.42
1:B:366:LYS:HD3	1:B:366:LYS:HA	1.78	0.42
1:A:268:ALA:HA	1:A:273:GLY:HA3	2.01	0.42
1:B:42:GLN:OE1	1:B:44:PHE:CE2	2.72	0.42
1:B:187:TRP:HH2	1:B:206:LEU:HD22	1.84	0.42
1:A:165:THR:HB	1:A:166:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:THR:HB	1:A:613:ASN:HB2	2.01	0.42
1:A:553:LEU:HD23	1:A:554:SER:N	2.35	0.42
1:B:131:GLY:HA3	3:B:6001:HOH:O	2.19	0.42
1:B:350:MET:HE3	1:B:350:MET:HB3	1.71	0.42
1:B:220:ILE:HG23	1:B:338:TYR:OH	2.20	0.42
1:B:518:VAL:O	1:B:619:LEU:HD11	2.19	0.42
1:A:132:ALA:HB1	1:A:144:LEU:HD22	2.02	0.42
1:A:263:SER:OG	1:A:408:ARG:HD3	2.18	0.42
1:A:380:MET:HB3	1:A:380:MET:HE2	1.72	0.42
1:A:556:ASN:N	1:A:556:ASN:HD22	2.17	0.42
1:A:418:LYS:HE3	1:A:479:ASP:O	2.19	0.42
1:A:578:GLU:HB2	1:A:581:SER:HB2	2.02	0.42
1:B:620:ALA:O	1:B:621:LYS:HG2	2.20	0.42
1:A:300:LEU:HD23	1:A:300:LEU:HA	1.76	0.42
1:B:134:ILE:HG23	1:B:142:VAL:CG1	2.50	0.42
1:B:370:TRP:HA	1:B:561:THR:O	2.20	0.42
1:B:546:ARG:NH1	1:B:578:GLU:OE2	2.53	0.42
1:B:557:ILE:HD12	1:B:568:PHE:CD1	2.55	0.42
1:B:659:THR:HG21	1:B:684:ARG:HH11	1.85	0.42
1:A:545:ASN:N	1:A:579:PRO:HB3	2.35	0.42
1:A:671:GLY:HA2	1:A:698:TRP:CE2	2.55	0.42
1:B:11:ARG:HG3	1:B:11:ARG:NH1	2.35	0.42
1:B:198:GLU:O	1:B:202:GLU:HB2	2.19	0.42
1:B:409:CYS:HB3	1:B:427:ASP:HB2	2.02	0.42
1:A:206:LEU:HD12	1:A:206:LEU:HA	1.91	0.41
1:A:216:GLU:OE2	1:A:218:ASN:HB2	2.20	0.41
1:B:29:VAL:CG1	1:B:31:LEU:HG	2.50	0.41
1:B:520:MET:HB2	1:B:520:MET:HE2	1.55	0.41
1:B:664:TRP:CZ3	1:B:679:MET:HB2	2.55	0.41
1:B:666:HIS:O	1:B:707:ALA:HA	2.19	0.41
1:B:565:LYS:HB2	1:B:599:LEU:HD11	2.01	0.41
1:B:660:LEU:HD22	1:B:713:SER:OG	2.20	0.41
1:B:425:GLN:HB2	1:B:426:PHE:CD2	2.56	0.41
1:A:428:ALA:N	1:A:429:PRO:CD	2.84	0.41
1:A:494:LEU:HG	1:A:498:LEU:HD23	2.02	0.41
1:A:402:ASN:HA	1:A:430:PHE:CE1	2.55	0.41
1:A:483:PHE:CD1	1:A:489:GLU:HG3	2.55	0.41
1:A:671:GLY:HA2	1:A:698:TRP:NE1	2.35	0.41
1:B:42:GLN:OE1	1:B:44:PHE:HE2	2.02	0.41
1:B:56:ARG:H	1:B:56:ARG:HG2	1.55	0.41
1:B:86:ILE:HD11	1:B:144:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:VAL:HG21	1:B:474:MET:SD	2.60	0.41
1:A:354:LEU:O	1:A:443:THR:HA	2.21	0.41
1:A:634:ILE:HD11	1:A:707:ALA:HB2	2.03	0.41
1:A:664:TRP:CE3	1:A:679:MET:HB2	2.56	0.41
1:A:234:ILE:HD13	1:A:300:LEU:HD21	2.03	0.41
1:A:498:LEU:HA	1:A:498:LEU:HD13	1.83	0.41
1:B:289:PRO:HD3	1:B:311:TYR:HB2	2.03	0.41
1:A:202:GLU:HA	1:A:206:LEU:HB2	2.02	0.41
1:A:354:LEU:HD23	1:A:618:VAL:HG11	2.03	0.41
1:A:400:GLN:O	1:A:406:MET:HA	2.21	0.41
1:A:568:PHE:HB2	1:A:593:GLU:O	2.21	0.41
1:B:344:ASN:O	1:B:347:ASN:HB2	2.21	0.41
1:B:676:MET:CE	1:B:693:GLU:HG3	2.50	0.41
1:A:165:THR:HG23	1:A:168:GLY:O	2.21	0.41
1:A:351:ASP:OD2	1:B:112:ASN:OD1	2.39	0.41
1:A:445:LYS:HB3	1:A:447:ASP:OD1	2.21	0.41
1:A:494:LEU:O	1:A:498:LEU:HD23	2.21	0.41
1:B:527:ALA:HB2	1:B:533:PHE:CB	2.43	0.41
1:B:549:ILE:CG2	1:B:610:ALA:HB1	2.48	0.41
1:B:609:THR:HG22	1:B:620:ALA:HB2	2.03	0.41
1:B:45:LEU:HD22	1:B:97:ASP:HB3	2.03	0.40
1:B:227:TYR:CD2	1:B:326:ARG:NH1	2.90	0.40
1:A:206:LEU:HD12	1:A:230:PHE:CZ	2.57	0.40
1:A:353:PHE:O	1:A:361:ASN:CB	2.69	0.40
1:A:654:ASN:CG	1:A:660:LEU:HG	2.46	0.40
1:B:60:ASN:O	1:B:61:LYS:C	2.65	0.40
1:B:300:LEU:HD23	1:B:300:LEU:HA	1.90	0.40
1:B:464:ILE:HG22	1:B:477:ILE:HG13	2.02	0.40
1:A:174:ARG:NH2	1:A:179:ASP:OD1	2.55	0.40
1:B:90:ARG:O	1:B:91:PRO:C	2.64	0.40
1:A:449:THR:HG22	1:A:450:HIS:N	2.36	0.40
1:A:543:SER:O	1:A:580:LEU:HD12	2.21	0.40
1:A:647:THR:HA	1:A:694:VAL:HA	2.04	0.40
1:B:192:ALA:O	1:B:381:THR:HG23	2.21	0.40
1:A:164:TRP:CD1	1:A:164:TRP:N	2.88	0.40
1:A:281:ASN:ND2	1:A:600:GLU:OE1	2.55	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	694/731 (95%)	631 (91%)	52 (8%)	11 (2%)	7	14
1	B	699/731 (96%)	613 (88%)	71 (10%)	15 (2%)	5	9
All	All	1393/1462 (95%)	1244 (89%)	123 (9%)	26 (2%)	6	11

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	GLU
1	A	281	ASN
1	B	45	LEU
1	B	53	PHE
1	B	55	GLU
1	B	613	ASN
1	A	139	ASP
1	A	470	GLY
1	B	56	ARG
1	B	219	ASP
1	B	505	PRO
1	A	509	GLU
1	A	613	ASN
1	B	487	GLN
1	A	10	GLY
1	A	296	VAL
1	A	472	ASP
1	B	268	ALA
1	B	362	SER
1	B	406	MET
1	A	136	MET
1	A	268	ALA
1	B	60	ASN
1	B	252	ARG
1	B	405	GLY

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Mol	Chain	Res	Type
1	B	91	PRO

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	616/644 (96%)	559 (91%)	57 (9%)	8	18
1	B	619/644 (96%)	533 (86%)	86 (14%)	3	7
All	All	1235/1288 (96%)	1092 (88%)	143 (12%)	5	11

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASP
1	A	47	VAL
1	A	58	ASP
1	A	59	THR
1	A	72	ASN
1	A	94	PRO
1	A	104	VAL
1	A	112	ASN
1	A	123	SER
1	A	140	ARG
1	A	165	THR
1	A	174	ARG
1	A	193	VAL
1	A	195	LEU
1	A	199	LYS
1	A	206	LEU
1	A	211	VAL
1	A	223	ARG
1	A	259	SER
1	A	290	SER
1	A	293	THR
1	A	340	SER

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Mol	Chain	Res	Type
1	A	354	LEU
1	A	364	LEU
1	A	387	VAL
1	A	397	SER
1	A	398	THR
1	A	403	SER
1	A	425	GLN
1	A	431	VAL
1	A	451	VAL
1	A	454	ASN
1	A	463	LEU
1	A	465	VAL
1	A	479	ASP
1	A	484	GLN
1	A	489	GLU
1	A	490	GLU
1	A	498	LEU
1	A	517	ASN
1	A	542	ASN
1	A	553	LEU
1	A	556	ASN
1	A	574	ASP
1	A	588	LEU
1	A	597	GLN
1	A	604	LEU
1	A	609	THR
1	A	621	LYS
1	A	626	VAL
1	A	633	ILE
1	A	639	THR
1	A	640	GLN
1	A	645	ASP
1	A	681	ARG
1	A	700	SER
1	A	721	LEU
1	B	12	ARG
1	B	14	VAL
1	B	25	ASP
1	B	26	LEU
1	B	47	VAL
1	B	59	THR
1	B	68	LYS

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Mol	Chain	Res	Type
1	B	76	VAL
1	B	104	VAL
1	B	110	GLN
1	B	115	THR
1	B	121	ILE
1	B	126	GLN
1	B	140	ARG
1	B	143	ARG
1	B	144	LEU
1	B	148	SER
1	B	165	THR
1	B	169	VAL
1	B	172	THR
1	B	174	ARG
1	B	189	GLU
1	B	193	VAL
1	B	202	GLU
1	B	206	LEU
1	B	217	VAL
1	B	223	ARG
1	B	235	LEU
1	B	259	SER
1	B	272	GLU
1	B	297	ASP
1	B	301	GLU
1	B	310	ARG
1	B	340	SER
1	B	347	ASN
1	B	354	LEU
1	B	360	VAL
1	B	363	LYS
1	B	397	SER
1	B	403	SER
1	B	406	MET
1	B	415	GLN
1	B	427	ASP
1	B	431	VAL
1	B	435	VAL
1	B	437	SER
1	B	445	LYS
1	B	451	VAL
1	B	463	LEU

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Mol	Chain	Res	Type
1	B	465	VAL
1	B	489	GLU
1	B	490	GLU
1	B	492	LEU
1	B	495	GLU
1	B	498	LEU
1	B	520	MET
1	B	523	GLU
1	B	525	GLU
1	B	526	ASN
1	B	538	THR
1	B	553	LEU
1	B	557	ILE
1	B	565	LYS
1	B	574	ASP
1	B	576	THR
1	B	578	GLU
1	B	588	LEU
1	B	589	ILE
1	B	604	LEU
1	B	609	THR
1	B	613	ASN
1	B	616	ARG
1	B	617	ASP
1	B	635	LYS
1	B	639	THR
1	B	640	GLN
1	B	647	THR
1	B	657	LYS
1	B	678	LYS
1	B	679	MET
1	B	683	ILE
1	B	696	ARG
1	B	713	SER
1	B	721	LEU
1	B	724	GLN
1	B	726	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS

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Mol	Chain	Res	Type
1	A	112	ASN
1	A	281	ASN
1	A	421	HIS
1	A	450	HIS
1	A	487	GLN
1	A	556	ASN
1	A	613	ASN
1	A	686	ASN
1	A	716	HIS
1	A	726	GLN
1	B	46	ASN
1	B	110	GLN
1	B	313	GLN
1	B	337	ASN
1	B	347	ASN
1	B	421	HIS
1	B	468	GLN
1	B	545	ASN
1	B	613	ASN
1	B	686	ASN
1	B	724	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	700/731 (95%)	-0.71	0 100 100	8, 31, 66, 83	0
1	B	705/731 (96%)	-0.72	0 100 100	4, 28, 71, 85	0
All	All	1405/1462 (96%)	-0.71	0 100 100	4, 29, 68, 85	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SR	B	732	1/1	0.96	0.03	45,45,45,45	0
2	SR	A	732	1/1	0.97	0.02	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.