



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:47 PM UTC

PDB ID : 1G2C / pdb_00001g2c
Title : HUMAN RESPIRATORY SYNCYTIAL VIRUS FUSION PROTEIN CORE
Authors : Zhao, X.; Singh, M.; Malashkevich, V.N.; Kim, P.S.
Deposited on : 2000-10-18
Resolution : 2.30 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

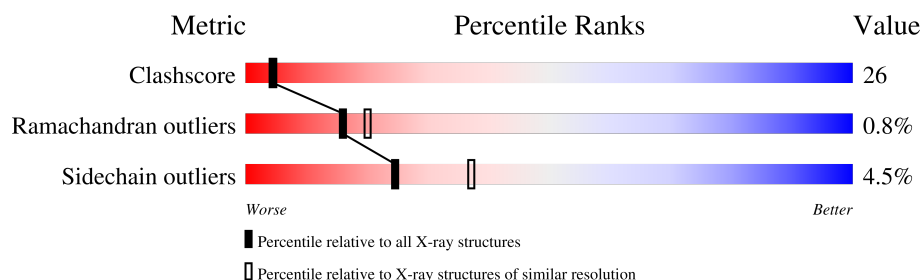
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

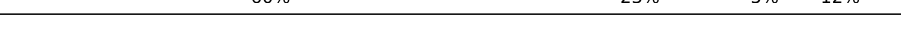
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	52	56% 33% 8% .
1	C	52	48% 40% . 8%
1	E	52	62% 25% 6% 8%
1	G	52	67% 25% . 6%
1	I	52	58% 31% 8% .
1	K	52	71% 15% 6% 8%
1	M	52	52% 37% . 10%
1	O	52	67% 23% 6% .

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Mol	Chain	Length	Quality of chain
1	Q	52	
1	S	52	
1	U	52	
1	W	52	
2	B	43	
2	D	43	
2	F	43	
2	H	43	
2	J	43	
2	L	43	
2	N	43	
2	P	43	
2	R	43	
2	T	43	
2	V	43	
2	X	43	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8942 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 FUSION PROTEIN (F).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	50	Total	C	N	O	0	0	0
			379	242	63	74			
1	C	48	Total	C	N	O	0	0	0
			361	232	59	70			
1	E	48	Total	C	N	O	0	0	0
			361	232	59	70			
1	G	49	Total	C	N	O	0	0	0
			369	236	61	72			
1	I	50	Total	C	N	O	0	0	0
			379	242	64	73			
1	K	48	Total	C	N	O	0	0	0
			362	231	61	70			
1	M	47	Total	C	N	O	0	0	0
			354	227	58	69			
1	O	50	Total	C	N	O	0	0	0
			379	244	63	72			
1	Q	49	Total	C	N	O	0	0	0
			369	236	61	72			
1	S	50	Total	C	N	O	0	0	0
			379	242	64	73			
1	U	50	Total	C	N	O	0	0	0
			379	242	63	74			
1	W	50	Total	C	N	O	0	0	0
			379	242	63	74			

- Molecule 2 is a protein called FUSION PROTEIN (F).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	40	Total	C	N	O	0	0	0
			314	197	53	64			
2	D	36	Total	C	N	O	0	0	0
			289	183	48	58			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	36	Total	C	N	O	0	0	0
			289	183	48	58			
2	H	37	Total	C	N	O	0	0	0
			296	188	49	59			
2	J	36	Total	C	N	O	0	0	0
			289	183	48	58			
2	L	40	Total	C	N	O	0	0	0
			327	210	52	65			
2	N	37	Total	C	N	O	0	0	0
			296	188	49	59			
2	P	37	Total	C	N	O	0	0	0
			296	188	49	59			
2	R	37	Total	C	N	O	0	0	0
			296	188	49	59			
2	T	38	Total	C	N	O	0	0	0
			304	192	51	61			
2	V	38	Total	C	N	O	0	0	0
			304	192	51	61			
2	X	38	Total	C	N	O	0	0	0
			304	192	51	61			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		
3	B	41	Total	O	0	0
			41	41		
3	C	26	Total	O	0	0
			26	26		
3	D	38	Total	O	0	0
			38	38		
3	E	28	Total	O	0	0
			28	28		
3	F	41	Total	O	0	0
			41	41		
3	G	38	Total	O	0	0
			38	38		
3	H	53	Total	O	0	0
			53	53		
3	I	70	Total	O	0	0
			70	70		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	45	Total 45	O 45	0	0
3	K	30	Total 30	O 30	0	0
3	L	40	Total 40	O 40	0	0
3	M	36	Total 36	O 36	0	0
3	N	42	Total 42	O 42	0	0
3	O	35	Total 35	O 35	0	0
3	P	32	Total 32	O 32	0	0
3	Q	32	Total 32	O 32	0	0
3	R	42	Total 42	O 42	0	0
3	S	26	Total 26	O 26	0	0
3	T	39	Total 39	O 39	0	0
3	U	22	Total 22	O 22	0	0
3	V	42	Total 42	O 42	0	0
3	W	17	Total 17	O 17	0	0
3	X	45	Total 45	O 45	0	0

3 Residue-property plots [i](#)

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

Chain A: 



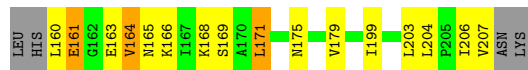
• Molecule 1: FUSION PROTEIN (F)

Chain C: 



• Molecule 1: FUSION PROTEIN (F)

Chain E: 



• Molecule 1: FUSION PROTEIN (F)

Chain G: 



• Molecule 1: FUSION PROTEIN (F)

Chain I: 



• Molecule 1: FUSION PROTEIN (F)

Chain K:  71% 15% 6% 8%



• Molecule 1: FUSION PROTEIN (F)

Chain M:  52% 37% 10%



• Molecule 1: FUSION PROTEIN (F)

Chain O:  67% 23% 6% 4%



• Molecule 1: FUSION PROTEIN (F)

Chain Q:  54% 37% 6% 3%



• Molecule 1: FUSION PROTEIN (F)

Chain S:  54% 33% 10% 3%



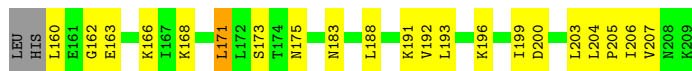
• Molecule 1: FUSION PROTEIN (F)

Chain U:  67% 25% 8% 0%



• Molecule 1: FUSION PROTEIN (F)

Chain W:  56% 38% 6% 0%



• Molecule 2: FUSION PROTEIN (F)

Chain B:  53% 30% 5% 5% 7%



• Molecule 2: FUSION PROTEIN (F)

Chain D:  51% 30% 16%



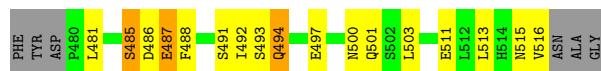
• Molecule 2: FUSION PROTEIN (F)

Chain F:  51% 30% 16%



• Molecule 2: FUSION PROTEIN (F)

Chain H:  47% 33% 7% 14%



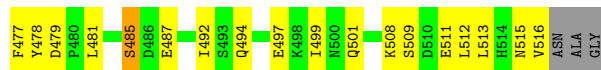
• Molecule 2: FUSION PROTEIN (F)

Chain J:  47% 35% 16%



• Molecule 2: FUSION PROTEIN (F)

Chain L:  51% 40% 7%



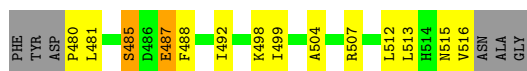
• Molecule 2: FUSION PROTEIN (F)

Chain N:  56% 26% 5% 14%



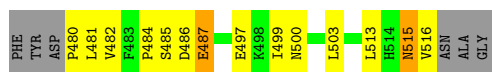
• Molecule 2: FUSION PROTEIN (F)

Chain P:  53% 28% 5% 14%



• Molecule 2: FUSION PROTEIN (F)

Chain R:  53% 28% 5% 14%



• Molecule 2: FUSION PROTEIN (F)

Chain T:  56% 28% 12%



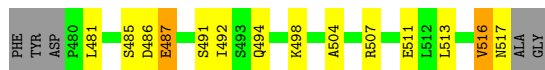
• Molecule 2: FUSION PROTEIN (F)

Chain V:  60% 23% 5% 12%



• Molecule 2: FUSION PROTEIN (F)

Chain X:  56% 28% 5% 12%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.90Å 71.54Å 76.45Å 81.34° 73.80° 60.72°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	94.7 (10.00-2.30)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.233 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8942	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	0/380	1.00	2/511 (0.4%)
1	C	0.50	0/362	0.97	1/489 (0.2%)
1	E	0.51	0/362	0.98	1/489 (0.2%)
1	G	0.47	0/370	0.87	0/500
1	I	0.44	0/381	0.94	3/515 (0.6%)
1	K	0.48	0/363	0.94	2/488 (0.4%)
1	M	0.55	0/355	1.00	1/479 (0.2%)
1	O	0.54	0/381	1.01	1/515 (0.2%)
1	Q	0.50	0/370	0.97	1/500 (0.2%)
1	S	0.43	0/381	0.96	3/515 (0.6%)
1	U	0.46	0/380	0.96	2/511 (0.4%)
1	W	0.44	0/380	0.92	0/511
2	B	0.49	0/319	1.08	1/429 (0.2%)
2	D	0.46	0/294	0.95	1/396 (0.3%)
2	F	0.48	0/294	1.12	1/396 (0.3%)
2	H	0.49	0/301	1.04	1/406 (0.2%)
2	J	0.47	0/294	0.94	0/396
2	L	0.53	0/334	1.17	4/452 (0.9%)
2	N	0.45	0/301	0.98	0/406
2	P	0.53	0/301	1.19	2/406 (0.5%)
2	R	0.49	0/301	1.01	2/406 (0.5%)
2	T	0.48	0/309	1.10	4/417 (1.0%)
2	V	0.49	0/309	1.04	1/417 (0.2%)
2	X	0.50	0/309	0.97	1/417 (0.2%)
All	All	0.49	0/8131	1.00	35/10967 (0.3%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	485	SER	N-CA-C	11.48	123.80	111.28
2	P	485	SER	N-CA-C	11.08	123.44	111.36
2	T	485	SER	N-CA-C	10.51	122.82	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	485	SER	N-CA-C	9.89	123.30	111.82
2	B	485	SER	N-CA-C	9.51	121.41	111.14
2	V	485	SER	N-CA-C	9.50	122.64	111.71
1	U	161	GLU	N-CA-C	-9.26	101.55	113.12
2	R	485	SER	N-CA-C	8.60	120.73	111.36
2	L	485	SER	N-CA-C	8.56	121.69	111.33
1	E	161	GLU	N-CA-C	-8.00	102.56	111.28
2	L	479	ASP	N-CA-C	7.95	123.28	112.55
2	D	485	SER	N-CA-C	7.46	122.07	113.19
2	X	485	SER	N-CA-C	7.15	119.16	111.36
2	L	479	ASP	CA-C-N	-6.76	111.91	120.23
2	L	479	ASP	C-N-CA	-6.76	111.91	120.23
1	I	163	GLU	N-CA-C	-6.08	106.00	113.41
1	A	208	ASN	N-CA-C	6.00	120.16	112.12
1	I	164	VAL	N-CA-C	-5.98	105.22	113.00
2	P	480	PRO	N-CA-CB	5.88	109.47	103.00
2	T	483	PHE	CA-C-N	5.74	127.02	119.84
2	T	483	PHE	C-N-CA	5.74	127.02	119.84
1	U	203	LEU	N-CA-C	5.65	117.13	110.97
1	K	163	GLU	N-CA-C	-5.59	105.27	111.36
2	T	487	GLU	N-CA-C	-5.58	104.59	111.40
1	S	203	LEU	N-CA-C	5.54	117.18	111.03
1	A	164	VAL	N-CA-C	-5.53	105.55	113.07
2	R	515	ASN	N-CA-C	-5.48	106.44	113.23
1	S	201	LYS	N-CA-C	5.43	119.07	112.23
1	C	203	LEU	N-CA-C	5.42	117.00	111.14
1	Q	203	LEU	N-CA-C	5.29	116.86	111.14
1	O	203	LEU	N-CA-C	5.18	116.78	111.03
1	I	200	ASP	N-CA-C	5.15	116.75	111.03
1	M	201	LYS	N-CA-C	5.07	118.62	112.23
1	K	201	LYS	N-CA-C	5.07	117.92	111.69
1	S	164	VAL	N-CA-C	-5.02	104.66	111.89

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	379	0	419	34	0
1	C	361	0	400	23	0
1	E	361	0	400	23	0
1	G	369	0	406	20	0
1	I	379	0	413	25	0
1	K	362	0	402	20	0
1	M	354	0	391	32	0
1	O	379	0	418	24	0
1	Q	369	0	406	37	0
1	S	379	0	413	35	0
1	U	379	0	419	30	0
1	W	379	0	419	27	0
2	B	314	0	304	22	0
2	D	289	0	281	19	0
2	F	289	0	281	15	0
2	H	296	0	290	25	0
2	J	289	0	281	20	0
2	L	327	0	311	35	0
2	N	296	0	290	23	0
2	P	296	0	290	22	0
2	R	296	0	290	20	0
2	T	304	0	296	17	0
2	V	304	0	296	19	0
2	X	304	0	296	22	0
3	A	28	0	0	9	0
3	B	41	0	0	3	0
3	C	26	0	0	1	0
3	D	38	0	0	1	0
3	E	28	0	0	1	0
3	F	41	0	0	2	0
3	G	38	0	0	0	0
3	H	53	0	0	2	0
3	I	70	0	0	4	0
3	J	45	0	0	3	0
3	K	30	0	0	3	0
3	L	40	0	0	2	0
3	M	36	0	0	5	0
3	N	42	0	0	6	0
3	O	35	0	0	1	0
3	P	32	0	0	0	0
3	Q	32	0	0	2	0
3	R	42	0	0	8	0
3	S	26	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	39	0	0	1	0
3	U	22	0	0	1	0
3	V	42	0	0	3	0
3	W	17	0	0	1	0
3	X	45	0	0	3	0
All	All	8942	0	8412	429	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 26.

All (429) 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:162:GLY:HA2	1:A:165:ASN:ND2	1.75	1.01
1:I:206:ILE:HD12	2:J:481:LEU:HD11	1.40	0.99
1:A:160:LEU:HD21	1:E:160:LEU:HG	1.44	0.96
1:O:171:LEU:HD13	2:R:513:LEU:HD11	1.51	0.91
3:M:751:HOH:O	1:Q:164:VAL:HG21	1.71	0.91
2:X:516:VAL:HG12	2:X:517:ASN:N	1.88	0.88
2:X:516:VAL:HG12	2:X:517:ASN:H	1.36	0.87
1:U:206:ILE:HD13	2:V:481:LEU:HD11	1.57	0.87
1:C:193:LEU:HD13	2:F:492:ILE:HD12	1.57	0.87
1:A:162:GLY:HA2	1:A:165:ASN:HD21	1.38	0.86
2:L:508:LYS:O	2:L:511:GLU:HG2	1.82	0.80
1:A:205:PRO:HB2	3:A:232:HOH:O	1.81	0.79
2:N:492:ILE:HD12	1:Q:193:LEU:HD13	1.63	0.79
1:G:160:LEU:CB	1:I:160:LEU:HD21	2.12	0.79
1:A:166:LYS:HG2	3:A:233:HOH:O	1.81	0.78
1:K:163:GLU:HB3	2:L:516:VAL:HG13	1.66	0.78
1:K:166:LYS:NZ	2:L:515:ASN:HB3	1.99	0.78
1:S:163:GLU:OE1	1:S:163:GLU:HA	1.83	0.77
2:B:480:PRO:O	2:B:482:VAL:HG23	1.84	0.77
2:B:497:GLU:HB3	3:B:557:HOH:O	1.83	0.77
2:H:492:ILE:HD12	1:K:193:LEU:HD13	1.65	0.77
1:O:206:ILE:HG13	1:O:207:VAL:HG23	1.67	0.76
1:O:207:VAL:HG11	1:Q:207:VAL:HG22	1.65	0.76
1:O:165:ASN:HB2	3:O:236:HOH:O	1.84	0.76
2:B:513:LEU:HD11	1:E:171:LEU:HD13	1.68	0.76
1:S:206:ILE:HD13	1:W:207:VAL:HG12	1.69	0.75
2:J:507:ARG:O	2:J:511:GLU:HG3	1.87	0.74
2:H:493:SER:O	2:H:497:GLU:HG3	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HG13	3:A:232:HOH:O	1.87	0.73
1:E:160:LEU:HD13	3:E:513:HOH:O	1.88	0.73
1:I:168:LYS:HE2	2:L:513:LEU:O	1.89	0.73
2:B:481:LEU:O	2:B:482:VAL:HB	1.88	0.73
1:U:203:LEU:O	1:U:206:ILE:HG12	1.89	0.73
1:I:193:LEU:HD13	2:L:492:ILE:HD12	1.71	0.72
1:G:206:ILE:HD12	2:H:481:LEU:HD11	1.70	0.72
2:B:516:VAL:HG12	2:B:517:ASN:ND2	2.06	0.71
2:H:500:ASN:HD22	2:P:487:GLU:H	1.38	0.71
2:D:500:ASN:HD21	2:H:486:ASP:H	1.37	0.71
2:L:494:GLN:HE22	2:P:498:LYS:CE	2.03	0.71
1:M:166:LYS:HD2	2:N:516:VAL:HA	1.73	0.71
1:S:166:LYS:HD2	2:T:516:VAL:HA	1.73	0.70
3:S:114:HOH:O	1:U:160:LEU:HD13	1.91	0.70
1:O:159:HIS:O	1:O:163:GLU:HG2	1.91	0.70
2:V:515:ASN:HA	3:V:554:HOH:O	1.91	0.70
2:B:498:LYS:HD3	2:B:501:GLN:NE2	2.05	0.70
2:B:513:LEU:O	1:E:168:LYS:HE2	1.90	0.70
1:G:201:LYS:HD2	1:G:201:LYS:N	2.06	0.70
2:B:481:LEU:HD13	1:E:204:LEU:HD22	1.72	0.70
1:M:168:LYS:HE2	2:P:513:LEU:O	1.91	0.70
2:R:513:LEU:O	2:R:516:VAL:HB	1.91	0.70
1:M:192:VAL:HG21	1:O:188:LEU:HD11	1.72	0.69
2:R:516:VAL:HG12	2:R:516:VAL:O	1.92	0.69
3:B:521:HOH:O	2:J:496:ASN:HB3	1.91	0.69
3:I:266:HOH:O	2:J:481:LEU:HD13	1.91	0.69
1:G:160:LEU:HB2	1:I:160:LEU:HD21	1.73	0.69
1:I:203:LEU:HD12	3:I:266:HOH:O	1.92	0.69
2:X:513:LEU:HA	2:X:516:VAL:HG23	1.73	0.69
2:B:493:SER:O	2:B:497:GLU:HG3	1.93	0.68
1:A:160:LEU:HD21	1:E:160:LEU:CG	2.21	0.68
1:A:191:LYS:HA	1:A:191:LYS:HE2	1.75	0.68
1:U:206:ILE:CD1	2:V:481:LEU:HD11	2.21	0.68
1:Q:166:LYS:HE2	3:Q:237:HOH:O	1.93	0.68
2:R:484:PRO:HA	2:T:500:ASN:OD1	1.94	0.68
2:D:511:GLU:OE1	2:D:511:GLU:HA	1.94	0.67
1:E:160:LEU:HA	1:E:163:GLU:HG2	1.75	0.67
2:H:513:LEU:HD11	1:K:171:LEU:HD13	1.76	0.67
1:M:160:LEU:O	1:M:164:VAL:HG23	1.95	0.67
1:S:168:LYS:HE2	2:V:516:VAL:HG23	1.76	0.67
1:G:160:LEU:HB3	1:I:160:LEU:HD21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:513:LEU:O	1:K:168:LYS:HE2	1.96	0.66
1:U:164:VAL:HG21	1:W:160:LEU:HD11	1.78	0.66
1:C:206:ILE:HD12	2:D:481:LEU:HD21	1.78	0.66
1:O:207:VAL:HG11	1:Q:207:VAL:CG2	2.25	0.66
2:N:515:ASN:HA	3:N:524:HOH:O	1.96	0.65
1:M:199:ILE:O	1:M:204:LEU:HG	1.96	0.65
1:C:183:ASN:HB3	2:D:498:LYS:NZ	2.13	0.64
1:S:159:HIS:HE1	1:S:163:GLU:OE2	1.80	0.64
1:O:168:LYS:HD2	2:R:516:VAL:HG11	1.79	0.64
1:M:204:LEU:HD22	2:P:481:LEU:HD23	1.79	0.64
1:Q:207:VAL:O	1:Q:208:ASN:HB3	1.96	0.64
2:L:508:LYS:HD3	3:L:548:HOH:O	1.96	0.64
1:A:162:GLY:O	1:A:166:LYS:HG3	1.98	0.63
2:B:480:PRO:O	2:B:482:VAL:N	2.30	0.63
1:S:171:LEU:HD13	2:V:513:LEU:HD11	1.78	0.63
2:D:500:ASN:HD22	2:H:487:GLU:H	1.44	0.63
1:I:193:LEU:HB2	2:L:492:ILE:HD13	1.81	0.63
3:N:624:HOH:O	1:Q:168:LYS:HE3	1.97	0.63
1:M:171:LEU:HD13	2:P:513:LEU:HD11	1.82	0.62
2:N:497:GLU:HG2	2:N:501:GLN:HE21	1.64	0.62
1:M:164:VAL:HG21	1:O:160:LEU:HD11	1.82	0.62
2:V:513:LEU:O	2:V:516:VAL:HG22	1.99	0.62
1:U:206:ILE:HD13	2:V:481:LEU:CD1	2.29	0.61
1:G:207:VAL:HG12	1:G:207:VAL:O	1.99	0.61
1:S:203:LEU:O	1:S:206:ILE:HG22	2.00	0.61
1:M:168:LYS:HE3	2:P:516:VAL:HB	1.82	0.60
2:T:516:VAL:HG12	2:T:517:ASN:N	2.14	0.60
2:J:487:GLU:OE1	2:J:487:GLU:N	2.31	0.60
1:W:207:VAL:HG12	1:W:207:VAL:O	2.00	0.60
2:T:513:LEU:O	1:W:168:LYS:HE2	2.00	0.60
1:M:160:LEU:HD23	1:Q:160:LEU:HD23	1.84	0.60
1:S:203:LEU:O	1:S:207:VAL:HG23	2.02	0.60
1:Q:162:GLY:O	1:Q:166:LYS:HG3	2.02	0.59
3:R:534:HOH:O	1:W:183:ASN:HB3	2.02	0.59
1:G:200:ASP:HB3	1:G:201:LYS:HD2	1.83	0.59
2:H:491:SER:HA	2:H:494:GLN:HE21	1.68	0.59
2:R:482:VAL:HG23	3:R:554:HOH:O	2.02	0.59
1:Q:160:LEU:O	1:Q:164:VAL:HG23	2.02	0.59
1:Q:163:GLU:OE1	2:R:516:VAL:HG13	2.03	0.59
2:N:513:LEU:O	1:Q:168:LYS:HE2	2.03	0.59
1:E:160:LEU:O	1:E:164:VAL:HG13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:207:VAL:HG12	1:K:207:VAL:O	2.02	0.59
1:S:207:VAL:HG11	1:U:206:ILE:CD1	2.33	0.59
1:S:168:LYS:CE	2:V:516:VAL:HG23	2.32	0.58
2:R:487:GLU:OE1	2:R:487:GLU:C	2.45	0.58
2:L:515:ASN:OD1	2:L:515:ASN:O	2.20	0.58
1:M:166:LYS:CD	2:N:516:VAL:HA	2.34	0.58
1:A:208:ASN:HD21	2:D:481:LEU:HD12	1.69	0.58
1:I:207:VAL:O	1:I:207:VAL:HG12	2.03	0.57
1:U:160:LEU:HD12	3:U:225:HOH:O	2.05	0.57
1:U:171:LEU:HD13	2:X:513:LEU:HD11	1.85	0.57
3:A:227:HOH:O	2:D:503:LEU:HD11	2.04	0.57
1:U:203:LEU:CD2	1:W:203:LEU:HD21	2.35	0.57
1:A:203:LEU:HD23	1:C:203:LEU:HD21	1.87	0.57
2:R:515:ASN:HB3	3:R:546:HOH:O	2.03	0.57
1:U:206:ILE:HG13	1:U:207:VAL:N	2.20	0.57
2:N:515:ASN:O	2:N:516:VAL:O	2.23	0.57
2:H:488:PHE:HE2	2:H:492:ILE:HD11	1.68	0.57
1:M:164:VAL:CG2	3:M:751:HOH:O	2.53	0.57
2:L:494:GLN:HE22	2:P:498:LYS:CD	2.18	0.56
1:U:203:LEU:HD23	1:W:203:LEU:HD21	1.86	0.56
1:E:175:ASN:O	1:E:179:VAL:HG23	2.05	0.56
2:T:487:GLU:C	2:T:487:GLU:OE1	2.49	0.56
2:X:513:LEU:HA	2:X:516:VAL:CG2	2.35	0.56
2:H:487:GLU:C	2:H:487:GLU:OE1	2.49	0.56
1:W:206:ILE:HD12	2:X:481:LEU:HD21	1.88	0.56
2:X:507:ARG:O	2:X:511:GLU:HG3	2.06	0.56
1:C:193:LEU:CD1	2:F:492:ILE:HD12	2.33	0.55
2:H:503:LEU:HD13	2:P:487:GLU:HA	1.88	0.55
1:W:162:GLY:O	1:W:166:LYS:HG2	2.06	0.55
1:I:206:ILE:CD1	2:J:481:LEU:HD11	2.26	0.55
1:S:168:LYS:HE2	2:V:516:VAL:CG2	2.36	0.55
1:A:207:VAL:HA	3:A:229:HOH:O	2.05	0.55
3:A:227:HOH:O	2:D:503:LEU:HD21	2.06	0.55
1:C:199:ILE:O	1:C:204:LEU:HG	2.06	0.55
2:N:488:PHE:HE2	2:N:492:ILE:HD11	1.71	0.55
2:J:507:ARG:HD3	3:J:530:HOH:O	2.07	0.55
2:F:488:PHE:CE2	2:F:492:ILE:HD11	2.42	0.55
1:M:164:VAL:HG23	3:M:751:HOH:O	2.07	0.55
1:A:176:LYS:HE2	3:A:214:HOH:O	2.07	0.55
1:C:166:LYS:HE2	3:C:222:HOH:O	2.07	0.55
2:D:500:ASN:HD21	2:H:486:ASP:N	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:513:LEU:HD11	1:Q:171:LEU:HD13	1.89	0.55
1:O:185:VAL:HG12	2:R:499:ILE:HD11	1.88	0.55
2:F:495:VAL:O	2:F:499:ILE:HG13	2.07	0.55
2:H:492:ILE:HD13	1:K:193:LEU:HB2	1.88	0.54
2:L:487:GLU:H	2:R:500:ASN:HD22	1.55	0.54
1:K:206:ILE:HD12	2:L:481:LEU:HD21	1.90	0.54
2:L:494:GLN:NE2	2:P:498:LYS:HD2	2.23	0.54
1:O:169:SER:OG	2:P:512:LEU:HD13	2.07	0.54
1:I:203:LEU:O	1:I:207:VAL:HG23	2.08	0.54
1:C:207:VAL:HG12	1:C:207:VAL:O	2.07	0.54
1:M:166:LYS:HE3	3:M:791:HOH:O	2.08	0.54
1:S:163:GLU:OE1	1:S:166:LYS:HD2	2.08	0.54
2:B:504:ALA:HB3	3:B:533:HOH:O	2.07	0.53
2:F:488:PHE:HE2	2:F:492:ILE:HD11	1.72	0.53
1:I:196:LYS:HD3	1:I:196:LYS:C	2.33	0.53
2:L:494:GLN:HE22	2:P:498:LYS:HD2	1.71	0.53
1:A:207:VAL:HG12	1:A:207:VAL:O	2.08	0.53
2:B:487:GLU:H	2:J:500:ASN:HD22	1.56	0.53
2:L:513:LEU:C	2:L:515:ASN:H	2.14	0.53
1:W:163:GLU:HA	1:W:163:GLU:OE1	2.09	0.53
2:L:487:GLU:HA	2:R:503:LEU:HD12	1.89	0.53
1:O:207:VAL:HG12	1:O:207:VAL:O	2.09	0.53
2:H:485:SER:OG	1:K:196:LYS:HE2	2.08	0.52
1:S:204:LEU:N	1:S:205:PRO:HD2	2.24	0.52
1:A:163:GLU:OE2	2:B:516:VAL:O	2.27	0.52
1:Q:206:ILE:HD12	2:R:481:LEU:HD11	1.91	0.52
1:W:188:LEU:O	1:W:192:VAL:HG23	2.09	0.52
1:W:193:LEU:HB3	3:W:226:HOH:O	2.09	0.52
1:C:183:ASN:HB3	2:D:498:LYS:HZ3	1.74	0.52
2:H:513:LEU:HA	2:H:516:VAL:HG23	1.92	0.52
2:T:487:GLU:HB2	3:T:548:HOH:O	2.10	0.52
1:M:163:GLU:OE1	1:M:166:LYS:HD2	2.10	0.52
1:W:203:LEU:O	1:W:207:VAL:HG23	2.09	0.52
1:K:166:LYS:HZ2	2:L:515:ASN:HB3	1.74	0.51
2:R:497:GLU:HG3	3:R:560:HOH:O	2.10	0.51
2:J:490:ALA:O	2:J:494:GLN:HG3	2.10	0.51
2:L:497:GLU:HG2	2:L:501:GLN:HE21	1.75	0.51
2:V:498:LYS:HE3	3:V:521:HOH:O	2.11	0.51
1:O:207:VAL:CG1	1:Q:207:VAL:HG22	2.35	0.51
1:Q:166:LYS:HD3	3:R:546:HOH:O	2.09	0.51
1:M:203:LEU:HD21	1:Q:203:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:160:LEU:HA	1:U:163:GLU:OE1	2.10	0.51
2:F:487:GLU:HG2	3:F:109:HOH:O	2.11	0.51
1:O:160:LEU:HA	1:O:163:GLU:HG2	1.93	0.51
1:U:168:LYS:HE2	2:X:513:LEU:O	2.11	0.50
1:Q:206:ILE:C	1:Q:207:VAL:O	2.50	0.50
1:S:196:LYS:HD3	1:S:196:LYS:C	2.36	0.50
1:S:188:LEU:O	1:S:192:VAL:HG23	2.12	0.50
2:D:491:SER:O	2:D:494:GLN:HG2	2.12	0.50
2:T:516:VAL:HG12	2:T:517:ASN:ND2	2.26	0.50
2:X:504:ALA:HA	2:X:507:ARG:NH1	2.27	0.50
1:S:172:LEU:O	1:S:176:LYS:HG3	2.12	0.50
1:A:206:ILE:C	1:A:208:ASN:H	2.18	0.50
1:C:204:LEU:N	1:C:205:PRO:HD2	2.27	0.50
1:W:196:LYS:HD3	1:W:196:LYS:C	2.37	0.50
1:G:201:LYS:N	1:G:201:LYS:CD	2.75	0.49
1:S:203:LEU:CD2	1:U:203:LEU:HD21	2.42	0.49
2:N:497:GLU:HG2	2:N:501:GLN:NE2	2.26	0.49
1:O:164:VAL:HG13	1:Q:167:ILE:HD12	1.94	0.49
2:J:514:HIS:HD2	3:J:552:HOH:O	1.95	0.49
1:S:168:LYS:HE2	2:V:513:LEU:O	2.12	0.49
1:O:160:LEU:HA	1:O:163:GLU:CG	2.42	0.49
1:A:171:LEU:HD13	2:D:513:LEU:HD11	1.93	0.49
1:C:196:LYS:C	1:C:196:LYS:HD3	2.38	0.49
1:E:166:LYS:HD2	2:F:512:LEU:HD22	1.95	0.49
1:I:193:LEU:HD13	2:L:492:ILE:CD1	2.41	0.49
1:I:200:ASP:OD2	2:L:485:SER:OG	2.30	0.49
2:B:486:ASP:H	2:J:500:ASN:HD21	1.61	0.49
1:C:164:VAL:HG11	1:E:163:GLU:HG3	1.95	0.49
2:L:512:LEU:O	2:L:515:ASN:HB3	2.12	0.49
1:M:204:LEU:HD22	2:P:481:LEU:CD2	2.41	0.49
2:N:492:ILE:HD13	1:Q:193:LEU:HB2	1.94	0.49
2:N:512:LEU:O	2:N:516:VAL:HG23	2.12	0.49
2:L:494:GLN:NE2	3:L:545:HOH:O	2.26	0.49
2:H:491:SER:HA	2:H:494:GLN:NE2	2.27	0.48
2:F:487:GLU:OE1	2:F:487:GLU:C	2.56	0.48
1:W:191:LYS:HA	1:W:191:LYS:HE2	1.94	0.48
1:C:203:LEU:O	1:C:207:VAL:HG23	2.13	0.48
1:K:163:GLU:HB3	2:L:516:VAL:CG1	2.40	0.48
1:M:188:LEU:HD11	1:Q:192:VAL:HG21	1.95	0.48
1:E:206:ILE:O	1:E:206:ILE:HG22	2.13	0.48
1:E:169:SER:OG	2:F:512:LEU:HD13	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:175:ASN:O	1:I:179:VAL:HG23	2.14	0.48
1:O:163:GLU:OE1	2:P:516:VAL:HG13	2.14	0.48
1:Q:196:LYS:HD3	1:Q:196:LYS:C	2.39	0.48
1:M:191:LYS:HD2	2:N:491:SER:CB	2.43	0.48
1:S:159:HIS:HE1	1:S:163:GLU:CD	2.21	0.48
1:A:196:LYS:HD3	1:A:196:LYS:C	2.39	0.48
1:O:168:LYS:HE2	2:R:513:LEU:O	2.14	0.48
1:U:207:VAL:HG21	1:W:203:LEU:HD11	1.96	0.48
1:A:165:ASN:OD1	1:A:166:LYS:N	2.47	0.48
2:B:498:LYS:O	2:B:501:GLN:HG2	2.14	0.48
1:I:186:SER:OG	2:L:499:ILE:HG21	2.13	0.48
1:S:207:VAL:CG1	1:U:206:ILE:HD12	2.44	0.48
1:U:193:LEU:HB2	2:X:492:ILE:HD13	1.95	0.48
2:R:480:PRO:HB2	3:R:554:HOH:O	2.13	0.48
1:S:188:LEU:HD11	1:W:192:VAL:HG21	1.95	0.47
1:A:162:GLY:CA	1:A:165:ASN:ND2	2.62	0.47
2:H:488:PHE:CE2	2:H:492:ILE:HD11	2.47	0.47
1:G:168:LYS:HE2	2:J:513:LEU:O	2.14	0.47
1:M:203:LEU:HD21	1:Q:203:LEU:CD2	2.45	0.47
1:O:203:LEU:CD2	1:Q:203:LEU:HD21	2.43	0.47
1:U:207:VAL:HG12	1:U:207:VAL:O	2.14	0.47
1:I:159:HIS:O	1:I:162:GLY:N	2.47	0.47
1:I:200:ASP:C	1:I:200:ASP:OD1	2.56	0.47
1:O:163:GLU:OE1	1:O:163:GLU:HA	2.14	0.47
1:Q:188:LEU:O	1:Q:192:VAL:HG23	2.14	0.47
1:C:162:GLY:O	1:C:166:LYS:N	2.48	0.47
1:E:206:ILE:HD12	2:F:481:LEU:HD21	1.95	0.47
2:R:486:ASP:OD2	2:T:507:ARG:CZ	2.63	0.47
1:S:163:GLU:C	1:S:165:ASN:N	2.72	0.47
1:S:185:VAL:HG12	2:V:499:ILE:HD11	1.96	0.47
2:V:512:LEU:HD23	3:V:527:HOH:O	2.14	0.47
1:A:160:LEU:O	1:A:164:VAL:HG23	2.15	0.47
1:A:162:GLY:C	1:A:163:GLU:OE1	2.58	0.47
1:A:191:LYS:O	1:A:194:ASP:HB2	2.15	0.47
2:L:509:SER:O	2:L:513:LEU:HG	2.15	0.47
1:C:160:LEU:HD23	1:E:160:LEU:HD21	1.96	0.46
1:K:166:LYS:NZ	2:L:515:ASN:CB	2.75	0.46
1:M:175:ASN:O	1:M:179:VAL:HG23	2.15	0.46
1:I:159:HIS:C	1:I:161:GLU:N	2.71	0.46
2:N:492:ILE:HD12	1:Q:193:LEU:CD1	2.40	0.46
2:P:487:GLU:OE1	2:P:487:GLU:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:174:THR:O	1:Q:178:VAL:HG23	2.15	0.46
2:D:496:ASN:ND2	3:D:542:HOH:O	2.47	0.46
1:G:181:LEU:O	1:G:185:VAL:HG23	2.16	0.46
1:M:191:LYS:HA	1:M:191:LYS:HE2	1.98	0.46
2:L:494:GLN:HE22	2:P:498:LYS:NZ	2.12	0.46
1:U:193:LEU:HD13	2:X:492:ILE:HD12	1.98	0.46
2:X:494:GLN:HG2	3:X:532:HOH:O	2.15	0.46
1:A:204:LEU:HB2	1:A:205:PRO:HD3	1.98	0.46
1:C:168:LYS:HE2	2:F:513:LEU:O	2.16	0.46
2:B:480:PRO:O	2:B:481:LEU:C	2.57	0.46
1:U:206:ILE:CD1	2:V:481:LEU:CD1	2.90	0.46
1:E:161:GLU:O	1:E:165:ASN:HB2	2.15	0.45
1:G:185:VAL:HG12	2:J:499:ILE:HD11	1.97	0.45
1:A:168:LYS:HE2	2:D:513:LEU:O	2.17	0.45
1:M:168:LYS:HD2	2:P:516:VAL:HG21	1.96	0.45
2:X:494:GLN:HG2	3:X:553:HOH:O	2.17	0.45
1:C:172:LEU:O	1:C:176:LYS:HG3	2.16	0.45
1:A:206:ILE:C	1:A:208:ASN:N	2.75	0.45
2:F:480:PRO:HA	3:F:603:HOH:O	2.15	0.45
1:G:203:LEU:CD2	1:I:203:LEU:HD21	2.46	0.45
2:T:513:LEU:HD11	1:W:171:LEU:HD13	1.98	0.45
1:A:203:LEU:HD11	1:E:207:VAL:HG21	1.98	0.45
1:M:195:LEU:O	1:M:199:ILE:HG13	2.17	0.45
1:U:208:ASN:OD1	2:X:481:LEU:HD12	2.16	0.45
1:I:191:LYS:HD2	2:J:491:SER:CB	2.47	0.45
2:N:507:ARG:NH1	2:X:486:ASP:OD1	2.49	0.45
3:N:769:HOH:O	1:Q:208:ASN:CG	2.60	0.45
1:K:166:LYS:HZ2	2:L:515:ASN:CB	2.29	0.45
2:T:513:LEU:HD21	1:W:171:LEU:HD13	1.98	0.45
1:K:201:LYS:O	1:K:205:PRO:HG2	2.16	0.45
1:I:160:LEU:O	1:I:164:VAL:HG23	2.17	0.45
2:N:487:GLU:C	2:N:487:GLU:OE1	2.60	0.45
2:T:508:LYS:O	2:T:511:GLU:HB3	2.17	0.45
2:R:513:LEU:HA	2:R:516:VAL:HG23	1.98	0.45
2:D:500:ASN:ND2	2:H:487:GLU:H	2.13	0.44
1:E:160:LEU:HD12	1:E:163:GLU:HG2	1.98	0.44
1:E:199:ILE:O	1:E:204:LEU:HG	2.17	0.44
1:M:204:LEU:HB2	1:M:205:PRO:HD3	1.99	0.44
1:Q:207:VAL:HG12	1:Q:208:ASN:N	2.32	0.44
1:S:207:VAL:HG12	1:S:207:VAL:O	2.17	0.44
1:W:191:LYS:HD2	2:X:491:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:203:LEU:HD23	1:I:203:LEU:HD21	1.98	0.44
1:G:203:LEU:O	1:G:207:VAL:HG23	2.18	0.44
1:I:196:LYS:HD3	1:I:197:ASN:N	2.33	0.44
2:J:497:GLU:HG3	3:J:545:HOH:O	2.17	0.44
2:P:488:PHE:O	2:P:492:ILE:HG12	2.17	0.44
1:S:203:LEU:HD23	1:U:203:LEU:HD21	2.00	0.44
1:A:162:GLY:CA	1:A:165:ASN:HD21	2.20	0.44
1:S:206:ILE:HG12	1:S:206:ILE:O	2.17	0.44
2:H:494:GLN:HE21	2:H:494:GLN:HB2	1.59	0.44
3:Q:238:HOH:O	2:X:487:GLU:HG2	2.17	0.44
2:L:487:GLU:HA	2:R:503:LEU:CD1	2.47	0.44
2:V:515:ASN:OD1	2:V:515:ASN:C	2.60	0.44
1:C:201:LYS:CD	1:C:201:LYS:N	2.80	0.44
2:F:499:ILE:O	2:F:502:SER:HB3	2.18	0.44
1:G:171:LEU:HD13	2:J:513:LEU:HD11	2.00	0.44
1:K:166:LYS:HZ2	2:L:515:ASN:CG	2.26	0.44
1:S:191:LYS:NZ	3:S:677:HOH:O	2.50	0.43
1:S:207:VAL:HG11	1:U:206:ILE:HD12	1.98	0.43
1:C:174:THR:O	1:C:177:ALA:HB3	2.18	0.43
1:C:191:LYS:HA	1:C:191:LYS:HE2	2.00	0.43
1:K:196:LYS:HD3	1:K:196:LYS:C	2.43	0.43
1:U:191:LYS:HA	1:U:191:LYS:HD3	1.80	0.43
1:E:160:LEU:HD12	1:E:163:GLU:CG	2.48	0.43
2:N:481:LEU:N	3:N:769:HOH:O	2.51	0.43
2:N:492:ILE:CD1	1:Q:193:LEU:HB2	2.48	0.43
1:G:201:LYS:HD2	1:G:201:LYS:H	1.83	0.43
1:O:166:LYS:NZ	2:P:515:ASN:OD1	2.37	0.43
1:O:200:ASP:OD1	1:O:200:ASP:C	2.61	0.43
1:Q:163:GLU:O	1:Q:167:ILE:HG13	2.19	0.43
1:C:183:ASN:HB2	2:D:498:LYS:HD3	1.99	0.43
2:H:481:LEU:HD23	2:H:481:LEU:HA	1.74	0.43
3:I:244:HOH:O	2:J:484:PRO:HG3	2.18	0.43
2:L:511:GLU:HG3	2:L:512:LEU:N	2.33	0.43
1:Q:207:VAL:HG12	1:Q:208:ASN:H	1.83	0.43
1:W:200:ASP:OD1	1:W:200:ASP:C	2.61	0.43
1:U:206:ILE:C	1:U:208:ASN:N	2.76	0.43
2:B:498:LYS:HD3	2:B:501:GLN:CD	2.43	0.43
1:O:206:ILE:HG13	1:O:207:VAL:N	2.34	0.43
2:X:516:VAL:CG1	2:X:517:ASN:H	2.10	0.43
2:L:508:LYS:HG3	2:L:511:GLU:OE2	2.19	0.43
1:M:185:VAL:HG12	2:P:499:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:507:ARG:HE	2:V:507:ARG:HB2	1.39	0.43
2:B:481:LEU:O	2:B:482:VAL:CB	2.60	0.43
2:N:481:LEU:HB2	3:N:769:HOH:O	2.18	0.43
1:U:200:ASP:OD1	1:U:200:ASP:C	2.61	0.43
2:V:513:LEU:O	2:V:516:VAL:CG2	2.66	0.43
1:E:207:VAL:O	1:E:207:VAL:HG12	2.18	0.42
1:G:175:ASN:HB3	2:J:506:ILE:HG23	2.01	0.42
1:M:203:LEU:CD2	1:O:203:LEU:HD21	2.49	0.42
2:T:506:ILE:HG23	1:W:175:ASN:HB3	2.00	0.42
2:B:483:PHE:O	2:B:485:SER:N	2.49	0.42
1:S:207:VAL:HG11	1:U:206:ILE:HD11	2.01	0.42
2:H:492:ILE:CD1	1:K:193:LEU:HD13	2.44	0.42
2:T:495:VAL:O	2:T:499:ILE:HG13	2.19	0.42
1:M:173:SER:OG	2:N:509:SER:HB2	2.19	0.42
1:S:163:GLU:OE1	1:S:163:GLU:CA	2.56	0.42
1:U:192:VAL:HG21	1:W:188:LEU:HD11	2.01	0.42
2:R:480:PRO:C	3:R:554:HOH:O	2.63	0.42
1:A:196:LYS:HG3	2:D:488:PHE:CD2	2.55	0.42
1:Q:200:ASP:CG	1:Q:201:LYS:HZ2	2.27	0.42
1:Q:203:LEU:O	1:Q:207:VAL:HG23	2.18	0.42
1:U:163:GLU:H	1:U:163:GLU:CD	2.27	0.42
2:X:516:VAL:CG1	2:X:517:ASN:N	2.61	0.42
1:Q:207:VAL:O	1:Q:208:ASN:CB	2.64	0.42
2:T:481:LEU:HA	2:T:481:LEU:HD23	1.88	0.42
2:D:507:ARG:CZ	3:H:560:HOH:O	2.68	0.42
1:G:207:VAL:HG11	3:I:266:HOH:O	2.20	0.42
2:H:501:GLN:NE2	3:H:556:HOH:O	2.53	0.42
2:N:516:VAL:HB	3:N:624:HOH:O	2.19	0.42
2:X:487:GLU:C	2:X:487:GLU:OE1	2.63	0.42
1:E:206:ILE:O	1:E:206:ILE:CG2	2.68	0.42
1:K:201:LYS:NZ	3:K:213:HOH:O	2.52	0.42
2:P:504:ALA:HA	2:P:507:ARG:HH21	1.84	0.42
1:S:163:GLU:OE2	2:T:516:VAL:O	2.38	0.42
1:M:160:LEU:HD21	1:Q:160:LEU:HB3	2.02	0.41
2:B:486:ASP:N	2:J:500:ASN:HD21	2.18	0.41
2:B:510:ASP:O	2:B:514:HIS:ND1	2.53	0.41
1:I:185:VAL:HG12	2:L:499:ILE:HD11	2.02	0.41
2:N:513:LEU:HA	2:N:516:VAL:HG23	2.02	0.41
2:X:511:GLU:HB2	3:X:562:HOH:O	2.18	0.41
1:C:201:LYS:O	1:C:205:PRO:HG3	2.19	0.41
1:S:203:LEU:HD11	1:W:207:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:499:ILE:O	2:V:502:SER:HB3	2.20	0.41
1:M:160:LEU:HG	3:M:751:HOH:O	2.20	0.41
2:P:487:GLU:OE1	2:P:487:GLU:C	2.63	0.41
1:A:207:VAL:O	1:A:207:VAL:CG1	2.68	0.41
2:D:495:VAL:O	2:D:499:ILE:HG13	2.21	0.41
2:H:503:LEU:CD1	2:P:487:GLU:HA	2.51	0.41
2:L:513:LEU:C	2:L:515:ASN:N	2.79	0.41
1:W:199:ILE:O	1:W:204:LEU:HG	2.21	0.41
1:A:206:ILE:N	3:A:232:HOH:O	2.53	0.41
3:R:534:HOH:O	2:X:498:LYS:HE3	2.20	0.41
1:S:160:LEU:HD23	1:S:160:LEU:HA	1.94	0.41
2:F:498:LYS:HD3	2:F:501:GLN:NE2	2.35	0.41
1:M:191:LYS:HD2	2:N:491:SER:HB2	2.02	0.41
1:A:203:LEU:HD21	1:E:203:LEU:CD2	2.51	0.41
1:M:203:LEU:HD11	1:Q:207:VAL:HG21	2.03	0.41
1:S:163:GLU:OE2	2:T:516:VAL:C	2.64	0.41
2:T:513:LEU:O	2:T:516:VAL:HG23	2.20	0.41
2:F:507:ARG:HG2	2:F:507:ARG:HH11	1.85	0.41
1:G:198:TYR:O	1:G:202:GLN:HB2	2.21	0.40
1:K:207:VAL:HG13	3:K:218:HOH:O	2.21	0.40
2:B:487:GLU:H	2:J:500:ASN:ND2	2.18	0.40
1:A:183:ASN:OD1	3:A:227:HOH:O	2.22	0.40
1:A:181:LEU:O	1:A:185:VAL:HG23	2.22	0.40
1:G:160:LEU:HD13	3:K:227:HOH:O	2.21	0.40
1:K:166:LYS:HE2	1:K:166:LYS:HB3	1.81	0.40
2:L:477:PHE:O	2:L:478:TYR:C	2.63	0.40
1:W:191:LYS:HE2	1:W:191:LYS:CA	2.51	0.40
1:C:206:ILE:O	1:C:206:ILE:HG22	2.21	0.40
2:H:511:GLU:O	2:H:515:ASN:ND2	2.54	0.40
1:S:201:LYS:O	1:S:205:PRO:HG3	2.21	0.40
2:V:491:SER:O	2:V:495:VAL:HG23	2.22	0.40
1:W:204:LEU:HB2	1:W:205:PRO:HD3	2.03	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	48/52 (92%)	47 (98%)	1 (2%)	0	100	100
1	C	46/52 (88%)	45 (98%)	0	1 (2%)	5	4
1	E	46/52 (88%)	44 (96%)	2 (4%)	0	100	100
1	G	47/52 (90%)	46 (98%)	1 (2%)	0	100	100
1	I	48/52 (92%)	48 (100%)	0	0	100	100
1	K	46/52 (88%)	44 (96%)	2 (4%)	0	100	100
1	M	45/52 (86%)	45 (100%)	0	0	100	100
1	O	48/52 (92%)	48 (100%)	0	0	100	100
1	Q	47/52 (90%)	46 (98%)	1 (2%)	0	100	100
1	S	48/52 (92%)	47 (98%)	0	1 (2%)	5	4
1	U	48/52 (92%)	45 (94%)	3 (6%)	0	100	100
1	W	48/52 (92%)	47 (98%)	1 (2%)	0	100	100
2	B	38/43 (88%)	33 (87%)	2 (5%)	3 (8%)	1	0
2	D	34/43 (79%)	32 (94%)	2 (6%)	0	100	100
2	F	34/43 (79%)	34 (100%)	0	0	100	100
2	H	35/43 (81%)	34 (97%)	1 (3%)	0	100	100
2	J	34/43 (79%)	31 (91%)	2 (6%)	1 (3%)	3	2
2	L	38/43 (88%)	35 (92%)	3 (8%)	0	100	100
2	N	35/43 (81%)	33 (94%)	2 (6%)	0	100	100
2	P	35/43 (81%)	35 (100%)	0	0	100	100
2	R	35/43 (81%)	35 (100%)	0	0	100	100
2	T	36/43 (84%)	34 (94%)	1 (3%)	1 (3%)	4	2
2	V	36/43 (84%)	35 (97%)	1 (3%)	0	100	100
2	X	36/43 (84%)	35 (97%)	0	1 (3%)	4	2
All	All	991/1140 (87%)	958 (97%)	25 (2%)	8 (1%)	16	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	481	LEU

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Mol	Chain	Res	Type
2	T	516	VAL
2	X	516	VAL
2	J	485	SER
2	B	517	ASN
2	B	482	VAL
1	C	161	GLU
1	S	207	VAL

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	46/48 (96%)	44 (96%)	2 (4%)	26	39
1	C	44/48 (92%)	41 (93%)	3 (7%)	14	20
1	E	44/48 (92%)	42 (96%)	2 (4%)	24	37
1	G	45/48 (94%)	43 (96%)	2 (4%)	25	38
1	I	46/48 (96%)	43 (94%)	3 (6%)	15	22
1	K	44/48 (92%)	42 (96%)	2 (4%)	24	37
1	M	43/48 (90%)	41 (95%)	2 (5%)	23	35
1	O	46/48 (96%)	44 (96%)	2 (4%)	26	39
1	Q	45/48 (94%)	43 (96%)	2 (4%)	25	38
1	S	46/48 (96%)	43 (94%)	3 (6%)	15	22
1	U	46/48 (96%)	44 (96%)	2 (4%)	26	39
1	W	46/48 (96%)	44 (96%)	2 (4%)	26	39
2	B	36/39 (92%)	34 (94%)	2 (6%)	19	28
2	D	34/39 (87%)	33 (97%)	1 (3%)	37	55
2	F	34/39 (87%)	33 (97%)	1 (3%)	37	55
2	H	35/39 (90%)	33 (94%)	2 (6%)	18	27
2	J	34/39 (87%)	33 (97%)	1 (3%)	37	55
2	L	38/39 (97%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	35/39 (90%)	33 (94%)	2 (6%)	18	27
2	P	35/39 (90%)	33 (94%)	2 (6%)	18	27
2	R	35/39 (90%)	34 (97%)	1 (3%)	37	55
2	T	36/39 (92%)	35 (97%)	1 (3%)	38	56
2	V	36/39 (92%)	34 (94%)	2 (6%)	19	28
2	X	36/39 (92%)	35 (97%)	1 (3%)	38	56
All	All	965/1044 (92%)	922 (96%)	43 (4%)	24	37

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	GLU
1	A	171	LEU
2	B	481	LEU
2	B	485	SER
1	C	161	GLU
1	C	165	ASN
1	C	171	LEU
2	D	481	LEU
1	E	164	VAL
1	E	171	LEU
2	F	487	GLU
1	G	165	ASN
1	G	171	LEU
2	H	487	GLU
2	H	494	GLN
1	I	161	GLU
1	I	163	GLU
1	I	171	LEU
2	J	481	LEU
1	K	171	LEU
1	K	173	SER
1	M	165	ASN
1	M	171	LEU
2	N	481	LEU
2	N	487	GLU
1	O	159	HIS
1	O	171	LEU
2	P	485	SER
2	P	487	GLU

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Mol	Chain	Res	Type
1	Q	171	LEU
1	Q	173	SER
2	R	487	GLU
1	S	165	ASN
1	S	171	LEU
1	S	173	SER
2	T	487	GLU
1	U	165	ASN
1	U	171	LEU
2	V	507	ARG
2	V	515	ASN
1	W	171	LEU
1	W	173	SER
2	X	487	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	ASN
2	B	501	GLN
2	B	517	ASN
1	C	165	ASN
2	D	500	ASN
2	D	514	HIS
1	E	165	ASN
2	F	501	GLN
2	F	515	ASN
1	G	208	ASN
2	H	494	GLN
2	H	500	ASN
2	H	515	ASN
1	I	208	ASN
2	J	500	ASN
2	J	514	HIS
1	K	208	ASN
2	L	494	GLN
2	L	501	GLN
2	L	514	HIS
2	N	500	ASN
2	N	501	GLN
2	N	515	ASN
1	Q	165	ASN

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Mol	Chain	Res	Type
1	Q	208	ASN
2	R	500	ASN
2	R	515	ASN
1	S	159	HIS
1	S	202	GLN
1	S	208	ASN
2	T	517	ASN
1	W	208	ASN
2	X	514	HIS
2	X	515	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.