



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:36 PM UTC

PDB ID : 1B6C / pdb_00001b6c
Title : CRYSTAL STRUCTURE OF THE CYTOPLASMIC DOMAIN OF THE
TYPE I TGF-BETA RECEPTOR IN COMPLEX WITH FKBP12
Authors : Huse, M.; Chen, Y.-G.; Massague, J.; Kuriyan, J.
Deposited on : 1999-01-13
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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
Mogul	:	2022.3.0, CSD as543be (2022)
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

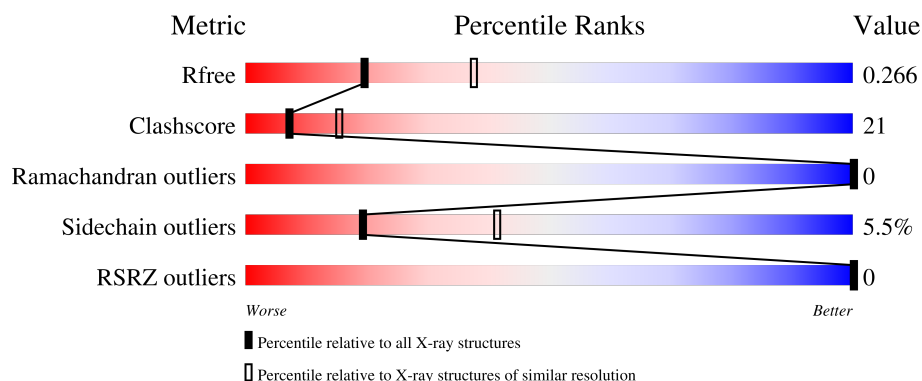
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	107	 66% 31% .
1	C	107	 65% 32% .
1	E	107	 66% 31% .
1	G	107	 66% 31% .
2	B	342	 57% 30% 8% 5%

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Mol	Chain	Length	Quality of chain
2	D	342	 54% 33% 8% 5%
2	F	342	 54% 30% 8% 8%
2	H	342	 56% 31% 8% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13748 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 FK506-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	107	Total	C	N	O	S	6	0	0
			831	527	146	154	4			
1	C	107	Total	C	N	O	S	6	0	0
			831	527	146	154	4			
1	E	107	Total	C	N	O	S	6	0	0
			831	527	146	154	4			
1	G	107	Total	C	N	O	S	6	0	0
			831	527	146	154	4			

- Molecule 2 is a protein called TGF-B SUPERFAMILY RECEPTOR TYPE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	326	Total	C	N	O	S	17	0	0
			2602	1642	467	477	16			
2	D	326	Total	C	N	O	S	17	0	0
			2602	1642	467	477	16			
2	F	314	Total	C	N	O	S	17	0	2
			2510	1584	452	458	16			
2	H	326	Total	C	N	O	S	17	0	0
			2602	1642	467	477	16			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

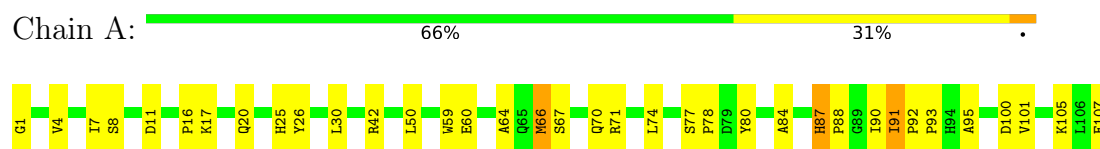
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	20	Total	O	0	0
			20	20		
4	C	2	Total	O	0	0
			2	2		
4	D	20	Total	O	0	0
			20	20		
4	E	2	Total	O	0	0
			2	2		
4	F	20	Total	O	0	0
			20	20		
4	G	2	Total	O	0	0
			2	2		
4	H	20	Total	O	0	0
			20	20		

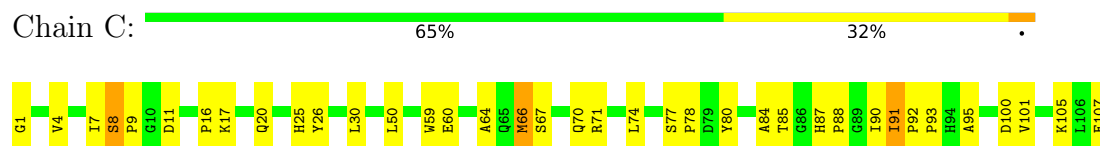
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

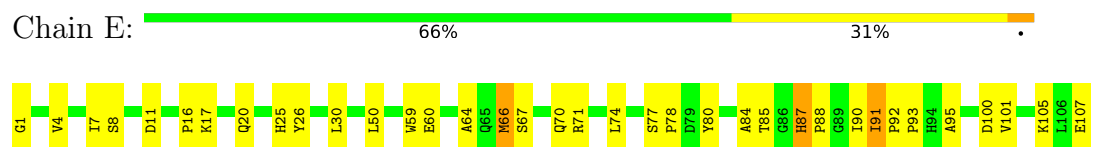
• Molecule 1: FK506-BINDING PROTEIN



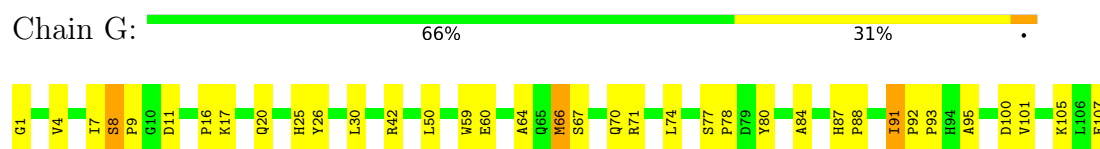
• Molecule 1: FK506-BINDING PROTEIN



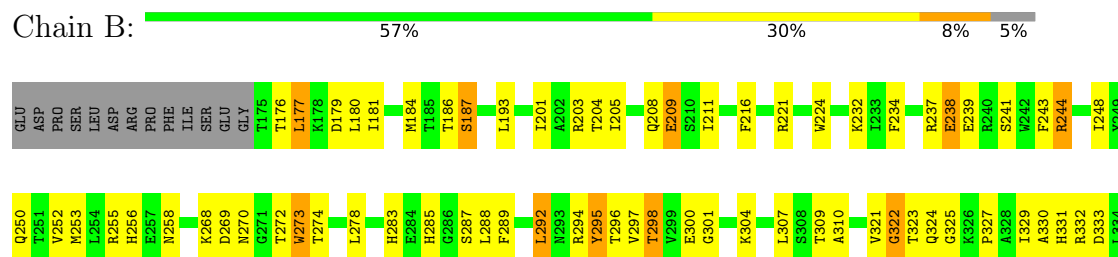
• Molecule 1: FK506-BINDING PROTEIN

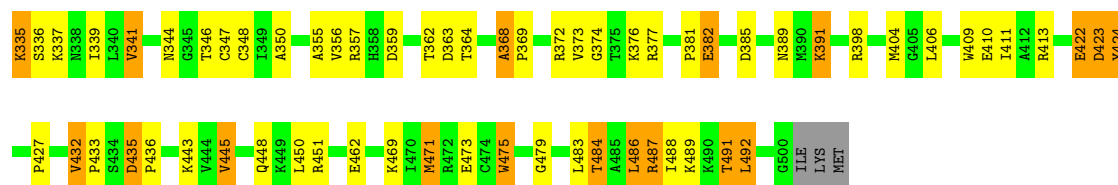


• Molecule 1: FK506-BINDING PROTEIN



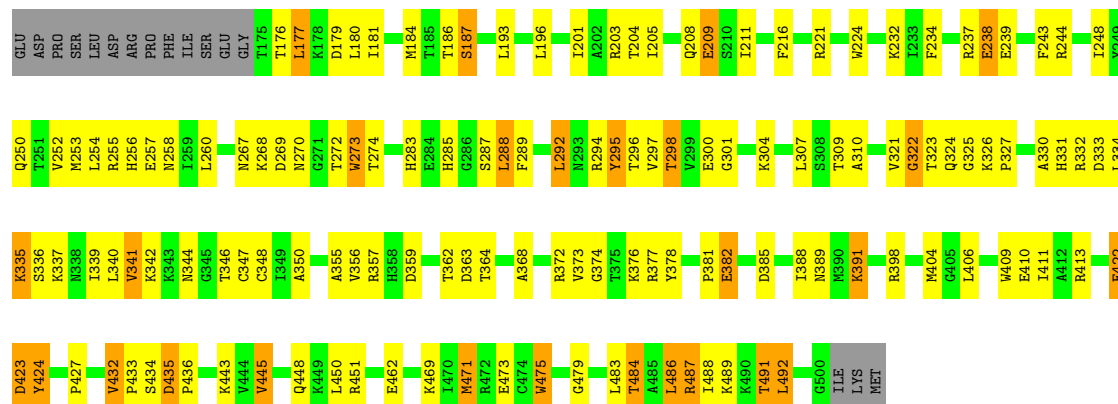
• Molecule 2: TGF-B SUPERFAMILY RECEPTOR TYPE I





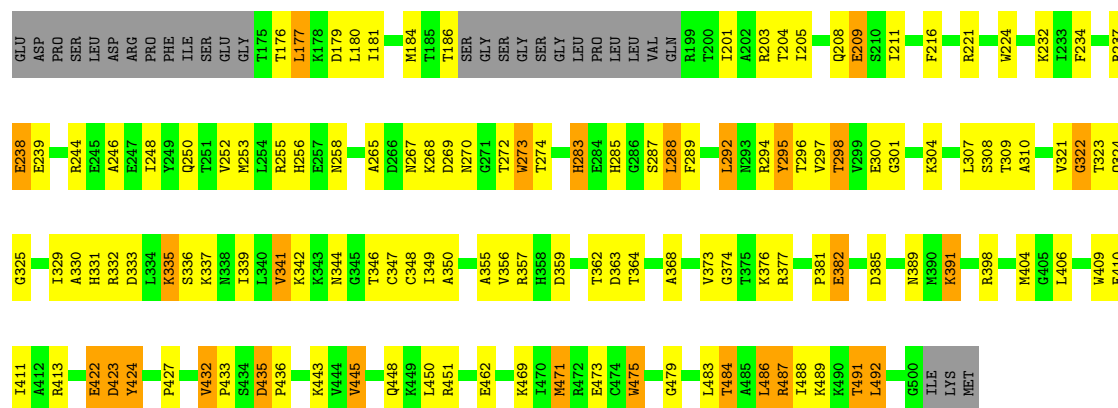
• Molecule 2: TGF-B SUPERFAMILY RECEPTOR TYPE I

Chain D: 54% 33% 8% 5%



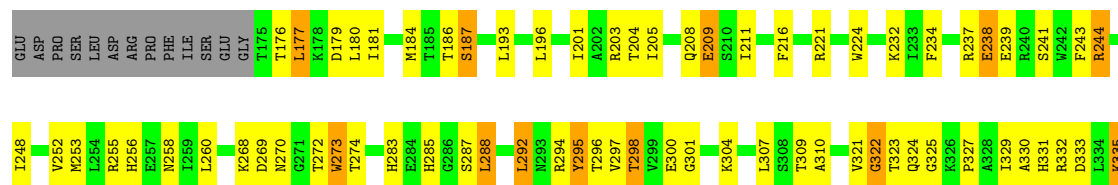
• Molecule 2: TGF-B SUPERFAMILY RECEPTOR TYPE I

Chain F: 54% 30% 8% 8%



• Molecule 2: TGF-B SUPERFAMILY RECEPTOR TYPE I

Chain H: 56% 31% 8% 5%



S336	K337	N338	I339	L340	V341	N344	G345	T346	C347	C348	T349	A350	A355	V356	R357	R358	D359	T362	D363	T364	A368	P369	R372	V373	G374	T375	K376	R377	Y378	P381	E382	D385	I388	N389	R390	K391	R398	M404	G405	L406	W409	E410	I411	A412	R413	E422	D423
Y424	P427	V432	P433	S434	D435	P436	K443	V444	V445	Q448	K449	L450	R451	E462	K469	I470	M471	R472	E473	G474	W475	G479	L483	T484	A485	L486	R487	I488	K489	R490	T491	L492	G500	ILE	LYS	MET											

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.58Å 81.06Å 90.53Å 86.23° 81.86° 63.92°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-2.60) 90.1 (30.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.60 (at 2.59Å)	Xtriage
Refinement program	CNS 0.3C	Depositor
R, R_{free}	0.249 , 0.269 0.248 , 0.266	Depositor DCC
R_{free} test set	5883 reflections (10.19%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 16.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.230 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13748	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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: SO4

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	0.61	0/850	1.26	12/1146 (1.0%)
1	C	0.60	0/850	1.26	12/1146 (1.0%)
1	E	0.59	0/850	1.26	12/1146 (1.0%)
1	G	0.59	0/850	1.26	12/1146 (1.0%)
2	B	0.71	2/2655 (0.1%)	1.16	24/3586 (0.7%)
2	D	0.71	2/2655 (0.1%)	1.15	23/3586 (0.6%)
2	F	0.74	3/2577 (0.1%)	1.16	22/3480 (0.6%)
2	H	0.73	3/2655 (0.1%)	1.16	23/3586 (0.6%)
All	All	0.70	10/13942 (0.1%)	1.18	140/18822 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	391	LYS	CG-CD	14.38	1.95	1.52
2	D	391	LYS	CG-CD	14.38	1.95	1.52
2	B	391	LYS	CG-CD	14.37	1.95	1.52
2	F	391	LYS	CG-CD	14.34	1.95	1.52
2	F	283	HIS	C-N	-9.93	1.19	1.33
2	H	283	HIS	C-N	7.52	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	471	MET	SD-CE	-7.12	1.61	1.79
2	B	471	MET	SD-CE	-6.99	1.62	1.79
2	D	471	MET	SD-CE	-6.94	1.62	1.79
2	H	471	MET	SD-CE	-6.89	1.62	1.79

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	324	GLN	OE1-CD-NE2	-9.84	112.76	122.60
2	H	324	GLN	OE1-CD-NE2	-9.82	112.78	122.60
2	B	324	GLN	OE1-CD-NE2	-9.81	112.78	122.60
2	D	324	GLN	OE1-CD-NE2	-9.76	112.84	122.60
2	B	376	LYS	N-CA-C	8.98	121.07	111.28
2	H	376	LYS	N-CA-C	8.98	121.07	111.28
2	D	376	LYS	N-CA-C	8.97	121.05	111.28
2	F	376	LYS	N-CA-C	8.97	121.05	111.28
1	A	66	MET	N-CA-C	-8.58	97.82	110.52
2	H	391	LYS	CB-CG-CD	-8.42	91.94	111.30
2	D	391	LYS	CB-CG-CD	-8.41	91.96	111.30
2	B	391	LYS	CB-CG-CD	-8.40	91.97	111.30
2	F	391	LYS	CB-CG-CD	-8.38	92.01	111.30
2	H	432	VAL	N-CA-C	8.35	116.04	109.19
2	B	432	VAL	N-CA-C	8.35	116.03	109.19
2	D	432	VAL	N-CA-C	8.22	115.93	109.19
2	F	432	VAL	N-CA-C	8.18	115.90	109.19
2	D	296	THR	N-CA-C	-8.17	98.37	110.46
2	F	296	THR	N-CA-C	-8.14	98.42	110.46
2	F	475	TRP	N-CA-C	8.12	122.90	112.92
2	H	296	THR	N-CA-C	-8.10	98.48	110.46
2	D	475	TRP	N-CA-C	8.07	122.85	112.92
2	H	475	TRP	N-CA-C	8.06	122.83	112.92
2	B	475	TRP	N-CA-C	8.05	122.82	112.92
2	B	296	THR	N-CA-C	-8.02	98.58	110.46
1	A	7	ILE	N-CA-C	-7.71	105.65	111.90
1	C	66	MET	N-CA-C	-7.60	99.27	110.52
1	C	7	ILE	N-CA-C	-7.60	105.75	111.90
1	G	7	ILE	N-CA-C	-7.59	105.75	111.90
1	E	7	ILE	N-CA-C	-7.58	105.76	111.90
2	H	368	ALA	CA-C-N	7.58	127.86	119.90
2	H	368	ALA	C-N-CA	7.58	127.86	119.90
1	E	66	MET	N-CA-C	-7.57	99.32	110.52
1	G	66	MET	N-CA-C	-7.56	99.33	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	368	ALA	CA-C-N	7.55	127.83	119.90
2	D	368	ALA	C-N-CA	7.55	127.83	119.90
2	B	368	ALA	CA-C-N	7.54	127.82	119.90
2	B	368	ALA	C-N-CA	7.54	127.82	119.90
2	F	368	ALA	CA-C-N	7.45	127.72	119.90
2	F	368	ALA	C-N-CA	7.45	127.72	119.90
2	H	445	VAL	N-CA-C	7.27	118.93	111.00
2	D	445	VAL	N-CA-C	7.26	118.91	111.00
2	B	445	VAL	N-CA-C	7.23	118.88	111.00
2	F	445	VAL	N-CA-C	7.20	118.84	111.00
1	G	8	SER	CA-C-N	6.89	126.86	119.76
1	G	8	SER	C-N-CA	6.89	126.86	119.76
1	E	8	SER	CA-C-N	6.82	126.79	119.76
1	E	8	SER	C-N-CA	6.82	126.79	119.76
2	H	283	HIS	O-C-N	6.76	133.27	122.99
1	C	8	SER	CA-C-N	6.74	126.70	119.76
1	C	8	SER	C-N-CA	6.74	126.70	119.76
1	A	8	SER	CA-C-N	6.73	126.69	119.76
1	A	8	SER	C-N-CA	6.73	126.69	119.76
2	H	324	GLN	CG-CD-NE2	6.68	126.42	116.40
2	F	324	GLN	CG-CD-NE2	6.68	126.42	116.40
2	D	324	GLN	CG-CD-NE2	6.66	126.39	116.40
2	B	324	GLN	CG-CD-NE2	6.66	126.39	116.40
1	G	91	ILE	CA-C-N	6.44	124.36	119.66
1	G	91	ILE	C-N-CA	6.44	124.36	119.66
1	A	91	ILE	CA-C-N	6.39	124.33	119.66
1	A	91	ILE	C-N-CA	6.39	124.33	119.66
1	E	91	ILE	CA-C-N	6.38	124.32	119.66
1	E	91	ILE	C-N-CA	6.38	124.32	119.66
1	C	91	ILE	CA-C-N	6.28	124.24	119.66
1	C	91	ILE	C-N-CA	6.28	124.24	119.66
1	C	67	SER	N-CA-C	-6.25	100.45	110.14
2	B	435	ASP	CA-C-N	6.25	126.00	119.76
2	B	435	ASP	C-N-CA	6.25	126.00	119.76
1	A	67	SER	N-CA-C	-6.22	100.50	110.14
1	E	67	SER	N-CA-C	-6.21	100.51	110.14
2	F	283	HIS	O-C-N	-6.18	114.65	123.06
1	E	87	HIS	CA-C-N	6.17	127.55	119.84
1	E	87	HIS	C-N-CA	6.17	127.55	119.84
1	C	87	HIS	CA-C-N	6.16	127.54	119.84
1	C	87	HIS	C-N-CA	6.16	127.54	119.84
2	H	435	ASP	CA-C-N	6.16	125.92	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	435	ASP	C-N-CA	6.16	125.92	119.76
1	G	67	SER	N-CA-C	-6.15	100.60	110.14
1	A	87	HIS	CA-C-N	6.14	127.52	119.84
1	A	87	HIS	C-N-CA	6.14	127.52	119.84
1	G	87	HIS	CA-C-N	6.14	127.51	119.84
1	G	87	HIS	C-N-CA	6.14	127.51	119.84
2	D	435	ASP	CA-C-N	6.14	125.90	119.76
2	D	435	ASP	C-N-CA	6.14	125.90	119.76
2	F	435	ASP	CA-C-N	6.14	125.90	119.76
2	F	435	ASP	C-N-CA	6.14	125.90	119.76
2	B	283	HIS	CA-C-N	6.08	128.71	120.38
2	B	283	HIS	C-N-CA	6.08	128.71	120.38
1	C	30	LEU	N-CA-C	-5.98	101.92	110.59
1	A	30	LEU	N-CA-C	-5.95	101.96	110.59
1	E	30	LEU	N-CA-C	-5.95	101.96	110.59
1	G	30	LEU	N-CA-C	-5.93	101.98	110.59
2	B	187	SER	N-CA-C	-5.92	101.42	110.30
2	H	187	SER	N-CA-C	-5.90	101.45	110.30
2	D	187	SER	N-CA-C	-5.86	101.51	110.30
2	B	295	TYR	N-CA-C	5.84	119.08	109.85
2	H	295	TYR	N-CA-C	5.79	118.99	109.72
2	F	295	TYR	N-CA-C	5.78	118.97	109.85
2	H	237	ARG	N-CA-C	5.77	118.34	111.71
2	D	295	TYR	N-CA-C	5.75	118.94	109.85
2	D	237	ARG	N-CA-C	5.73	118.30	111.71
2	B	237	ARG	N-CA-C	5.73	118.30	111.71
2	F	237	ARG	N-CA-C	5.70	118.26	111.71
2	B	283	HIS	O-C-N	-5.66	115.90	123.14
2	D	324	GLN	N-CA-C	-5.56	106.81	113.21
2	F	324	GLN	N-CA-C	-5.56	106.81	113.21
2	B	324	GLN	N-CA-C	-5.51	106.87	113.21
2	H	324	GLN	N-CA-C	-5.39	107.01	113.21
2	H	179	ASP	N-CA-C	-5.34	105.35	111.07
2	F	423	ASP	N-CA-C	-5.34	103.34	110.55
2	F	179	ASP	N-CA-C	-5.33	105.36	111.07
2	H	423	ASP	N-CA-C	-5.32	103.36	110.55
2	B	179	ASP	N-CA-C	-5.32	105.38	111.07
2	D	423	ASP	N-CA-C	-5.30	103.39	110.55
2	H	322	GLY	N-CA-C	5.30	117.45	112.04
2	B	322	GLY	N-CA-C	5.30	117.45	112.04
2	H	462	GLU	N-CA-C	5.27	117.71	111.33
2	B	423	ASP	N-CA-C	-5.27	103.44	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	179	ASP	N-CA-C	-5.27	105.44	111.07
2	D	462	GLU	N-CA-C	5.26	117.70	111.33
2	B	462	GLU	N-CA-C	5.25	117.69	111.33
2	D	322	GLY	N-CA-C	5.21	117.36	112.04
2	F	462	GLU	N-CA-C	5.19	117.61	111.33
2	F	322	GLY	N-CA-C	5.18	117.33	112.04
2	D	288	LEU	N-CA-C	-5.13	105.69	111.28
2	F	288	LEU	N-CA-C	-5.11	105.71	111.28
1	E	77	SER	CA-C-N	5.10	126.22	119.84
1	E	77	SER	C-N-CA	5.10	126.22	119.84
2	H	288	LEU	N-CA-C	-5.09	105.73	111.28
1	A	77	SER	CA-C-N	5.07	126.17	119.84
1	A	77	SER	C-N-CA	5.07	126.17	119.84
2	B	176	THR	N-CA-C	5.07	117.39	110.55
1	G	77	SER	CA-C-N	5.07	126.17	119.84
1	G	77	SER	C-N-CA	5.07	126.17	119.84
2	H	176	THR	N-CA-C	5.06	117.38	110.55
2	D	176	THR	N-CA-C	5.05	117.37	110.55
1	C	77	SER	CA-C-N	5.04	126.14	119.84
1	C	77	SER	C-N-CA	5.04	126.14	119.84
2	D	434	SER	N-CA-C	-5.03	103.41	110.50
2	F	176	THR	N-CA-C	5.03	117.34	110.55

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	424	TYR	Sidechain
2	D	424	TYR	Sidechain
2	F	424	TYR	Sidechain
2	H	424	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	831	0	831	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	831	0	831	20	0
1	E	831	0	831	27	0
1	G	831	0	831	19	0
2	B	2602	0	2606	126	0
2	D	2602	0	2606	127	0
2	F	2510	0	2525	131	0
2	H	2602	0	2606	123	0
3	B	5	0	0	1	0
3	D	5	0	0	1	0
3	F	5	0	0	1	0
3	H	5	0	0	1	0
4	A	2	0	0	0	0
4	B	20	0	0	0	0
4	C	2	0	0	0	0
4	D	20	0	0	0	0
4	E	2	0	0	0	0
4	F	20	0	0	0	0
4	G	2	0	0	0	0
4	H	20	0	0	0	0
All	All	13748	0	13667	565	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 21.

All (565) 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)
2:H:484:THR:HG22	2:H:487:ARG:H	1.28	0.97
2:B:484:THR:HG22	2:B:487:ARG:H	1.28	0.97
2:D:484:THR:HG22	2:D:487:ARG:H	1.28	0.94
2:F:484:THR:HG22	2:F:487:ARG:H	1.28	0.94
2:H:310:ALA:HA	2:H:404:MET:HE1	1.52	0.92
2:H:216:PHE:CE2	2:H:372:ARG:HD2	2.04	0.92
2:F:310:ALA:HA	2:F:404:MET:HE1	1.52	0.91
2:D:310:ALA:HA	2:D:404:MET:HE1	1.52	0.89
2:D:216:PHE:CE2	2:D:372:ARG:HD2	2.07	0.89
2:F:443:LYS:HG2	2:F:448:GLN:HE21	1.39	0.87
2:B:310:ALA:HA	2:B:404:MET:HE1	1.52	0.87
2:H:443:LYS:HG2	2:H:448:GLN:HE21	1.39	0.87
2:B:443:LYS:HG2	2:B:448:GLN:HE21	1.39	0.86
2:D:443:LYS:HG2	2:D:448:GLN:HE21	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:180:LEU:HG	2:F:184:MET:HE2	1.58	0.85
2:B:180:LEU:HG	2:B:184:MET:HE2	1.58	0.84
2:D:180:LEU:HG	2:D:184:MET:HE2	1.58	0.84
2:H:180:LEU:HG	2:H:184:MET:HE2	1.58	0.83
1:A:66:MET:HA	1:A:70:GLN:OE1	1.78	0.83
2:D:409:TRP:HB2	2:D:471:MET:HE3	1.62	0.81
2:B:248:ILE:CD1	2:B:355:ALA:HB3	2.11	0.81
2:F:409:TRP:HB2	2:F:471:MET:HE3	1.62	0.81
2:B:409:TRP:HB2	2:B:471:MET:HE3	1.62	0.81
2:H:409:TRP:HB2	2:H:471:MET:HE3	1.62	0.80
2:B:469:LYS:O	2:B:473:GLU:HG2	1.82	0.80
2:B:193:LEU:CD1	2:B:201:ILE:HD12	2.12	0.80
1:E:66:MET:HA	1:E:70:GLN:OE1	1.82	0.80
2:D:209:GLU:OE2	2:D:221:ARG:NH1	2.16	0.79
2:D:469:LYS:O	2:D:473:GLU:HG2	1.82	0.79
2:F:469:LYS:O	2:F:473:GLU:HG2	1.82	0.79
1:A:88:PRO:HG3	2:B:243:PHE:CD1	2.18	0.79
2:B:209:GLU:OE2	2:B:221:ARG:NH1	2.16	0.79
1:C:66:MET:HA	1:C:70:GLN:OE1	1.82	0.79
2:F:209:GLU:OE2	2:F:221:ARG:NH1	2.16	0.79
2:H:209:GLU:OE2	2:H:221:ARG:NH1	2.16	0.79
2:D:193:LEU:CD1	2:D:201:ILE:HD12	2.12	0.79
2:F:252:VAL:HG11	2:F:329:ILE:HD11	1.65	0.79
1:G:66:MET:HA	1:G:70:GLN:OE1	1.82	0.79
2:H:193:LEU:CD1	2:H:201:ILE:HD12	2.12	0.79
2:H:469:LYS:O	2:H:473:GLU:HG2	1.82	0.79
2:D:309:THR:HG22	2:D:404:MET:HE2	1.66	0.78
2:B:309:THR:HG22	2:B:404:MET:HE2	1.66	0.78
2:F:309:THR:HG22	2:F:404:MET:HE2	1.65	0.77
2:H:309:THR:HG22	2:H:404:MET:HE2	1.66	0.76
2:H:409:TRP:HD1	2:H:471:MET:HE1	1.52	0.75
2:F:256:HIS:HD2	2:F:258:ASN:H	1.34	0.75
2:H:256:HIS:HD2	2:H:258:ASN:H	1.35	0.74
2:F:409:TRP:HD1	2:F:471:MET:HE1	1.51	0.74
2:H:193:LEU:HD13	2:H:201:ILE:HD12	1.69	0.74
2:B:413:ARG:NH1	2:B:423:ASP:O	2.21	0.74
2:B:409:TRP:HD1	2:B:471:MET:HE1	1.52	0.73
2:F:413:ARG:NH1	2:F:423:ASP:O	2.21	0.73
2:D:409:TRP:HD1	2:D:471:MET:HE1	1.51	0.73
2:B:256:HIS:HD2	2:B:258:ASN:H	1.35	0.73
2:H:413:ARG:NH1	2:H:423:ASP:O	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:256:HIS:HD2	2:D:258:ASN:H	1.35	0.73
2:D:413:ARG:NH1	2:D:423:ASP:O	2.21	0.73
2:D:193:LEU:HD13	2:D:201:ILE:HD12	1.69	0.73
2:B:193:LEU:HD13	2:B:201:ILE:HD12	1.69	0.72
2:H:331:HIS:HD2	2:H:333:ASP:H	1.37	0.72
2:B:252:VAL:HG11	2:B:329:ILE:HD11	1.72	0.72
2:B:298:THR:HG22	2:B:300:GLU:N	2.05	0.71
2:F:298:THR:HG22	2:F:300:GLU:N	2.05	0.71
2:D:331:HIS:HD2	2:D:333:ASP:H	1.37	0.71
2:F:331:HIS:HD2	2:F:333:ASP:H	1.37	0.71
1:A:88:PRO:HG3	2:B:243:PHE:CE1	2.25	0.71
2:D:298:THR:HG22	2:D:300:GLU:N	2.06	0.71
2:H:298:THR:HG22	2:H:300:GLU:N	2.06	0.70
2:F:484:THR:CG2	2:F:487:ARG:H	2.04	0.70
2:B:331:HIS:HD2	2:B:333:ASP:H	1.37	0.70
2:B:216:PHE:HD2	2:B:238:GLU:HG2	1.57	0.69
2:D:216:PHE:HD2	2:D:238:GLU:HG2	1.56	0.69
2:B:484:THR:CG2	2:B:487:ARG:H	2.03	0.69
2:F:216:PHE:HD2	2:F:238:GLU:HG2	1.57	0.69
2:D:484:THR:CG2	2:D:487:ARG:H	2.04	0.69
2:H:216:PHE:HD2	2:H:238:GLU:HG2	1.57	0.69
2:B:248:ILE:HD12	2:B:355:ALA:HB3	1.76	0.68
2:F:283:HIS:CE1	2:F:342:LYS:HG2	2.28	0.68
1:G:88:PRO:HG3	2:H:243:PHE:CE1	2.28	0.68
1:G:88:PRO:HG3	2:H:243:PHE:CD1	2.28	0.68
2:H:484:THR:CG2	2:H:487:ARG:H	2.03	0.67
2:D:310:ALA:HA	2:D:404:MET:CE	2.25	0.67
2:B:310:ALA:HA	2:B:404:MET:CE	2.25	0.67
2:H:298:THR:HG22	2:H:301:GLY:H	1.60	0.67
2:F:473:GLU:HB3	2:F:483:LEU:HG	1.77	0.66
1:G:42:ARG:HD2	2:H:184:MET:HG2	1.76	0.66
2:F:298:THR:HG22	2:F:301:GLY:H	1.60	0.66
2:B:298:THR:HG22	2:B:301:GLY:H	1.60	0.66
2:F:269:ASP:HA	2:F:274:THR:HA	1.78	0.66
2:F:310:ALA:HA	2:F:404:MET:CE	2.25	0.66
2:H:473:GLU:HB3	2:H:483:LEU:HG	1.78	0.66
2:D:298:THR:HG22	2:D:301:GLY:H	1.61	0.65
2:H:269:ASP:HA	2:H:274:THR:HA	1.78	0.65
2:H:310:ALA:HA	2:H:404:MET:CE	2.25	0.65
2:B:473:GLU:HB3	2:B:483:LEU:HG	1.77	0.65
2:D:269:ASP:HA	2:D:274:THR:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:ASP:HA	2:B:274:THR:HA	1.78	0.64
2:D:473:GLU:HB3	2:D:483:LEU:HG	1.78	0.64
1:E:88:PRO:CB	2:F:246:ALA:HB3	2.28	0.63
1:E:90:ILE:CG1	2:F:250:GLN:HG2	2.28	0.63
2:D:216:PHE:CD2	2:D:238:GLU:HG2	2.34	0.62
1:E:90:ILE:HG13	2:F:250:GLN:HG2	1.79	0.62
2:D:409:TRP:CD1	2:D:471:MET:HE1	2.35	0.61
2:H:216:PHE:CD2	2:H:238:GLU:HG2	2.35	0.61
2:B:216:PHE:CD2	2:B:238:GLU:HG2	2.35	0.61
2:D:331:HIS:CD2	2:D:333:ASP:H	2.18	0.61
2:F:211:ILE:HD11	2:F:221:ARG:HB2	1.83	0.61
2:H:211:ILE:HD11	2:H:221:ARG:HB2	1.83	0.60
2:B:211:ILE:HD11	2:B:221:ARG:HB2	1.83	0.60
2:D:211:ILE:HD11	2:D:221:ARG:HB2	1.83	0.60
2:D:473:GLU:CB	2:D:483:LEU:HG	2.32	0.60
2:F:216:PHE:CD2	2:F:238:GLU:HG2	2.35	0.60
2:F:298:THR:HG22	2:F:300:GLU:H	1.67	0.59
2:B:256:HIS:CD2	2:B:258:ASN:H	2.20	0.59
2:B:298:THR:HG22	2:B:300:GLU:H	1.67	0.59
2:H:331:HIS:CD2	2:H:333:ASP:H	2.18	0.59
2:F:331:HIS:CD2	2:F:333:ASP:H	2.18	0.59
2:B:473:GLU:CB	2:B:483:LEU:HG	2.32	0.59
2:F:204:THR:HG22	2:F:204:THR:O	2.02	0.59
2:F:473:GLU:CB	2:F:483:LEU:HG	2.32	0.59
2:H:248:ILE:CD1	2:H:355:ALA:HB3	2.31	0.59
2:H:260:LEU:HD13	2:H:340:LEU:HD12	1.85	0.59
2:H:473:GLU:CB	2:H:483:LEU:HG	2.32	0.59
2:D:336:SER:OG	2:D:410:GLU:OE1	2.21	0.58
2:H:377:ARG:HD2	3:H:504:SO4:O2	2.03	0.58
2:D:488:ILE:O	2:D:492:LEU:HB2	2.03	0.58
2:F:256:HIS:CD2	2:F:258:ASN:H	2.19	0.58
2:D:204:THR:O	2:D:204:THR:HG22	2.02	0.58
2:B:409:TRP:CD1	2:B:471:MET:HE1	2.36	0.58
2:D:377:ARG:HD2	3:D:504:SO4:O2	2.03	0.58
2:F:377:ARG:HD2	3:F:504:SO4:O2	2.03	0.58
2:B:204:THR:HG22	2:B:204:THR:O	2.02	0.58
2:B:336:SER:OG	2:B:410:GLU:OE1	2.21	0.58
2:H:204:THR:HG22	2:H:204:THR:O	2.02	0.58
2:H:298:THR:HG22	2:H:300:GLU:H	1.68	0.58
2:B:331:HIS:CD2	2:B:333:ASP:H	2.19	0.58
2:D:232:LYS:HD2	2:D:234:PHE:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:298:THR:HG22	2:D:300:GLU:H	1.67	0.57
2:F:488:ILE:O	2:F:492:LEU:HB2	2.04	0.57
1:C:4:VAL:HG22	1:C:74:LEU:HD22	1.87	0.57
2:F:298:THR:CG2	2:F:300:GLU:H	2.18	0.57
2:H:443:LYS:HG2	2:H:448:GLN:NE2	2.17	0.57
2:B:298:THR:CG2	2:B:300:GLU:H	2.17	0.57
2:B:377:ARG:HD2	3:B:158:SO4:O2	2.03	0.57
2:D:298:THR:CG2	2:D:300:GLU:H	2.18	0.57
2:F:258:ASN:C	2:F:348:CYS:HA	2.29	0.57
2:H:488:ILE:O	2:H:492:LEU:HB2	2.04	0.57
2:B:232:LYS:HD2	2:B:234:PHE:CZ	2.39	0.57
1:E:4:VAL:HG22	1:E:74:LEU:HD22	1.87	0.57
2:F:232:LYS:HD2	2:F:234:PHE:CZ	2.39	0.57
1:G:4:VAL:HG22	1:G:74:LEU:HD22	1.87	0.57
2:B:422:GLU:OE1	2:H:434:SER:HB3	2.05	0.57
2:F:336:SER:OG	2:F:410:GLU:OE1	2.21	0.57
2:B:216:PHE:CE2	2:B:372:ARG:HD2	2.40	0.57
2:H:336:SER:OG	2:H:410:GLU:OE1	2.21	0.57
2:H:232:LYS:HD2	2:H:234:PHE:CZ	2.39	0.56
2:H:409:TRP:CD1	2:H:471:MET:HE1	2.36	0.56
2:B:488:ILE:O	2:B:492:LEU:HB2	2.04	0.56
2:H:256:HIS:CD2	2:H:258:ASN:H	2.20	0.56
2:B:443:LYS:HG2	2:B:448:GLN:NE2	2.17	0.56
1:G:1:GLY:HA2	1:G:80:TYR:CD1	2.41	0.56
2:D:256:HIS:CD2	2:D:258:ASN:H	2.19	0.56
2:B:252:VAL:HG13	2:B:327:PRO:HD2	1.88	0.56
2:F:272:THR:HG1	2:F:273:TRP:HE3	1.53	0.56
2:H:298:THR:CG2	2:H:300:GLU:H	2.18	0.56
2:D:248:ILE:CD1	2:D:355:ALA:HB3	2.36	0.56
2:D:288:LEU:HG	2:D:292:LEU:HD22	1.88	0.56
2:F:409:TRP:CD1	2:F:471:MET:HE1	2.35	0.56
1:A:1:GLY:HA2	1:A:80:TYR:CD1	2.41	0.56
1:C:1:GLY:HA2	1:C:80:TYR:CD1	2.41	0.56
2:F:288:LEU:HG	2:F:292:LEU:HD22	1.88	0.56
2:F:346:THR:CG2	2:F:347:CYS:N	2.70	0.55
2:B:288:LEU:HG	2:B:292:LEU:HD22	1.88	0.55
2:H:288:LEU:HG	2:H:292:LEU:HD22	1.88	0.55
1:E:1:GLY:HA2	1:E:80:TYR:CD1	2.41	0.55
1:A:4:VAL:HG22	1:A:74:LEU:HD22	1.87	0.55
2:D:177:LEU:HD13	2:D:224:TRP:CZ3	2.42	0.55
2:B:253:MET:HE1	2:B:255:ARG:CZ	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:331:HIS:HE1	2:F:350:ALA:O	1.90	0.55
2:H:346:THR:CG2	2:H:347:CYS:N	2.69	0.55
2:F:443:LYS:HG2	2:F:448:GLN:NE2	2.17	0.54
2:B:346:THR:CG2	2:B:347:CYS:N	2.70	0.54
2:H:177:LEU:HD13	2:H:224:TRP:CZ3	2.42	0.54
2:B:331:HIS:HE1	2:B:350:ALA:O	1.90	0.54
2:D:346:THR:CG2	2:D:347:CYS:N	2.70	0.54
2:B:177:LEU:HD13	2:B:224:TRP:CZ3	2.42	0.54
2:D:253:MET:HE1	2:D:255:ARG:CZ	2.37	0.54
1:E:88:PRO:HB2	2:F:246:ALA:CB	2.37	0.54
2:F:253:MET:HE1	2:F:255:ARG:CZ	2.37	0.54
1:E:85:THR:HG21	2:F:267:ASN:HD22	1.73	0.54
2:F:432:VAL:HG13	2:F:433:PRO:HD2	1.90	0.54
2:B:177:LEU:HD11	2:B:201:ILE:HD13	1.90	0.54
2:D:331:HIS:HE1	2:D:350:ALA:O	1.91	0.54
2:H:323:THR:C	2:H:325:GLY:H	2.15	0.54
2:F:323:THR:C	2:F:325:GLY:H	2.15	0.53
2:B:323:THR:C	2:B:325:GLY:H	2.15	0.53
2:D:177:LEU:HD11	2:D:201:ILE:HD13	1.90	0.53
2:D:443:LYS:HG2	2:D:448:GLN:NE2	2.16	0.53
2:B:432:VAL:HG13	2:B:433:PRO:HD2	1.90	0.53
2:D:432:VAL:HG13	2:D:433:PRO:HD2	1.90	0.53
2:F:177:LEU:HD13	2:F:224:TRP:CZ3	2.42	0.53
2:H:331:HIS:HE1	2:H:350:ALA:O	1.91	0.53
2:D:323:THR:C	2:D:325:GLY:H	2.15	0.53
2:H:177:LEU:HD11	2:H:201:ILE:HD13	1.90	0.53
2:H:253:MET:HE1	2:H:255:ARG:CZ	2.37	0.53
2:H:248:ILE:HD12	2:H:355:ALA:HB3	1.91	0.53
2:D:258:ASN:C	2:D:348:CYS:HA	2.34	0.53
2:F:201:ILE:O	2:F:205:ILE:HG13	2.09	0.53
2:F:177:LEU:HD11	2:F:201:ILE:HD13	1.90	0.52
2:F:180:LEU:HG	2:F:184:MET:CE	2.36	0.52
2:H:432:VAL:HG13	2:H:433:PRO:HD2	1.90	0.52
2:D:433:PRO:O	2:D:436:PRO:HG3	2.10	0.52
2:D:252:VAL:HG13	2:D:327:PRO:HD2	1.91	0.52
2:B:272:THR:HG1	2:B:273:TRP:HE3	1.58	0.52
1:E:16:PRO:HG2	1:E:64:ALA:HA	1.92	0.52
2:H:180:LEU:HG	2:H:184:MET:CE	2.36	0.52
2:D:258:ASN:O	2:D:348:CYS:HA	2.09	0.52
2:B:288:LEU:HD21	2:B:411:ILE:HD11	1.92	0.52
2:F:433:PRO:O	2:F:436:PRO:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:201:ILE:O	2:H:205:ILE:HG13	2.09	0.52
2:B:201:ILE:O	2:B:205:ILE:HG13	2.10	0.52
2:D:201:ILE:O	2:D:205:ILE:HG13	2.09	0.52
1:A:16:PRO:HG2	1:A:64:ALA:HA	1.91	0.52
2:B:433:PRO:O	2:B:436:PRO:HG3	2.10	0.52
2:D:270:ASN:C	2:D:272:THR:H	2.18	0.51
2:H:208:GLN:C	2:H:209:GLU:HG3	2.35	0.51
2:H:216:PHE:CE2	2:H:372:ARG:CD	2.85	0.51
2:F:208:GLN:C	2:F:209:GLU:HG3	2.35	0.51
1:G:16:PRO:HG2	1:G:64:ALA:HA	1.92	0.51
2:F:270:ASN:C	2:F:272:THR:H	2.18	0.51
1:C:16:PRO:HG2	1:C:64:ALA:HA	1.91	0.51
2:B:244:ARG:NH1	2:B:368:ALA:HB2	2.26	0.51
2:D:193:LEU:HD11	2:D:201:ILE:HD12	1.92	0.51
2:F:288:LEU:HD21	2:F:411:ILE:HD11	1.92	0.51
2:B:346:THR:HG22	2:B:347:CYS:N	2.26	0.51
2:D:208:GLN:C	2:D:209:GLU:HG3	2.35	0.51
2:H:288:LEU:HD21	2:H:411:ILE:HD11	1.92	0.51
2:D:180:LEU:HG	2:D:184:MET:CE	2.36	0.51
2:D:288:LEU:HD21	2:D:411:ILE:HD11	1.91	0.51
2:F:346:THR:HG22	2:F:347:CYS:N	2.26	0.51
2:H:232:LYS:HD2	2:H:234:PHE:CE1	2.46	0.51
2:F:248:ILE:CD1	2:F:355:ALA:HB3	2.41	0.50
2:H:433:PRO:O	2:H:436:PRO:HG3	2.10	0.50
1:A:42:ARG:HD2	2:B:184:MET:HG2	1.93	0.50
2:D:272:THR:HG1	2:D:273:TRP:HE3	1.57	0.50
2:D:346:THR:HG22	2:D:347:CYS:N	2.26	0.50
2:D:283:HIS:CE1	2:D:342:LYS:HG2	2.46	0.50
2:B:270:ASN:C	2:B:272:THR:H	2.18	0.50
2:F:232:LYS:HD2	2:F:234:PHE:CE1	2.46	0.50
2:H:193:LEU:HD11	2:H:201:ILE:HD12	1.92	0.50
2:H:270:ASN:C	2:H:272:THR:H	2.18	0.50
2:F:258:ASN:O	2:F:348:CYS:HA	2.12	0.50
2:H:344:ASN:OD1	2:H:346:THR:HB	2.12	0.50
2:D:232:LYS:HD2	2:D:234:PHE:CE1	2.46	0.50
2:F:344:ASN:OD1	2:F:346:THR:HB	2.12	0.50
2:D:248:ILE:HD12	2:D:355:ALA:HB3	1.94	0.50
2:B:180:LEU:HG	2:B:184:MET:CE	2.36	0.49
2:B:232:LYS:HD2	2:B:234:PHE:CE1	2.47	0.49
1:E:88:PRO:HB2	2:F:246:ALA:HB3	1.94	0.49
2:B:344:ASN:OD1	2:B:346:THR:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:432:VAL:CG1	2:F:436:PRO:HG3	2.43	0.49
2:H:272:THR:HG1	2:H:273:TRP:HE3	1.59	0.49
2:D:432:VAL:HG13	2:D:433:PRO:CD	2.43	0.49
2:F:336:SER:OG	2:F:410:GLU:CD	2.56	0.49
1:A:50:LEU:HD12	1:A:60:GLU:HG3	1.95	0.49
2:D:344:ASN:OD1	2:D:346:THR:HB	2.12	0.49
2:B:432:VAL:CG1	2:B:436:PRO:HG3	2.43	0.49
1:C:88:PRO:HG3	2:D:243:PHE:CD1	2.48	0.49
2:B:336:SER:OG	2:B:410:GLU:CD	2.56	0.48
2:H:432:VAL:HG13	2:H:433:PRO:CD	2.43	0.48
2:B:208:GLN:C	2:B:209:GLU:HG3	2.35	0.48
2:D:432:VAL:CG1	2:D:436:PRO:HG3	2.43	0.48
2:H:346:THR:HG22	2:H:347:CYS:N	2.26	0.48
2:B:432:VAL:HG13	2:B:433:PRO:CD	2.43	0.48
1:C:50:LEU:HD12	1:C:60:GLU:HG3	1.95	0.48
2:H:492:LEU:HD12	2:H:492:LEU:HA	1.73	0.48
2:B:186:THR:O	2:B:187:SER:C	2.57	0.48
2:F:362:THR:O	2:F:364:THR:HG23	2.14	0.48
2:F:432:VAL:HG13	2:F:433:PRO:CD	2.43	0.48
1:E:88:PRO:HB3	2:F:246:ALA:HB3	1.96	0.48
2:B:362:THR:O	2:B:364:THR:HG23	2.14	0.48
2:D:362:THR:O	2:D:364:THR:HG23	2.14	0.48
2:D:186:THR:O	2:D:187:SER:C	2.57	0.48
2:D:385:ASP:OD1	2:D:385:ASP:C	2.57	0.48
2:H:432:VAL:CG1	2:H:436:PRO:HG3	2.43	0.48
2:D:398:ARG:HD3	2:D:479:GLY:C	2.39	0.48
1:E:50:LEU:HD12	1:E:60:GLU:HG3	1.95	0.48
2:H:385:ASP:C	2:H:385:ASP:OD1	2.57	0.48
2:B:389:ASN:ND2	2:B:391:LYS:H	2.12	0.47
1:C:90:ILE:HG13	2:D:250:GLN:HG2	1.94	0.47
2:D:336:SER:OG	2:D:410:GLU:CD	2.56	0.47
2:F:389:ASN:C	2:F:389:ASN:HD22	2.22	0.47
2:F:450:LEU:O	2:F:451:ARG:HD3	2.14	0.47
2:B:297:VAL:HG22	2:B:298:THR:N	2.30	0.47
2:F:389:ASN:ND2	2:F:391:LYS:H	2.12	0.47
1:G:50:LEU:HD12	1:G:60:GLU:HG3	1.95	0.47
2:F:385:ASP:C	2:F:385:ASP:OD1	2.57	0.47
2:H:336:SER:OG	2:H:410:GLU:CD	2.57	0.47
2:H:389:ASN:C	2:H:389:ASN:HD22	2.23	0.47
2:D:389:ASN:ND2	2:D:391:LYS:H	2.13	0.47
2:B:193:LEU:HD11	2:B:201:ILE:HD12	1.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:450:LEU:O	2:B:451:ARG:HD3	2.15	0.47
2:H:297:VAL:HG22	2:H:298:THR:N	2.30	0.47
2:H:409:TRP:CB	2:H:471:MET:HE3	2.40	0.47
2:D:450:LEU:O	2:D:451:ARG:HD3	2.14	0.47
2:F:363:ASP:OD1	2:F:363:ASP:O	2.33	0.47
2:F:398:ARG:HD3	2:F:479:GLY:C	2.39	0.47
2:H:362:THR:O	2:H:364:THR:HG23	2.14	0.47
2:B:363:ASP:OD1	2:B:363:ASP:O	2.33	0.47
2:F:297:VAL:HG22	2:F:298:THR:N	2.30	0.47
2:B:184:MET:CE	2:B:193:LEU:HD22	2.45	0.47
2:B:385:ASP:OD1	2:B:385:ASP:C	2.57	0.47
2:D:184:MET:CE	2:D:193:LEU:HD22	2.45	0.47
2:D:260:LEU:HD13	2:D:340:LEU:HD12	1.97	0.47
1:G:26:TYR:HA	1:G:100:ASP:O	2.15	0.47
2:D:297:VAL:HG22	2:D:298:THR:N	2.30	0.47
2:F:252:VAL:HG11	2:F:329:ILE:CD1	2.42	0.47
2:B:398:ARG:HD3	2:B:479:GLY:C	2.39	0.46
2:H:238:GLU:O	2:H:239:GLU:C	2.58	0.46
2:H:398:ARG:HD3	2:H:479:GLY:C	2.39	0.46
2:B:432:VAL:HG12	2:B:433:PRO:O	2.15	0.46
2:D:389:ASN:C	2:D:389:ASN:HD22	2.22	0.46
2:F:432:VAL:HG12	2:F:433:PRO:O	2.15	0.46
2:B:484:THR:HG23	2:B:486:LEU:H	1.80	0.46
2:F:489:LYS:HD2	2:F:489:LYS:C	2.41	0.46
2:H:186:THR:O	2:H:187:SER:C	2.57	0.46
2:H:389:ASN:ND2	2:H:391:LYS:H	2.12	0.46
2:H:450:LEU:O	2:H:451:ARG:HD3	2.15	0.46
2:H:489:LYS:HD2	2:H:489:LYS:C	2.41	0.46
1:A:91:ILE:HA	1:A:92:PRO:HD3	1.83	0.46
1:C:26:TYR:CZ	2:D:196:LEU:HD22	2.50	0.46
2:F:492:LEU:HD12	2:F:492:LEU:HA	1.73	0.46
2:B:238:GLU:O	2:B:239:GLU:C	2.59	0.46
2:D:484:THR:HG23	2:D:486:LEU:H	1.80	0.46
1:G:8:SER:HA	1:G:9:PRO:HD3	1.80	0.46
2:H:184:MET:CE	2:H:193:LEU:HD22	2.45	0.46
2:B:471:MET:HE2	2:B:475:TRP:CH2	2.51	0.46
2:B:489:LYS:C	2:B:489:LYS:HD2	2.41	0.46
2:H:363:ASP:OD1	2:H:363:ASP:O	2.33	0.46
2:H:432:VAL:HG12	2:H:433:PRO:O	2.16	0.46
2:B:389:ASN:HD22	2:B:389:ASN:C	2.22	0.46
2:D:413:ARG:NH1	2:D:422:GLU:HB3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:492:LEU:HD12	2:D:492:LEU:HA	1.73	0.46
1:E:26:TYR:HA	1:E:100:ASP:O	2.15	0.46
2:F:471:MET:HE2	2:F:475:TRP:CH2	2.51	0.46
2:H:270:ASN:C	2:H:272:THR:N	2.74	0.46
1:E:90:ILE:HG12	2:F:250:GLN:HG2	1.97	0.46
2:B:413:ARG:NH1	2:B:422:GLU:HB3	2.31	0.46
2:F:484:THR:HG23	2:F:486:LEU:H	1.80	0.46
2:H:413:ARG:NH1	2:H:422:GLU:HB3	2.31	0.46
2:D:363:ASP:OD1	2:D:363:ASP:O	2.33	0.46
2:D:432:VAL:HG12	2:D:433:PRO:O	2.16	0.46
2:F:270:ASN:C	2:F:272:THR:N	2.74	0.46
2:H:244:ARG:HG2	2:H:368:ALA:CB	2.46	0.46
2:H:373:VAL:HG22	2:H:374:GLY:H	1.81	0.46
2:B:357:ARG:HD2	2:B:359:ASP:OD1	2.17	0.45
2:D:489:LYS:C	2:D:489:LYS:HD2	2.41	0.45
1:C:26:TYR:HA	1:C:100:ASP:O	2.16	0.45
2:D:270:ASN:C	2:D:272:THR:N	2.74	0.45
1:A:26:TYR:HA	1:A:100:ASP:O	2.16	0.45
2:F:258:ASN:ND2	2:F:308:SER:HB2	2.31	0.45
2:H:471:MET:HE2	2:H:475:TRP:CH2	2.51	0.45
2:D:410:GLU:OE1	2:D:424:TYR:OH	2.27	0.45
2:D:471:MET:HE2	2:D:475:TRP:CH2	2.51	0.45
2:F:413:ARG:NH1	2:F:422:GLU:HB3	2.31	0.45
2:H:357:ARG:HD2	2:H:359:ASP:OD1	2.16	0.45
2:H:484:THR:HG23	2:H:486:LEU:H	1.80	0.45
2:D:381:PRO:HD2	2:D:382:GLU:OE2	2.17	0.45
2:D:294:ARG:HD2	2:D:295:TYR:CE1	2.52	0.45
2:H:294:ARG:HD2	2:H:295:TYR:CE1	2.52	0.45
2:B:373:VAL:HG22	2:B:374:GLY:H	1.81	0.45
2:B:381:PRO:HD2	2:B:382:GLU:OE2	2.17	0.45
2:D:216:PHE:CZ	2:D:372:ARG:HD2	2.52	0.45
2:D:331:HIS:O	2:D:332:ARG:HB2	2.17	0.45
2:F:373:VAL:HG22	2:F:374:GLY:H	1.81	0.45
2:H:331:HIS:O	2:H:332:ARG:HB2	2.17	0.45
2:D:406:LEU:HB3	2:D:427:PRO:HG2	1.99	0.45
1:E:90:ILE:HG12	2:F:250:GLN:CG	2.46	0.45
2:F:381:PRO:HD2	2:F:382:GLU:OE2	2.17	0.45
1:A:17:LYS:N	1:A:20:GLN:OE1	2.49	0.45
2:B:294:ARG:HD2	2:B:295:TYR:CE1	2.52	0.45
2:B:484:THR:HG22	2:B:487:ARG:N	2.12	0.45
1:C:85:THR:HG21	2:D:267:ASN:HD22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:238:GLU:O	2:D:239:GLU:C	2.59	0.45
2:F:294:ARG:HD2	2:F:295:TYR:CE1	2.52	0.45
2:H:381:PRO:HD2	2:H:382:GLU:OE2	2.17	0.45
2:D:373:VAL:HG22	2:D:374:GLY:H	1.82	0.44
2:F:216:PHE:HD2	2:F:238:GLU:CG	2.28	0.44
2:D:357:ARG:HD2	2:D:359:ASP:OD1	2.16	0.44
2:D:484:THR:HG22	2:D:487:ARG:N	2.13	0.44
1:C:11:ASP:C	1:C:11:ASP:OD1	2.61	0.44
1:C:17:LYS:N	1:C:20:GLN:OE1	2.49	0.44
2:F:238:GLU:O	2:F:239:GLU:C	2.58	0.44
2:H:368:ALA:HA	2:H:369:PRO:HD3	1.68	0.44
2:H:432:VAL:HG11	2:H:436:PRO:CG	2.48	0.44
1:A:1:GLY:HA2	1:A:80:TYR:CG	2.52	0.44
2:D:435:ASP:N	2:D:436:PRO:HD3	2.32	0.44
2:F:406:LEU:HB3	2:F:427:PRO:HG2	2.00	0.44
2:F:409:TRP:CB	2:F:471:MET:HE3	2.39	0.44
2:H:216:PHE:HD2	2:H:238:GLU:CG	2.28	0.44
2:F:357:ARG:HD2	2:F:359:ASP:OD1	2.17	0.44
2:F:432:VAL:HG11	2:F:436:PRO:CG	2.47	0.44
1:A:84:ALA:O	1:A:93:PRO:CB	2.66	0.44
2:B:435:ASP:N	2:B:436:PRO:HD3	2.32	0.44
1:C:1:GLY:HA2	1:C:80:TYR:CG	2.53	0.44
1:C:84:ALA:O	1:C:93:PRO:CB	2.66	0.44
2:D:389:ASN:ND2	2:D:389:ASN:C	2.76	0.44
1:G:1:GLY:HA2	1:G:80:TYR:CG	2.52	0.44
2:B:331:HIS:O	2:B:332:ARG:HB2	2.17	0.44
2:D:177:LEU:O	2:D:181:ILE:HG13	2.18	0.44
2:D:203:ARG:NH1	2:D:268:LYS:HG3	2.33	0.44
2:F:331:HIS:O	2:F:332:ARG:HB2	2.17	0.44
2:B:406:LEU:HB3	2:B:427:PRO:HG2	2.00	0.44
2:D:177:LEU:HD13	2:D:224:TRP:CE3	2.53	0.44
1:E:84:ALA:O	1:E:93:PRO:CB	2.66	0.44
2:H:252:VAL:HG11	2:H:329:ILE:HD11	1.99	0.44
2:H:435:ASP:N	2:H:436:PRO:HD3	2.33	0.44
2:B:177:LEU:O	2:B:181:ILE:HG13	2.18	0.44
2:B:278:LEU:HD12	2:B:278:LEU:HA	1.87	0.44
2:D:335:LYS:HD3	2:D:337:LYS:HB2	2.00	0.44
2:D:432:VAL:HG11	2:D:436:PRO:CG	2.48	0.44
2:F:177:LEU:O	2:F:181:ILE:HG13	2.18	0.44
2:H:216:PHE:HE2	2:H:372:ARG:HD2	1.74	0.44
2:B:203:ARG:NH1	2:B:268:LYS:HG3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:VAL:HG12	2:B:322:GLY:N	2.33	0.43
2:B:335:LYS:HD3	2:B:337:LYS:HB2	2.00	0.43
1:E:90:ILE:HD11	2:F:250:GLN:CD	2.43	0.43
2:F:335:LYS:HD3	2:F:337:LYS:HB2	2.00	0.43
1:G:84:ALA:O	1:G:93:PRO:CB	2.66	0.43
2:H:406:LEU:HB3	2:H:427:PRO:HG2	2.00	0.43
2:B:216:PHE:HD2	2:B:238:GLU:CG	2.28	0.43
2:D:321:VAL:HG12	2:D:322:GLY:N	2.33	0.43
2:F:203:ARG:NH1	2:F:268:LYS:HG3	2.33	0.43
2:B:389:ASN:ND2	2:B:389:ASN:C	2.76	0.43
2:D:382:GLU:CD	2:D:382:GLU:H	2.26	0.43
1:E:1:GLY:HA2	1:E:80:TYR:CG	2.53	0.43
1:E:11:ASP:C	1:E:11:ASP:OD1	2.61	0.43
2:B:382:GLU:H	2:B:382:GLU:CD	2.26	0.43
2:H:177:LEU:HD13	2:H:224:TRP:CE3	2.53	0.43
1:A:11:ASP:OD1	1:A:11:ASP:C	2.61	0.43
2:B:177:LEU:HD13	2:B:224:TRP:CE3	2.53	0.43
2:B:432:VAL:HG11	2:B:436:PRO:CG	2.48	0.43
2:F:484:THR:HG22	2:F:487:ARG:N	2.13	0.43
2:H:331:HIS:HD2	2:H:333:ASP:N	2.12	0.43
2:H:389:ASN:C	2:H:389:ASN:ND2	2.76	0.43
2:D:257:GLU:O	2:D:342:LYS:NZ	2.47	0.43
2:F:410:GLU:OE1	2:F:424:TYR:OH	2.26	0.43
2:F:177:LEU:HD13	2:F:224:TRP:CE3	2.53	0.43
2:F:382:GLU:CD	2:F:382:GLU:H	2.26	0.43
1:G:11:ASP:OD1	1:G:11:ASP:C	2.61	0.43
1:C:8:SER:HA	1:C:9:PRO:HD3	1.81	0.43
1:E:87:HIS:HE1	2:F:265:ALA:O	2.02	0.43
2:F:435:ASP:N	2:F:436:PRO:HD3	2.32	0.43
2:H:177:LEU:O	2:H:181:ILE:HG13	2.18	0.43
2:B:270:ASN:C	2:B:272:THR:N	2.74	0.43
2:B:391:LYS:O	2:B:391:LYS:HG2	2.19	0.43
2:H:203:ARG:NH1	2:H:268:LYS:HG3	2.33	0.43
1:E:17:LYS:N	1:E:20:GLN:OE1	2.49	0.43
2:F:432:VAL:CG1	2:F:436:PRO:CG	2.97	0.43
2:H:382:GLU:CD	2:H:382:GLU:H	2.26	0.43
1:E:91:ILE:HA	1:E:92:PRO:HD3	1.83	0.42
2:H:391:LYS:O	2:H:391:LYS:HG2	2.19	0.42
2:B:252:VAL:HG11	2:B:329:ILE:CD1	2.46	0.42
2:B:487:ARG:O	2:B:491:THR:HG23	2.19	0.42
2:H:321:VAL:HG12	2:H:322:GLY:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:335:LYS:HD3	2:H:337:LYS:HB2	2.00	0.42
2:B:368:ALA:HA	2:B:369:PRO:HD3	1.68	0.42
2:H:330:ALA:HB3	2:H:356:VAL:HG22	2.01	0.42
1:A:90:ILE:HD11	2:B:250:GLN:CD	2.44	0.42
1:C:91:ILE:HA	1:C:92:PRO:HD3	1.83	0.42
2:F:391:LYS:HG2	2:F:391:LYS:O	2.19	0.42
2:B:244:ARG:HG2	2:B:368:ALA:CB	2.49	0.42
2:D:432:VAL:CG1	2:D:436:PRO:CG	2.97	0.42
1:E:78:PRO:HG3	1:E:95:ALA:C	2.45	0.42
1:E:90:ILE:HD11	2:F:250:GLN:OE1	2.20	0.42
2:B:330:ALA:HB3	2:B:356:VAL:HG22	2.02	0.42
2:D:184:MET:HE3	2:D:193:LEU:HD22	2.02	0.42
2:B:409:TRP:CB	2:B:471:MET:HE3	2.40	0.42
2:D:331:HIS:HD2	2:D:333:ASP:N	2.12	0.42
2:F:321:VAL:HG12	2:F:322:GLY:N	2.33	0.42
2:F:330:ALA:HB3	2:F:356:VAL:HG22	2.02	0.42
1:C:71:ARG:HA	1:C:101:VAL:O	2.20	0.42
1:C:78:PRO:HG3	1:C:95:ALA:C	2.45	0.42
2:D:216:PHE:HD2	2:D:238:GLU:CG	2.28	0.42
1:E:88:PRO:HB2	2:F:246:ALA:HB1	2.02	0.42
1:G:105:LYS:HE3	1:G:107:GLU:OE2	2.20	0.42
2:H:487:ARG:O	2:H:491:THR:HG23	2.20	0.42
1:A:105:LYS:HE3	1:A:107:GLU:OE2	2.20	0.42
2:B:177:LEU:HD12	2:B:177:LEU:HA	1.87	0.42
2:D:330:ALA:HB3	2:D:356:VAL:HG22	2.01	0.42
2:D:487:ARG:O	2:D:491:THR:HG23	2.19	0.42
1:G:71:ARG:HA	1:G:101:VAL:O	2.20	0.42
2:H:432:VAL:CG1	2:H:436:PRO:CG	2.97	0.42
1:A:90:ILE:HG13	2:B:250:GLN:HG2	2.02	0.42
2:B:432:VAL:CG1	2:B:436:PRO:CG	2.97	0.42
2:F:177:LEU:HD12	2:F:177:LEU:HA	1.87	0.42
1:A:71:ARG:HA	1:A:101:VAL:O	2.20	0.41
2:F:389:ASN:C	2:F:389:ASN:ND2	2.76	0.41
2:B:248:ILE:HD13	2:B:355:ALA:HB3	1.97	0.41
2:D:391:LYS:O	2:D:391:LYS:HG2	2.19	0.41
2:D:409:TRP:HD1	2:D:471:MET:CE	2.27	0.41
2:F:487:ARG:O	2:F:491:THR:HG23	2.19	0.41
2:H:378:TYR:OH	2:H:410:GLU:OE2	2.38	0.41
2:B:184:MET:HE3	2:B:193:LEU:HD22	2.02	0.41
2:B:285:HIS:HB2	2:B:341:VAL:O	2.20	0.41
2:D:378:TYR:OH	2:D:410:GLU:OE2	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:PRO:HG3	1:G:95:ALA:C	2.45	0.41
2:H:252:VAL:HG13	2:H:327:PRO:HD2	2.02	0.41
2:D:285:HIS:HB2	2:D:341:VAL:O	2.20	0.41
2:D:445:VAL:HG13	2:D:451:ARG:NH1	2.36	0.41
2:F:204:THR:O	2:F:204:THR:CG2	2.69	0.41
1:G:26:TYR:CZ	2:H:196:LEU:HD22	2.56	0.41
1:A:78:PRO:HG3	1:A:95:ALA:C	2.45	0.41
2:B:410:GLU:OE1	2:B:424:TYR:OH	2.26	0.41
1:C:105:LYS:HE3	1:C:107:GLU:OE2	2.20	0.41
2:D:254:LEU:HD21	2:D:326:LYS:HE2	2.02	0.41
2:D:334:LEU:HD23	2:D:334:LEU:HA	1.90	0.41
2:F:180:LEU:HD12	2:F:180:LEU:HA	1.96	0.41
2:H:285:HIS:HB2	2:H:341:VAL:O	2.21	0.41
2:B:186:THR:HG22	2:B:187:SER:N	2.35	0.41
2:D:287:SER:HA	2:D:339:ILE:O	2.21	0.41
1:C:90:ILE:CG1	2:D:250:GLN:HG2	2.50	0.41
2:F:216:PHE:HB3	2:F:238:GLU:HG2	2.03	0.41
2:F:409:TRP:HD1	2:F:471:MET:CE	2.27	0.41
2:B:216:PHE:HB3	2:B:238:GLU:HG2	2.03	0.41
2:B:445:VAL:HG13	2:B:451:ARG:NH1	2.35	0.41
2:D:186:THR:HG22	2:D:187:SER:N	2.36	0.41
1:E:71:ARG:HA	1:E:101:VAL:O	2.20	0.41
2:F:331:HIS:HD2	2:F:333:ASP:N	2.12	0.41
2:H:388:ILE:HG23	2:H:388:ILE:O	2.21	0.41
2:H:445:VAL:HG13	2:H:451:ARG:NH1	2.35	0.41
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.93	0.41
2:B:253:MET:HE1	2:B:255:ARG:NH1	2.36	0.41
2:B:287:SER:HA	2:B:339:ILE:O	2.21	0.41
2:F:287:SER:HA	2:F:339:ILE:O	2.21	0.41
2:F:289:PHE:HB2	2:F:336:SER:HB2	2.03	0.41
2:B:238:GLU:HB3	2:B:241:SER:HB2	2.03	0.40
2:B:289:PHE:HB2	2:B:336:SER:HB2	2.03	0.40
2:D:272:THR:OG1	2:D:273:TRP:HE3	2.04	0.40
1:E:105:LYS:HE3	1:E:107:GLU:OE2	2.20	0.40
1:G:91:ILE:HA	1:G:92:PRO:HD3	1.83	0.40
2:H:184:MET:HE3	2:H:193:LEU:HD22	2.02	0.40
2:B:272:THR:OG1	2:B:273:TRP:HE3	2.04	0.40
2:F:285:HIS:HB2	2:F:341:VAL:O	2.20	0.40
2:F:445:VAL:HG13	2:F:451:ARG:NH1	2.36	0.40
2:F:253:MET:HE1	2:F:255:ARG:NH1	2.36	0.40
1:G:17:LYS:N	1:G:20:GLN:OE1	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:253:MET:HE1	2:H:255:ARG:NH1	2.36	0.40
2:B:258:ASN:O	2:B:348:CYS:HA	2.21	0.40
2:D:253:MET:HE1	2:D:255:ARG:NH1	2.36	0.40
2:D:289:PHE:HB2	2:D:336:SER:HB2	2.03	0.40
2:D:388:ILE:O	2:D:388:ILE:HG23	2.21	0.40
2:H:186:THR:HG22	2:H:187:SER:N	2.36	0.40
2:H:272:THR:OG1	2:H:273:TRP:HE3	2.04	0.40
2:D:409:TRP:CB	2:D:471:MET:HE3	2.40	0.40
2:F:258:ASN:O	2:F:349:ILE:N	2.45	0.40
2:H:238:GLU:HB3	2:H:241:SER:HB2	2.03	0.40
2:H:258:ASN:O	2:H:348:CYS:HA	2.22	0.40
2:H:287:SER:HA	2:H:339:ILE:O	2.21	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	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
1	C	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
1	E	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
1	G	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	B	324/342 (95%)	306 (94%)	18 (6%)	0	100	100
2	D	324/342 (95%)	307 (95%)	17 (5%)	0	100	100
2	F	312/342 (91%)	295 (95%)	17 (5%)	0	100	100
2	H	324/342 (95%)	307 (95%)	17 (5%)	0	100	100
All	All	1704/1796 (95%)	1611 (94%)	93 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	89/89 (100%)	87 (98%)	2 (2%)	45	72
1	C	89/89 (100%)	87 (98%)	2 (2%)	45	72
1	E	89/89 (100%)	87 (98%)	2 (2%)	45	72
1	G	89/89 (100%)	87 (98%)	2 (2%)	45	72
2	B	279/294 (95%)	261 (94%)	18 (6%)	15	35
2	D	279/294 (95%)	261 (94%)	18 (6%)	15	35
2	F	270/294 (92%)	252 (93%)	18 (7%)	15	33
2	H	279/294 (95%)	261 (94%)	18 (6%)	15	35
All	All	1463/1532 (96%)	1383 (94%)	80 (6%)	19	41

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	59	TRP
2	B	177	LEU
2	B	209	GLU
2	B	238	GLU
2	B	244	ARG
2	B	273	TRP
2	B	292	LEU
2	B	298	THR
2	B	304	LYS
2	B	307	LEU
2	B	335	LYS
2	B	341	VAL
2	B	382	GLU
2	B	422	GLU
2	B	484	THR
2	B	486	LEU
2	B	487	ARG
2	B	491	THR

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Mol	Chain	Res	Type
2	B	492	LEU
1	C	25	HIS
1	C	59	TRP
2	D	177	LEU
2	D	209	GLU
2	D	238	GLU
2	D	244	ARG
2	D	273	TRP
2	D	292	LEU
2	D	298	THR
2	D	304	LYS
2	D	307	LEU
2	D	335	LYS
2	D	341	VAL
2	D	382	GLU
2	D	422	GLU
2	D	484	THR
2	D	486	LEU
2	D	487	ARG
2	D	491	THR
2	D	492	LEU
1	E	25	HIS
1	E	59	TRP
2	F	177	LEU
2	F	209	GLU
2	F	238	GLU
2	F	244	ARG
2	F	273	TRP
2	F	292	LEU
2	F	298	THR
2	F	304	LYS
2	F	307	LEU
2	F	335	LYS
2	F	341	VAL
2	F	382	GLU
2	F	422	GLU
2	F	484	THR
2	F	486	LEU
2	F	487	ARG
2	F	491	THR
2	F	492	LEU
1	G	25	HIS

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Mol	Chain	Res	Type
1	G	59	TRP
2	H	177	LEU
2	H	209	GLU
2	H	238	GLU
2	H	244	ARG
2	H	273	TRP
2	H	292	LEU
2	H	298	THR
2	H	304	LYS
2	H	307	LEU
2	H	335	LYS
2	H	341	VAL
2	H	382	GLU
2	H	422	GLU
2	H	484	THR
2	H	486	LEU
2	H	487	ARG
2	H	491	THR
2	H	492	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	256	HIS
2	B	258	ASN
2	B	283	HIS
2	B	315	HIS
2	B	331	HIS
2	B	389	ASN
2	B	448	GLN
2	B	459	GLN
2	B	494	GLN
2	B	498	GLN
1	C	87	HIS
2	D	256	HIS
2	D	258	ASN
2	D	267	ASN
2	D	283	HIS
2	D	331	HIS
2	D	389	ASN
2	D	448	GLN
2	D	494	GLN

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Mol	Chain	Res	Type
2	D	498	GLN
1	E	87	HIS
2	F	258	ASN
2	F	267	ASN
2	F	283	HIS
2	F	315	HIS
2	F	331	HIS
2	F	389	ASN
2	F	448	GLN
2	F	459	GLN
2	F	494	GLN
2	F	498	GLN
2	H	256	HIS
2	H	283	HIS
2	H	315	HIS
2	H	331	HIS
2	H	389	ASN
2	H	448	GLN
2	H	459	GLN
2	H	494	GLN
2	H	498	GLN

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	B	158	-	4,4,4	0.51	0	6,6,6	0.18	0
3	SO4	H	504	-	4,4,4	0.52	0	6,6,6	0.18	0
3	SO4	D	504	-	4,4,4	0.55	0	6,6,6	0.19	0
3	SO4	F	504	-	4,4,4	0.54	0	6,6,6	0.18	0

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.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	158	SO4	1	0
3	H	504	SO4	1	0
3	D	504	SO4	1	0
3	F	504	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	283:HIS	C	284:GLU	N	1.19

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	107/107 (100%)	-1.54	0 100 100	30, 40, 51, 57	2 (1%)
1	C	107/107 (100%)	-1.60	0 100 100	30, 40, 52, 58	2 (1%)
1	E	107/107 (100%)	-1.54	0 100 100	30, 40, 52, 58	2 (1%)
1	G	107/107 (100%)	-1.58	0 100 100	30, 40, 51, 57	2 (1%)
2	B	326/342 (95%)	-1.60	0 100 100	13, 31, 64, 85	5 (1%)
2	D	326/342 (95%)	-1.55	0 100 100	15, 32, 64, 86	5 (1%)
2	F	314/342 (91%)	-1.49	0 100 100	16, 33, 66, 86	5 (1%)
2	H	326/342 (95%)	-1.58	0 100 100	15, 31, 64, 86	5 (1%)
All	All	1720/1796 (95%)	-1.56	0 100 100	13, 35, 60, 86	28 (1%)

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($\text{\AA}^2$)	Q<0.9
3	SO4	F	504	5/5	0.98	0.07	64,64,65,66	0
3	SO4	D	504	5/5	0.99	0.07	63,64,64,65	0
3	SO4	B	158	5/5	0.99	0.04	61,61,62,62	0
3	SO4	H	504	5/5	0.99	0.03	62,62,62,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.