



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:16 AM UTC

PDB ID : 5OTB / pdb_00005otb
Title : Structure of caprine serum albumin in P1 space group
Authors : Talaj, J.A.; Bujacz, A.; Bujacz, G.
Deposited on : 2017-08-21
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
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

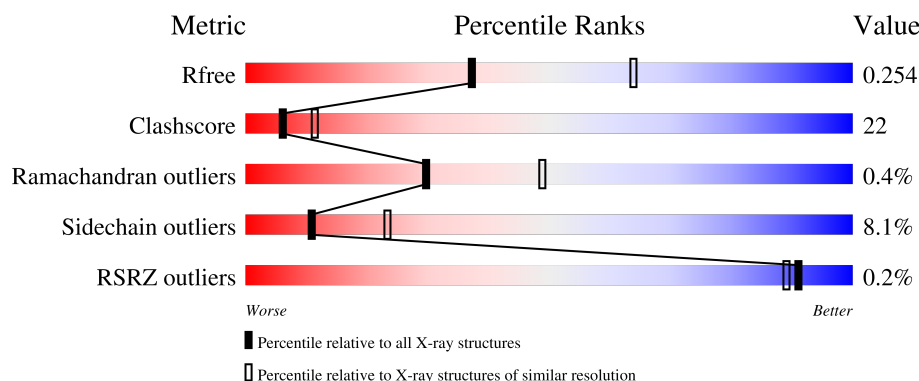
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	180053	5829 (2.50-2.50)
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	583	51% 41% 8%
1	B	583	53% 39% 8%
1	C	583	50% 42% 8%
1	D	583	53% 40% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PRO	A	602	-	-	X	-
3	PRO	B	602	-	-	X	-
3	PRO	D	602	-	-	X	-

2 Entry composition [i](#)

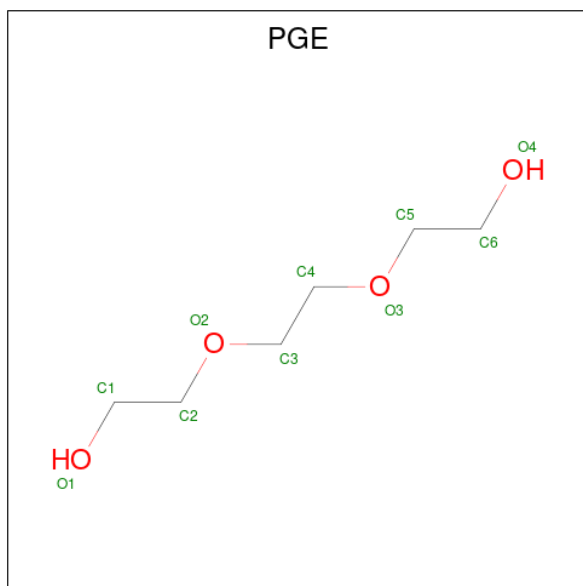
There are 5 unique types of molecules in this entry. The entry contains 19131 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4628	2922	777	890	39			
1	B	581	Total	C	N	O	S	0	0	0
			4627	2922	777	889	39			
1	C	581	Total	C	N	O	S	0	0	0
			4628	2922	777	890	39			
1	D	581	Total	C	N	O	S	0	1	0
			4634	2927	778	890	39			

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



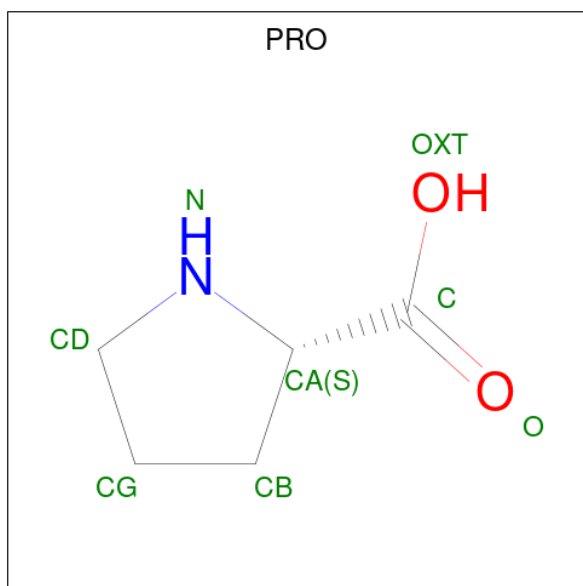
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	5	1	2		
3	A	1	Total	C	N	O	0	0
			8	5	1	2		
3	B	1	Total	C	N	O	0	0
			8	5	1	2		
3	B	1	Total	C	N	O	0	0
			8	5	1	2		
3	C	1	Total	C	N	O	0	0
			8	5	1	2		
3	C	1	Total	C	N	O	0	0
			8	5	1	2		
3	C	1	Total	C	N	O	0	0
			8	5	1	2		
3	D	1	Total	C	N	O	0	0
			8	5	1	2		
3	D	1	Total	C	N	O	0	0
			8	5	1	2		
3	D	1	Total	C	N	O	0	0
			8	5	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

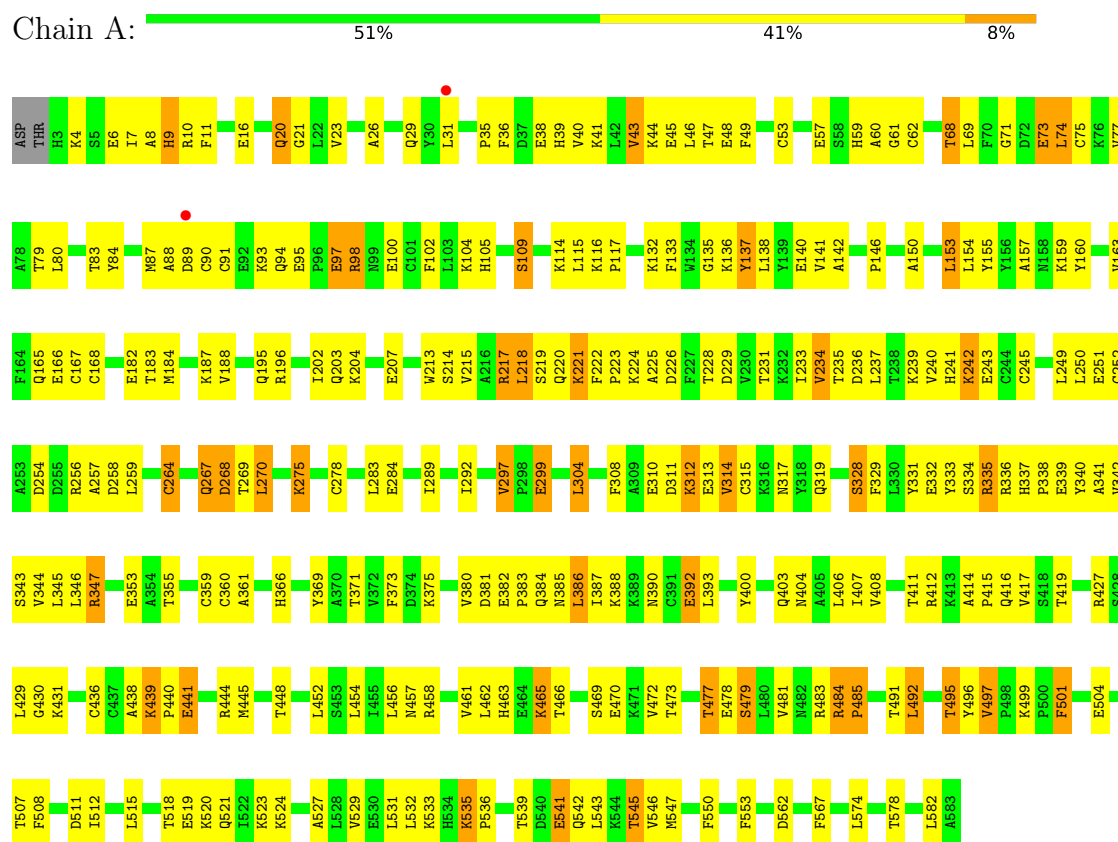
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	124	Total	O	0	0
			124	124		
5	C	124	Total	O	0	0
			124	124		
5	D	126	Total	O	0	0
			126	126		

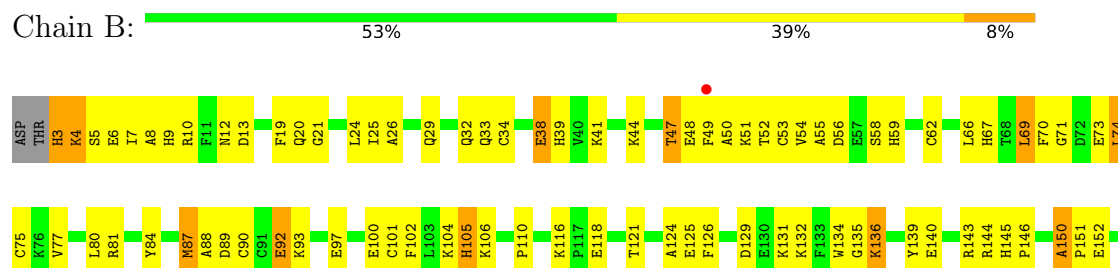
3 Residue-property plots [i](#)

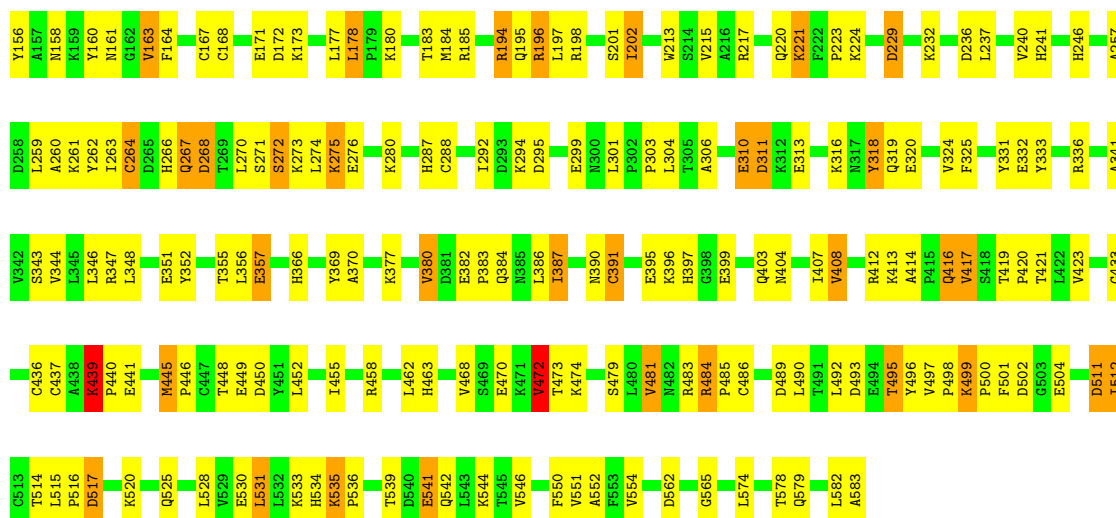
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



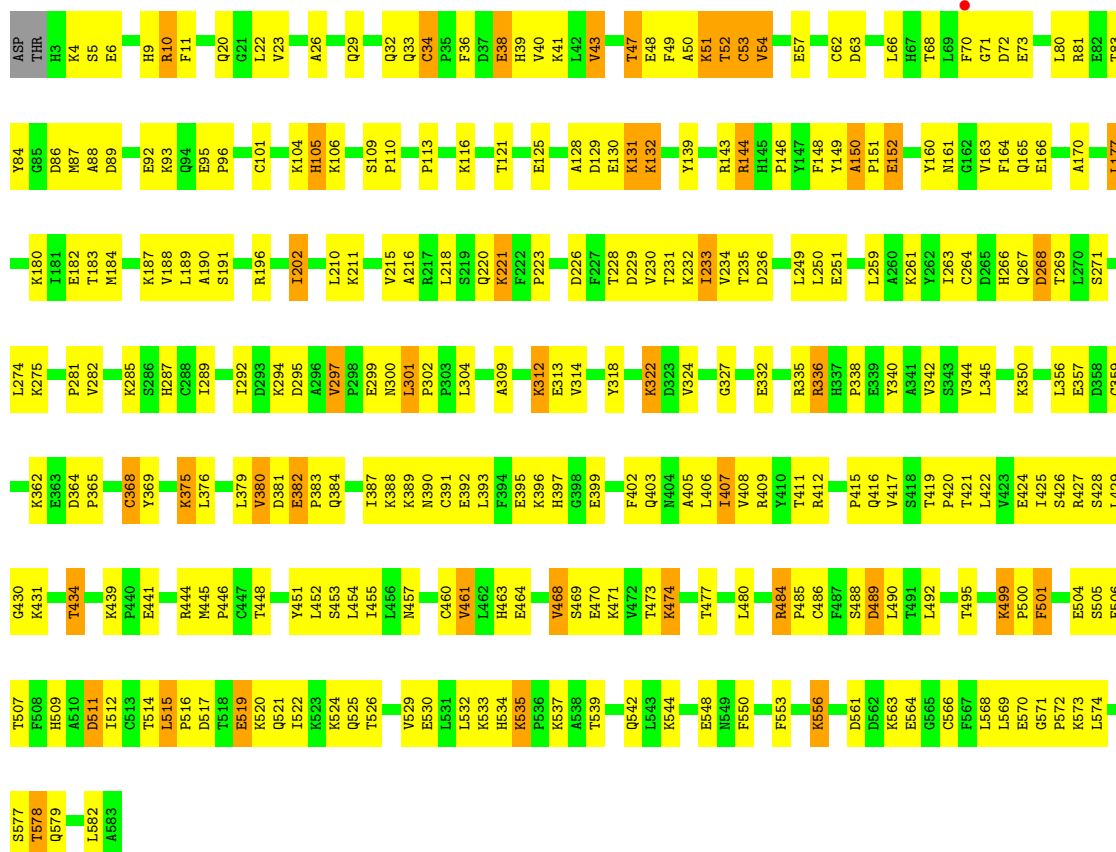
• Molecule 1: Albumin





• Molecule 1: Albumin

Chain C: 50% 42% 8%



• Molecule 1: Albumin

Chain D: 53% 40% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.75Å 80.93Å 110.53Å 90.01° 75.90° 72.22°	Depositor
Resolution (Å)	40.00 – 2.50 40.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.00-2.50) 98.1 (40.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.197 , 0.246 (Not available) , 0.254	Depositor DCC
R_{free} test set	1707 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19131	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.27% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.24	13/4724 (0.3%)	1.45	46/6376 (0.7%)
1	B	1.21	5/4723 (0.1%)	1.46	53/6374 (0.8%)
1	C	1.19	12/4724 (0.3%)	1.42	41/6376 (0.6%)
1	D	1.26	13/4733 (0.3%)	1.46	59/6387 (0.9%)
All	All	1.23	43/18904 (0.2%)	1.45	199/25513 (0.8%)

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150	ALA	C-O	-7.60	1.17	1.24
1	C	150	ALA	CA-C	-7.08	1.44	1.52
1	A	270	LEU	CA-C	6.79	1.57	1.52
1	D	124	ALA	CA-C	6.29	1.60	1.52
1	D	502	ASP	C-O	6.15	1.31	1.24
1	C	522	ILE	N-CA	-6.11	1.39	1.46
1	B	525	GLN	C-O	6.02	1.31	1.24
1	D	449	GLU	C-O	5.94	1.31	1.24
1	D	209	ALA	N-CA	-5.91	1.39	1.46
1	C	463	HIS	CA-C	-5.90	1.44	1.52
1	C	381	ASP	CA-CB	5.88	1.59	1.53
1	A	335	ARG	CA-C	5.80	1.60	1.52
1	D	24	LEU	N-CA	5.71	1.53	1.46
1	D	194	ARG	CA-C	-5.61	1.45	1.52
1	A	89	ASP	N-CA	5.55	1.53	1.46
1	C	132	LYS	CA-C	5.53	1.59	1.52
1	C	480	LEU	N-CA	-5.53	1.39	1.46
1	B	391	CYS	N-CA	5.52	1.53	1.46
1	A	283	LEU	CA-C	5.50	1.59	1.52
1	D	164	PHE	N-CA	-5.49	1.39	1.46
1	D	245	CYS	CA-C	-5.48	1.45	1.52
1	D	148	PHE	C-O	5.46	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	20	GLN	CA-C	-5.45	1.45	1.52
1	A	203	GLN	CA-C	-5.44	1.48	1.52
1	D	502	ASP	C-N	5.39	1.41	1.33
1	A	166	GLU	N-CA	-5.39	1.39	1.46
1	B	158	ASN	N-CA	5.24	1.52	1.46
1	B	168	CYS	N-CA	-5.23	1.39	1.46
1	B	136	LYS	CA-C	5.20	1.59	1.52
1	C	191	SER	C-O	-5.18	1.17	1.24
1	A	454	LEU	N-CA	-5.17	1.39	1.46
1	A	400	TYR	CA-C	5.15	1.59	1.52
1	D	18	ASN	CG-OD1	-5.13	1.13	1.23
1	A	157	ALA	CA-C	-5.13	1.46	1.52
1	A	547	MET	N-CA	5.12	1.52	1.46
1	D	156	TYR	C-O	-5.11	1.17	1.24
1	C	322	LYS	C-O	-5.10	1.18	1.24
1	D	163	VAL	CA-CB	-5.08	1.47	1.54
1	A	79	THR	N-CA	5.07	1.52	1.46
1	C	170	ALA	N-CA	5.07	1.52	1.46
1	C	282	VAL	CA-C	5.07	1.58	1.52
1	A	270	LEU	N-CA	5.07	1.51	1.46
1	A	524	LYS	N-CA	5.05	1.52	1.46

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	497	VAL	N-CA-C	-10.93	98.86	109.02
1	B	497	VAL	CB-CA-C	9.63	120.44	111.00
1	D	150	ALA	CA-C-N	-9.36	108.67	119.05
1	D	150	ALA	C-N-CA	-9.36	108.67	119.05
1	C	152	GLU	N-CA-C	-9.29	101.94	113.18
1	A	109	SER	CA-C-N	9.29	128.92	119.82
1	A	109	SER	C-N-CA	9.29	128.92	119.82
1	B	267	GLN	N-CA-C	8.87	123.36	112.54
1	B	357	GLU	N-CA-C	-8.85	101.91	112.89
1	D	252	CYS	N-CA-C	-8.48	101.61	111.03
1	D	364	ASP	CA-C-N	-8.46	109.98	119.28
1	D	364	ASP	C-N-CA	-8.46	109.98	119.28
1	A	527	ALA	N-CA-C	-8.26	100.97	112.45
1	B	472	VAL	N-CA-C	-8.26	104.71	111.81
1	C	282	VAL	N-CA-C	8.15	118.92	110.36
1	C	34	CYS	N-CA-C	8.07	118.88	109.60
1	D	320	GLU	N-CA-C	8.01	120.09	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	302	PRO	CA-C-N	-7.91	109.95	119.84
1	C	302	PRO	C-N-CA	-7.91	109.95	119.84
1	D	417	VAL	N-CA-C	-7.91	99.37	109.58
1	A	535	LYS	CA-C-N	7.89	127.81	119.05
1	A	535	LYS	C-N-CA	7.89	127.81	119.05
1	D	187	LYS	N-CA-C	-7.74	102.79	111.14
1	C	535	LYS	CA-C-N	7.72	127.77	119.28
1	C	535	LYS	C-N-CA	7.72	127.77	119.28
1	A	219	SER	N-CA-C	-7.66	102.87	112.90
1	B	87	MET	N-CA-C	-7.46	103.15	111.28
1	A	150	ALA	CA-C-N	-7.45	110.73	118.85
1	A	150	ALA	C-N-CA	-7.45	110.73	118.85
1	C	53	CYS	N-CA-C	-7.42	103.95	113.16
1	C	380	VAL	N-CA-C	7.42	118.18	110.62
1	C	170	ALA	N-CA-C	7.38	119.84	110.24
1	D	243	GLU	N-CA-C	-7.36	103.19	111.14
1	D	112	LEU	CA-C-N	7.35	127.77	119.83
1	D	112	LEU	C-N-CA	7.35	127.77	119.83
1	A	74	LEU	N-CA-C	-7.27	103.29	111.07
1	A	114	LYS	N-CA-C	-7.22	101.00	110.53
1	B	74	LEU	N-CA-C	-7.19	102.54	111.75
1	C	511	ASP	N-CA-C	-7.17	103.50	111.82
1	C	514	THR	N-CA-C	-7.15	104.68	113.41
1	A	43	VAL	N-CA-C	7.07	119.93	111.09
1	A	100	GLU	N-CA-C	-7.06	103.67	111.36
1	C	324	VAL	N-CA-C	-7.04	103.81	110.42
1	B	163	VAL	CB-CA-C	-6.98	102.89	112.24
1	C	128	ALA	N-CA-C	6.97	118.96	111.36
1	C	327	GLY	N-CA-C	-6.91	104.48	112.50
1	B	202	ILE	CB-CA-C	-6.91	102.81	112.14
1	D	109	SER	CA-C-N	-6.87	111.25	119.84
1	D	109	SER	C-N-CA	-6.87	111.25	119.84
1	A	256	ARG	N-CA-C	-6.86	103.59	112.23
1	C	220	GLN	N-CA-C	-6.69	104.14	112.90
1	D	445	MET	CA-C-N	-6.67	111.94	119.28
1	D	445	MET	C-N-CA	-6.67	111.94	119.28
1	D	160	TYR	N-CA-C	6.62	119.05	111.11
1	D	289	ILE	CB-CA-C	-6.62	103.09	112.22
1	A	137	TYR	N-CA-C	-6.60	104.70	112.89
1	A	495	THR	N-CA-C	6.58	119.46	111.82
1	D	106	LYS	N-CA-C	6.56	119.74	109.96
1	B	53	CYS	N-CA-C	-6.56	105.14	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	LYS	N-CA-C	-6.55	104.06	111.07
1	D	282	VAL	CB-CA-C	-6.54	103.59	111.97
1	A	477	THR	N-CA-C	6.54	121.26	113.28
1	C	368	CYS	N-CA-C	-6.53	105.86	113.88
1	B	484	ARG	CA-C-N	6.48	126.24	119.05
1	B	484	ARG	C-N-CA	6.48	126.24	119.05
1	B	183	THR	CB-CA-C	-6.46	100.07	110.79
1	A	329	PHE	N-CA-C	-6.45	104.33	111.36
1	D	8	ALA	N-CA-C	-6.42	106.07	114.04
1	B	511	ASP	N-CA-C	-6.38	104.42	111.82
1	C	434	THR	N-CA-C	-6.36	104.43	111.36
1	A	328	SER	N-CA-C	-6.33	104.61	112.90
1	D	295	ASP	N-CA-C	-6.32	101.59	110.50
1	A	73	GLU	N-CA-C	-6.28	107.46	114.62
1	A	297	VAL	CA-C-N	-6.28	113.51	119.85
1	A	297	VAL	C-N-CA	-6.28	113.51	119.85
1	B	535	LYS	CA-C-N	6.26	127.67	119.84
1	B	535	LYS	C-N-CA	6.26	127.67	119.84
1	C	275	LYS	N-CA-C	-6.16	105.02	112.54
1	B	514	THR	N-CA-C	-6.15	104.84	112.90
1	D	347	ARG	N-CA-C	-6.13	105.06	112.54
1	A	380	VAL	N-CA-C	6.10	116.84	110.62
1	A	245	CYS	N-CA-C	-6.08	105.13	112.54
1	D	72	ASP	N-CA-C	-6.05	105.73	113.23
1	A	235	THR	CB-CA-C	6.02	120.91	110.79
1	D	466	THR	CA-C-N	-6.00	113.78	120.14
1	D	466	THR	C-N-CA	-6.00	113.78	120.14
1	B	468	VAL	N-CA-C	5.99	116.35	111.62
1	C	188	VAL	N-CA-C	5.93	116.71	110.72
1	B	318	TYR	N-CA-C	-5.93	103.59	111.24
1	B	264	CYS	N-CA-C	-5.86	104.81	111.14
1	A	133	PHE	CA-C-N	5.85	128.92	120.79
1	A	133	PHE	C-N-CA	5.85	128.92	120.79
1	A	195	GLN	N-CA-C	-5.85	105.04	111.82
1	A	231	THR	N-CA-C	-5.83	104.29	111.75
1	B	196	ARG	N-CA-C	-5.83	104.84	111.07
1	B	19	PHE	N-CA-C	-5.82	104.84	111.07
1	A	188	VAL	N-CA-C	5.81	115.94	110.30
1	B	4	LYS	N-CA-C	5.81	117.69	111.36
1	A	562	ASP	N-CA-C	-5.80	99.82	109.46
1	A	381	ASP	N-CA-C	5.80	119.62	112.54
1	B	135	GLY	N-CA-C	5.79	120.83	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	291	GLU	N-CA-C	-5.79	103.94	113.50
1	C	453	SER	N-CA-C	-5.77	104.96	112.23
1	D	120	ASP	CB-CA-C	-5.76	101.06	110.85
1	D	427	ARG	N-CA-C	-5.74	104.94	111.14
1	D	278	CYS	N-CA-C	5.72	119.98	112.89
1	D	392	GLU	N-CA-C	-5.70	103.83	112.04
1	D	62	CYS	N-CA-C	5.65	118.17	111.33
1	D	156	TYR	CA-C-N	5.65	128.42	120.28
1	D	156	TYR	C-N-CA	5.65	128.42	120.28
1	D	202	ILE	CB-CA-C	-5.64	104.75	111.81
1	C	9	HIS	N-CA-C	-5.64	105.12	112.23
1	B	445	MET	CA-C-N	-5.63	112.80	119.84
1	B	445	MET	C-N-CA	-5.63	112.80	119.84
1	B	299	GLU	N-CA-C	5.63	117.22	111.14
1	B	105	HIS	N-CA-C	5.62	120.12	113.16
1	B	416	GLN	N-CA-C	-5.61	106.28	113.01
1	B	531	LEU	N-CA-C	-5.57	105.11	111.07
1	C	144	ARG	N-CA-C	-5.57	106.53	113.38
1	C	515	LEU	N-CA-C	5.56	116.71	109.64
1	D	460	CYS	CA-C-N	-5.55	112.22	120.82
1	D	460	CYS	C-N-CA	-5.55	112.22	120.82
1	C	448	THR	N-CA-C	5.54	117.32	111.28
1	D	106	LYS	CA-C-N	-5.54	115.29	123.05
1	D	106	LYS	C-N-CA	-5.54	115.29	123.05
1	A	484	ARG	O-C-N	5.54	124.75	120.38
1	B	499	LYS	CA-C-N	-5.53	112.93	119.84
1	B	499	LYS	C-N-CA	-5.53	112.93	119.84
1	B	320	GLU	N-CA-C	5.52	117.74	111.11
1	C	68	THR	N-CA-C	-5.52	105.18	111.14
1	A	61	GLY	N-CA-C	5.51	122.69	115.36
1	C	393	LEU	N-CA-C	-5.51	104.14	111.24
1	A	196	ARG	N-CA-C	-5.48	105.38	111.36
1	B	178	LEU	CA-C-N	-5.48	112.99	119.84
1	B	178	LEU	C-N-CA	-5.48	112.99	119.84
1	C	375	LYS	N-CA-C	-5.47	104.16	112.04
1	B	502	ASP	N-CA-C	5.46	116.92	110.97
1	C	489	ASP	N-CA-C	5.46	118.15	111.82
1	D	337	HIS	CA-C-N	-5.40	114.21	120.04
1	D	337	HIS	C-N-CA	-5.40	114.21	120.04
1	C	304	LEU	CA-C-N	5.37	127.74	120.38
1	C	304	LEU	C-N-CA	5.37	127.74	120.38
1	A	20	GLN	N-CA-C	-5.37	105.47	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	121	THR	N-CA-C	-5.35	105.44	111.28
1	C	106	LYS	N-CA-C	-5.35	100.68	109.40
1	C	113	PRO	CA-C-O	-5.34	115.07	121.48
1	A	355	THR	CB-CA-C	-5.33	102.76	110.96
1	B	280	LYS	CA-C-N	-5.32	115.10	120.21
1	B	280	LYS	C-N-CA	-5.32	115.10	120.21
1	D	428	SER	CB-CA-C	-5.32	102.47	110.92
1	B	185	ARG	CB-CA-C	-5.27	102.57	110.90
1	D	505	SER	N-CA-C	5.27	117.31	107.99
1	A	75	CYS	N-CA-C	5.25	117.69	111.33
1	D	348	LEU	N-CA-C	-5.23	105.22	111.03
1	D	414	ALA	N-CA-C	5.22	117.63	108.75
1	D	511	ASP	N-CA-C	-5.22	105.55	112.34
1	A	62	CYS	N-CA-C	5.21	117.87	111.82
1	C	202	ILE	CB-CA-C	-5.21	105.10	112.14
1	A	9	HIS	CA-C-N	5.21	127.21	120.44
1	A	9	HIS	C-N-CA	5.21	127.21	120.44
1	D	300	ASN	N-CA-C	5.20	115.88	108.54
1	A	267	GLN	N-CA-C	5.20	117.35	111.11
1	A	242	LYS	N-CA-C	-5.20	105.52	111.14
1	D	113	PRO	CB-CA-C	-5.20	105.09	111.64
1	B	479	SER	N-CA-C	5.19	117.86	110.24
1	B	47	THR	N-CA-C	-5.19	105.71	111.36
1	A	264	CYS	N-CA-C	-5.17	105.82	111.82
1	D	344	VAL	CB-CA-C	-5.17	105.08	112.22
1	D	34	CYS	N-CA-C	5.17	116.20	109.64
1	D	293	ASP	N-CA-C	5.16	117.52	110.55
1	A	23	VAL	CB-CA-C	-5.14	105.39	111.97
1	A	202	ILE	CB-CA-C	-5.14	104.19	112.16
1	D	112	LEU	N-CA-C	-5.14	102.56	110.58
1	A	545	THR	N-CA-CB	5.14	117.86	110.20
1	B	69	LEU	N-CA-C	5.13	116.68	111.14
1	D	167	CYS	N-CA-C	5.13	119.58	112.45
1	D	22	LEU	CA-C-N	5.12	127.10	120.70
1	D	22	LEU	C-N-CA	5.12	127.10	120.70
1	C	10	ARG	N-CA-C	-5.12	104.67	112.04
1	B	150	ALA	CA-C-N	-5.10	113.67	119.28
1	B	150	ALA	C-N-CA	-5.10	113.67	119.28
1	B	163	VAL	N-CA-C	-5.10	105.44	111.00
1	C	301	LEU	CA-C-N	-5.10	115.13	120.38
1	C	301	LEU	C-N-CA	-5.10	115.13	120.38
1	B	288	CYS	N-CA-C	-5.08	105.82	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	166	GLU	N-CA-C	5.08	116.50	111.07
1	D	501	PHE	N-CA-C	5.07	121.59	110.80
1	D	256	ARG	N-CA-C	-5.06	105.95	111.82
1	B	145	HIS	CA-C-N	5.05	126.16	119.84
1	B	145	HIS	C-N-CA	5.05	126.16	119.84
1	C	180	LYS	N-CA-C	-5.04	106.30	112.90
1	C	359	CYS	N-CA-C	5.04	117.66	111.82
1	B	423	VAL	CA-C-N	-5.03	113.59	120.44
1	B	423	VAL	C-N-CA	-5.03	113.59	120.44
1	D	246	HIS	CA-C-N	-5.02	115.55	122.63
1	D	246	HIS	C-N-CA	-5.02	115.55	122.63
1	B	439	LYS	CA-C-N	-5.01	114.57	119.93
1	B	439	LYS	C-N-CA	-5.01	114.57	119.93
1	C	70	PHE	N-CA-C	5.01	116.55	111.14

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	4628	0	4537	222	0
1	B	4627	0	4537	209	1
1	C	4628	0	4537	209	1
1	D	4634	0	4550	195	2
2	A	10	0	14	1	0
2	B	10	0	14	1	0
2	C	10	0	14	0	0
3	A	16	0	14	12	0
3	B	16	0	14	6	0
3	C	24	0	21	6	0
3	D	32	0	28	15	0
4	C	7	0	10	1	0
4	D	7	0	10	2	0
5	A	108	0	0	6	0
5	B	124	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	124	0	0	9	0
5	D	126	0	0	9	0
All	All	19131	0	18300	830	2

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 22.

All (830) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:PRO:O	1:B:500:PRO:HD3	1.31	1.26
1:A:116:LYS:HE3	1:B:116:LYS:HE3	1.28	1.08
1:C:86:ASP:O	1:C:89:ASP:HB2	1.60	1.02
1:B:539:THR:HB	1:B:542:GLN:HB2	1.44	0.99
1:C:499:LYS:HG3	1:C:500:PRO:HD2	1.45	0.98
1:D:382:GLU:HB2	1:D:383:PRO:HD3	1.47	0.96
1:B:56:ASP:HB3	1:B:59:HIS:HB2	1.47	0.96
1:B:498:PRO:HB3	1:B:536:PRO:HG2	1.49	0.95
1:C:517:ASP:HA	1:C:520:LYS:HD2	1.46	0.95
1:B:484:ARG:HB3	1:B:485:PRO:HD3	1.45	0.95
1:A:415:PRO:HD2	1:A:416:GLN:NE2	1.83	0.94
1:D:390:ASN:HB3	4:D:601:PEG:H42	1.49	0.93
1:C:569:LEU:HD22	1:C:570:GLU:HG2	1.50	0.93
1:A:80:LEU:HB2	1:A:88:ALA:HB2	1.52	0.91
1:C:383:PRO:O	1:C:387:ILE:HD13	1.70	0.90
1:C:29:GLN:HG2	1:C:146:PRO:HA	1.55	0.88
1:D:341:ALA:H	1:D:445:MET:HE3	1.39	0.87
1:B:74:LEU:O	1:B:77:VAL:HB	1.74	0.86
1:D:89:ASP:O	1:D:92:GLU:HB2	1.75	0.86
1:C:457:ASN:O	1:C:461:VAL:HG13	1.77	0.84
1:C:504:GLU:O	1:C:507:THR:HG22	1.79	0.83
1:B:498:PRO:O	1:B:500:PRO:CD	2.24	0.82
1:D:88:ALA:O	1:D:91:CYS:HB2	1.80	0.82
1:B:131:LYS:HD2	3:B:602:PRO:CB	2.09	0.82
1:A:87:MET:HE3	1:A:105:HIS:CB	2.10	0.81
1:C:460:CYS:O	1:C:464:GLU:HB2	1.81	0.81
1:B:50:ALA:O	1:B:54:VAL:HG23	1.81	0.81
1:C:131:LYS:HG3	3:C:603:PRO:HG3	1.64	0.80
1:C:451:TYR:HA	1:C:454:LEU:HD12	1.64	0.79
1:D:81:ARG:HG2	1:D:88:ALA:HB3	1.63	0.79
1:D:310:GLU:HA	1:D:366:HIS:NE2	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ARG:HD3	1:A:102:PHE:HE2	1.47	0.78
1:A:71:GLY:HA2	1:A:74:LEU:HD12	1.65	0.78
1:A:213:TRP:CD1	3:A:602:PRO:N	2.50	0.78
1:B:131:LYS:HD2	3:B:602:PRO:HB3	1.65	0.78
1:A:26:ALA:HB2	1:A:249:LEU:HD12	1.66	0.78
1:D:341:ALA:HB2	1:D:445:MET:HG2	1.66	0.78
1:A:213:TRP:HD1	3:A:602:PRO:N	1.81	0.78
1:C:87:MET:HE3	1:C:105:HIS:HB2	1.65	0.78
1:D:463:HIS:HE1	1:D:473:THR:HB	1.49	0.78
1:B:32:GLN:O	1:B:143:ARG:NE	2.18	0.77
1:B:275:LYS:HE3	1:B:275:LYS:O	1.84	0.77
1:D:264:CYS:O	1:D:267:GLN:HG2	1.85	0.77
1:A:38:GLU:OE2	1:A:41:LYS:HE3	1.86	0.76
1:C:511:ASP:O	1:C:515:LEU:HG	1.85	0.76
1:C:556:LYS:HE3	1:C:570:GLU:OE2	1.86	0.76
1:C:5:SER:HB3	1:C:62:CYS:O	1.85	0.76
1:D:382:GLU:HB2	1:D:383:PRO:CD	2.16	0.75
1:A:264:CYS:O	1:A:267:GLN:HG3	1.87	0.75
1:C:561:ASP:OD1	1:D:435:LYS:HD3	1.85	0.75
1:D:525:GLN:O	1:D:529:VAL:HG23	1.87	0.75
1:A:550:PHE:CD1	1:A:574:LEU:HD21	2.22	0.74
1:C:382:GLU:HB3	1:C:383:PRO:HD2	1.68	0.74
1:A:484:ARG:N	1:A:485:PRO:HD2	2.01	0.74
1:A:463:HIS:CD2	1:A:472:VAL:HG12	2.23	0.74
1:B:100:GLU:O	1:B:104:LYS:HG3	1.87	0.74
1:C:419:THR:HG21	1:C:526:THR:HG23	1.67	0.74
1:C:289:ILE:O	1:C:292:ILE:HG22	1.88	0.74
1:D:86:ASP:O	1:D:89:ASP:OD1	2.06	0.73
1:B:390:ASN:ND2	2:B:601:PGE:H32	2.04	0.73
1:D:550:PHE:CE2	1:D:574:LEU:HD21	2.23	0.73
1:A:87:MET:O	1:A:90:CYS:HB2	1.88	0.73
1:B:531:LEU:HD11	1:B:582:LEU:HD11	1.69	0.73
1:A:213:TRP:HZ3	1:A:217:ARG:HD2	1.53	0.73
1:B:220:GLN:O	1:B:223:PRO:HD3	1.89	0.72
1:B:156:TYR:O	1:B:184:MET:HE1	1.90	0.72
1:C:318:TYR:OH	1:C:357:GLU:OE1	2.07	0.72
1:A:87:MET:HE3	1:A:105:HIS:HB3	1.72	0.72
1:A:98:ARG:HD3	1:A:102:PHE:CE2	2.26	0.71
1:A:217:ARG:HG3	1:A:218:LEU:N	2.05	0.71
1:C:471:LYS:HD3	1:C:490:LEU:HD22	1.72	0.71
1:C:51:LYS:O	1:C:54:VAL:HG12	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:LYS:HG3	1:C:500:PRO:CD	2.20	0.71
1:D:531:LEU:HD11	1:D:546:VAL:HG11	1.72	0.71
1:A:214:SER:HA	1:A:217:ARG:HG2	1.73	0.70
1:B:262:TYR:C	1:B:262:TYR:CD2	2.69	0.70
1:A:473:THR:O	1:A:477:THR:OG1	2.09	0.70
1:A:497:VAL:CG1	1:A:499:LYS:HE2	2.21	0.70
1:C:268:ASP:OD2	1:C:268:ASP:N	2.21	0.69
1:D:550:PHE:CD2	1:D:574:LEU:HD21	2.27	0.69
1:B:34:CYS:HB2	1:B:39:HIS:CE1	2.26	0.69
1:B:44:LYS:O	1:B:48:GLU:HG2	1.93	0.69
1:C:89:ASP:O	1:C:92:GLU:HB3	1.93	0.69
1:C:569:LEU:CD2	1:C:570:GLU:HG2	2.23	0.69
1:B:386:LEU:HD12	1:B:387:ILE:HD13	1.73	0.69
1:D:131:LYS:HE3	3:D:602:PRO:CA	2.23	0.69
1:A:412:ARG:HB3	1:A:492:LEU:HG	1.74	0.69
1:B:484:ARG:HB3	1:B:485:PRO:CD	2.22	0.69
1:C:407:ILE:HD12	1:C:525:GLN:HG2	1.74	0.68
1:A:116:LYS:HE3	1:B:116:LYS:CE	2.15	0.68
1:C:419:THR:CG2	1:C:526:THR:HG23	2.21	0.68
1:A:404:ASN:O	1:A:408:VAL:HG23	1.93	0.68
1:B:77:VAL:O	1:B:77:VAL:HG12	1.93	0.68
1:A:463:HIS:HE1	1:A:469:SER:H	1.42	0.68
1:B:213:TRP:HZ3	1:B:217:ARG:HD2	1.58	0.68
1:C:399:GLU:O	1:C:403:GLN:HG3	1.92	0.67
1:C:121:THR:O	1:C:125:GLU:HG3	1.95	0.67
1:D:160:TYR:HB2	1:D:184:MET:HE1	1.75	0.67
1:D:26:ALA:HB2	1:D:249:LEU:HD12	1.75	0.67
1:D:390:ASN:CB	4:D:601:PEG:H42	2.25	0.67
1:B:67:HIS:HE1	1:B:246:HIS:HE1	1.41	0.67
1:B:264:CYS:O	1:B:267:GLN:HG2	1.95	0.66
1:A:95:GLU:OE1	1:A:98:ARG:HD2	1.95	0.66
1:C:259:LEU:O	1:C:263:ILE:HG13	1.95	0.66
1:A:80:LEU:CB	1:A:88:ALA:HB2	2.26	0.66
1:B:272:SER:HB2	1:B:295:ASP:OD1	1.95	0.66
1:B:131:LYS:HD2	3:B:602:PRO:HB2	1.76	0.66
1:B:71:GLY:O	1:B:75:CYS:HB2	1.96	0.66
1:B:539:THR:CB	1:B:542:GLN:HB2	2.24	0.66
1:C:38:GLU:O	1:C:41:LYS:HG2	1.95	0.65
1:C:439:LYS:O	1:C:444:ARG:NH2	2.30	0.65
1:D:412:ARG:HD3	1:D:492:LEU:HD22	1.78	0.65
1:B:413:LYS:HE2	1:B:490:LEU:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:GLU:OE1	1:B:336:ARG:NH2	2.29	0.65
1:A:390:ASN:HB3	2:A:601:PGE:H2	1.79	0.65
1:A:39:HIS:O	1:A:43:VAL:HG23	1.97	0.64
1:C:150:ALA:HB3	1:C:151:PRO:HD3	1.79	0.64
1:A:539:THR:HG22	1:A:541:GLU:H	1.62	0.64
1:B:562:ASP:OD2	1:B:565:GLY:HA3	1.96	0.64
1:A:497:VAL:HG11	1:A:499:LYS:HE2	1.79	0.64
1:A:135:GLY:HA2	1:A:138:LEU:HD12	1.80	0.64
1:B:414:ALA:HB1	1:B:417:VAL:HG23	1.81	0.63
1:D:302:PRO:O	1:D:336:ARG:NH1	2.30	0.63
1:B:29:GLN:HE21	1:B:146:PRO:HA	1.64	0.63
1:B:246:HIS:O	1:B:246:HIS:ND1	2.32	0.63
1:C:530:GLU:HA	1:C:533:LYS:HB2	1.81	0.63
1:D:304:LEU:O	1:D:308:PHE:HD2	1.81	0.63
1:C:4:LYS:O	1:C:63:ASP:HA	1.99	0.63
1:B:152:GLU:OE2	1:B:287:HIS:ND1	2.25	0.63
1:D:36:PHE:HB2	1:D:139:TYR:CE2	2.34	0.62
1:C:417:VAL:HG13	5:C:765:HOH:O	1.98	0.62
1:D:470:GLU:HA	1:D:473:THR:HG22	1.81	0.62
1:B:458:ARG:CZ	1:B:462:LEU:HD21	2.30	0.62
1:B:84:TYR:HB2	1:B:87:MET:HB2	1.81	0.62
1:A:492:LEU:HD12	1:A:492:LEU:H	1.64	0.62
1:A:315:CYS:O	1:A:319:GLN:HG3	2.00	0.62
1:D:470:GLU:N	1:D:470:GLU:CD	2.58	0.62
1:D:412:ARG:HB3	1:D:492:LEU:HD22	1.81	0.61
1:A:29:GLN:HG2	1:A:146:PRO:HA	1.83	0.61
1:B:515:LEU:HD22	1:B:516:PRO:HD2	1.82	0.61
1:B:550:PHE:O	1:B:554:VAL:HG23	1.99	0.61
1:D:369:TYR:O	1:D:372:VAL:HG12	2.00	0.61
1:B:66:LEU:HA	1:B:69:LEU:HD12	1.82	0.61
1:D:31:LEU:HD11	1:D:74:LEU:HD22	1.80	0.61
1:D:131:LYS:HE3	3:D:602:PRO:CB	2.29	0.61
1:A:312:LYS:HD2	1:A:312:LYS:O	2.00	0.61
1:B:89:ASP:O	1:B:92:GLU:HB2	2.00	0.61
1:C:5:SER:CB	1:C:62:CYS:O	2.48	0.61
1:B:66:LEU:O	1:B:70:PHE:HD2	1.84	0.60
1:C:569:LEU:O	1:C:572:PRO:HD2	2.01	0.60
1:A:383:PRO:HA	1:A:386:LEU:HD23	1.84	0.60
1:A:427:ARG:HG2	1:A:427:ARG:HH11	1.65	0.60
1:B:56:ASP:CB	1:B:59:HIS:HB2	2.28	0.60
1:C:266:HIS:HB3	1:C:269:THR:OG1	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ILE:HG13	1:C:210:LEU:HD22	1.83	0.60
3:D:604:PRO:HB3	5:D:817:HOH:O	2.00	0.60
1:A:77:VAL:O	1:A:80:LEU:HG	2.02	0.60
1:D:44:LYS:HD2	1:D:45:GLU:HG2	1.83	0.60
1:D:74:LEU:O	1:D:77:VAL:HB	2.02	0.60
1:A:87:MET:HE3	1:A:105:HIS:HB2	1.83	0.59
1:A:346:LEU:HD12	3:A:602:PRO:HG2	1.84	0.59
1:C:251:GLU:OE1	1:C:251:GLU:N	2.30	0.59
1:C:473:THR:O	1:C:477:THR:OG1	2.16	0.59
1:B:38:GLU:O	1:B:41:LYS:HG2	2.01	0.59
1:D:213:TRP:HB3	3:D:603:PRO:OXT	2.03	0.59
1:A:80:LEU:HB2	1:A:88:ALA:CB	2.31	0.59
1:A:346:LEU:HD12	3:A:602:PRO:HB2	1.84	0.59
1:C:515:LEU:HB3	1:C:519:GLU:HB2	1.85	0.59
1:D:31:LEU:HD11	1:D:74:LEU:CD2	2.32	0.59
1:A:532:LEU:HD21	1:A:543:LEU:HD11	1.85	0.58
1:A:10:ARG:NH1	1:A:254:ASP:OD2	2.37	0.58
1:A:109:SER:HB3	1:A:465:LYS:NZ	2.19	0.58
1:A:214:SER:O	1:A:218:LEU:HB2	2.03	0.58
1:A:550:PHE:HD1	1:A:574:LEU:HD21	1.65	0.58
1:C:226:ASP:HB3	1:C:228:THR:H	1.68	0.58
1:D:351:GLU:HG2	1:D:379:LEU:HD11	1.85	0.58
1:A:220:GLN:HG2	1:A:338:PRO:HA	1.86	0.58
1:A:539:THR:HB	1:A:542:GLN:HG3	1.85	0.58
1:B:273:LYS:HB2	1:B:292:ILE:HD11	1.86	0.58
1:C:403:GLN:HG2	1:C:430:GLY:HA3	1.84	0.58
1:A:59:HIS:CG	1:A:60:ALA:N	2.71	0.57
1:A:207:GLU:OE1	1:A:242:LYS:HD3	2.04	0.57
1:B:414:ALA:HB1	1:B:417:VAL:CG2	2.33	0.57
1:D:232:LYS:HE2	1:D:236:ASP:OD2	2.04	0.57
1:A:484:ARG:H	1:A:485:PRO:HD2	1.68	0.57
1:A:87:MET:CE	1:A:105:HIS:HB2	2.33	0.57
1:D:178:LEU:N	1:D:179:PRO:CD	2.66	0.57
1:D:152:GLU:OE2	1:D:287:HIS:ND1	2.30	0.57
1:A:457:ASN:O	1:A:461:VAL:HG13	2.04	0.57
1:D:167:CYS:HB3	1:D:177:LEU:HD12	1.87	0.57
1:D:29:GLN:HG2	1:D:146:PRO:HA	1.85	0.57
1:C:412:ARG:HG2	1:C:492:LEU:HD13	1.87	0.57
1:C:419:THR:HB	1:C:420:PRO:HD3	1.87	0.57
1:C:501:PHE:HB3	1:C:579:GLN:NE2	2.20	0.57
1:C:578:THR:HG22	1:C:579:GLN:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LEU:HD12	1:B:336:ARG:HG3	1.85	0.57
1:B:408:VAL:HG13	1:B:412:ARG:NH1	2.20	0.57
1:A:93:LYS:HE3	1:A:97:GLU:HB3	1.85	0.56
1:C:553:PHE:HE1	1:C:570:GLU:HB2	1.69	0.56
1:A:93:LYS:HE2	1:D:276:GLU:HG3	1.88	0.56
1:B:387:ILE:HD12	1:B:448:THR:HG21	1.86	0.56
1:C:501:PHE:HD1	1:C:534:HIS:CE1	2.22	0.56
1:D:350:LYS:HD3	1:D:481:VAL:HG11	1.86	0.56
1:A:497:VAL:HG13	1:A:499:LYS:HE2	1.86	0.56
1:D:87:MET:HE2	1:D:102:PHE:CD1	2.39	0.56
1:D:156:TYR:HB3	1:D:184:MET:HE3	1.87	0.56
1:B:332:GLU:HB3	1:B:336:ARG:HH21	1.71	0.56
1:D:500:PRO:O	1:D:504:GLU:HG2	2.06	0.56
1:A:226:ASP:HB3	1:A:228:THR:H	1.70	0.56
1:A:313:GLU:O	1:A:317:ASN:OD1	2.24	0.56
1:B:412:ARG:O	1:B:492:LEU:HA	2.04	0.56
1:A:518:THR:O	1:A:521:GLN:HB2	2.06	0.56
1:B:6:GLU:OE2	1:B:10:ARG:NH2	2.39	0.56
1:D:393:LEU:HD23	1:D:402:PHE:CE1	2.39	0.56
1:A:462:LEU:O	1:A:465:LYS:HB3	2.06	0.56
1:D:218:LEU:HD23	1:D:218:LEU:O	2.06	0.56
1:D:463:HIS:CE1	1:D:473:THR:HB	2.38	0.56
1:D:540:ASP:O	1:D:544:LYS:HG2	2.06	0.56
1:A:249:LEU:O	1:A:252:CYS:HB3	2.06	0.56
1:D:6:GLU:C	1:D:8:ALA:H	2.14	0.56
1:C:573:LYS:O	1:C:577:SER:HB3	2.07	0.55
1:D:393:LEU:HD23	1:D:402:PHE:HE1	1.70	0.55
1:B:263:ILE:HG23	1:B:270:LEU:HD13	1.89	0.55
1:C:412:ARG:CG	1:C:492:LEU:HD13	2.35	0.55
1:D:294:LYS:HD2	1:D:338:PRO:HB3	1.86	0.55
1:D:190:ALA:O	1:D:191:SER:C	2.48	0.55
1:A:159:LYS:HE2	1:A:284:GLU:OE1	2.07	0.55
1:C:271:SER:OG	1:C:295:ASP:HB2	2.07	0.55
1:D:263:ILE:HG23	1:D:270:LEU:HD13	1.88	0.55
1:D:429:LEU:HD23	1:D:455:ILE:HD13	1.87	0.55
1:A:346:LEU:HD12	3:A:602:PRO:CB	2.37	0.55
1:A:49:PHE:CE2	1:A:69:LEU:HD21	2.42	0.55
1:B:273:LYS:O	1:B:276:GLU:HB3	2.07	0.55
1:D:167:CYS:HB3	1:D:177:LEU:CD1	2.37	0.55
1:B:81:ARG:NH1	1:B:81:ARG:HB3	2.22	0.55
1:C:390:ASN:HB3	3:C:604:PRO:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PHE:CD1	1:A:11:PHE:C	2.85	0.55
1:B:528:LEU:O	1:B:531:LEU:HB3	2.07	0.55
1:C:501:PHE:CD2	1:C:501:PHE:N	2.71	0.55
1:A:214:SER:HB3	1:A:234:VAL:HG22	1.89	0.54
1:A:343:SER:HA	3:A:602:PRO:HG2	1.87	0.54
1:A:41:LYS:O	1:A:45:GLU:HG3	2.07	0.54
1:C:6:GLU:OE2	1:C:10:ARG:NH2	2.40	0.54
1:C:499:LYS:CG	1:C:500:PRO:HD2	2.28	0.54
1:D:131:LYS:HE3	3:D:602:PRO:HA	1.89	0.54
1:A:458:ARG:O	1:A:461:VAL:HG22	2.07	0.54
1:A:518:THR:HA	1:A:521:GLN:OE1	2.07	0.54
1:B:237:LEU:HD11	1:B:241:HIS:CE1	2.41	0.54
1:B:213:TRP:HA	1:B:346:LEU:HD11	1.90	0.54
1:B:578:THR:HG22	1:B:579:GLN:HG3	1.89	0.54
1:D:218:LEU:HD21	1:D:222:PHE:CD2	2.43	0.54
1:B:306:ALA:HA	1:B:310:GLU:HG3	1.89	0.54
1:B:448:THR:O	1:B:452:LEU:HG	2.07	0.54
1:C:50:ALA:C	1:C:52:THR:H	2.15	0.54
1:D:470:GLU:CD	1:D:470:GLU:H	2.15	0.54
1:A:187:LYS:HE2	5:A:743:HOH:O	2.08	0.54
1:B:470:GLU:HA	1:B:473:THR:HG22	1.90	0.54
1:D:500:PRO:O	1:D:504:GLU:CG	2.56	0.54
1:D:499:LYS:O	1:D:534:HIS:ND1	2.41	0.54
1:A:213:TRP:CZ3	1:A:217:ARG:HD2	2.39	0.54
1:C:431:LYS:O	1:C:434:THR:N	2.40	0.54
1:C:516:PRO:HG2	1:C:519:GLU:HG2	1.89	0.54
1:A:458:ARG:CZ	1:A:462:LEU:HD21	2.38	0.54
1:B:535:LYS:HG3	1:B:582:LEU:HB3	1.90	0.54
1:C:416:GLN:O	1:C:468:VAL:HG21	2.08	0.54
1:C:484:ARG:HB3	1:C:485:PRO:HD3	1.89	0.54
1:C:362:LYS:HD2	1:C:368:CYS:SG	2.47	0.53
1:A:419:THR:OG1	1:A:533:LYS:NZ	2.38	0.53
1:A:520:LYS:HE2	5:A:792:HOH:O	2.06	0.53
1:B:20:GLN:O	1:B:21:GLY:C	2.52	0.53
1:D:59:HIS:CG	1:D:60:ALA:H	2.25	0.53
1:A:340:TYR:HA	1:A:445:MET:HE3	1.90	0.53
1:B:5:SER:HB3	1:B:62:CYS:O	2.08	0.53
1:C:129:ASP:HB3	5:C:772:HOH:O	2.07	0.53
1:D:334:SER:OG	1:D:345:LEU:HD13	2.08	0.53
1:C:49:PHE:O	1:C:52:THR:HG22	2.08	0.53
1:D:470:GLU:N	1:D:470:GLU:OE1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:TYR:OH	1:A:159:LYS:HE3	2.09	0.53
1:B:129:ASP:HB3	1:B:132:LYS:HB3	1.91	0.53
1:C:382:GLU:HB3	1:C:383:PRO:CD	2.36	0.53
1:D:391:CYS:O	1:D:395:GLU:HG2	2.08	0.53
1:A:343:SER:HA	3:A:602:PRO:CG	2.39	0.53
1:B:67:HIS:HE1	1:B:246:HIS:CE1	2.24	0.53
1:B:106:LYS:HG2	1:B:146:PRO:HB2	1.90	0.53
1:C:218:LEU:HD21	4:C:602:PEG:H42	1.91	0.53
1:C:309:ALA:O	1:C:369:TYR:HE1	1.91	0.53
1:C:419:THR:HG23	1:C:529:VAL:HG11	1.90	0.53
1:C:407:ILE:O	1:C:411:THR:OG1	2.18	0.53
1:A:382:GLU:O	1:A:385:ASN:HB2	2.07	0.53
1:A:511:ASP:O	1:A:515:LEU:HG	2.08	0.53
1:B:483:ARG:O	1:B:484:ARG:C	2.50	0.53
1:D:59:HIS:CG	1:D:60:ALA:N	2.77	0.53
1:B:259:LEU:O	1:B:263:ILE:HG13	2.08	0.53
1:B:8:ALA:O	1:B:12:ASN:ND2	2.42	0.52
1:B:463:HIS:HE1	1:B:473:THR:HB	1.74	0.52
1:D:283:LEU:O	1:D:284:GLU:C	2.51	0.52
1:D:467:PRO:HB2	3:D:605:PRO:HD3	1.91	0.52
1:D:484:ARG:HB3	1:D:485:PRO:HD3	1.91	0.52
1:A:492:LEU:H	1:A:492:LEU:CD1	2.22	0.52
1:B:56:ASP:O	1:B:59:HIS:N	2.36	0.52
1:C:427:ARG:HG2	1:C:427:ARG:HH11	1.73	0.52
1:B:102:PHE:O	1:B:105:HIS:N	2.39	0.52
1:C:149:TYR:CD1	1:C:151:PRO:HD2	2.45	0.52
1:C:211:LYS:O	1:C:215:VAL:HG23	2.09	0.52
1:C:221:LYS:HA	1:C:294:LYS:HG2	1.91	0.52
1:C:452:LEU:HD13	1:C:484:ARG:HG3	1.90	0.52
1:D:271:SER:OG	1:D:295:ASP:HB2	2.09	0.52
1:A:16:GLU:OE2	3:A:603:PRO:HG3	2.09	0.52
1:B:455:ILE:O	1:B:458:ARG:HB3	2.10	0.52
1:C:384:GLN:HA	1:C:384:GLN:OE1	2.09	0.52
1:C:486:CYS:O	1:C:489:ASP:HB2	2.09	0.52
1:D:243:GLU:OE2	1:D:251:GLU:HB3	2.09	0.52
1:A:332:GLU:OE1	1:A:336:ARG:NH1	2.43	0.52
1:C:148:PHE:CD1	1:C:149:TYR:N	2.78	0.52
1:A:16:GLU:O	1:A:20:GLN:HG3	2.08	0.52
1:C:407:ILE:HG13	1:C:426:SER:HB2	1.92	0.52
1:D:294:LYS:HE3	1:D:338:PRO:HB2	1.90	0.52
1:D:407:ILE:HG13	1:D:426:SER:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LEU:HB3	1:B:336:ARG:NH1	2.25	0.52
1:B:399:GLU:O	1:B:403:GLN:HG3	2.09	0.52
1:D:340:TYR:HA	1:D:445:MET:HE3	1.92	0.52
1:A:387:ILE:HG22	1:A:388:LYS:N	2.24	0.52
1:B:463:HIS:CE1	1:B:472:VAL:HG12	2.45	0.52
1:C:229:ASP:O	1:C:233:ILE:HG13	2.10	0.52
1:C:417:VAL:HB	1:C:422:LEU:HD21	1.92	0.52
1:B:266:HIS:O	1:B:270:LEU:HG	2.10	0.52
1:C:86:ASP:O	1:C:89:ASP:CB	2.47	0.52
1:C:471:LYS:HA	1:C:474:LYS:HE2	1.91	0.52
1:D:30:TYR:HE1	1:D:103:LEU:HD23	1.75	0.52
1:D:217:ARG:NH2	1:D:290:ALA:O	2.43	0.52
1:B:194:ARG:NH1	5:B:708:HOH:O	2.42	0.52
1:D:151:PRO:O	1:D:154:LEU:HB2	2.10	0.52
1:A:403:GLN:HG2	1:A:430:GLY:HA3	1.92	0.51
1:B:25:ILE:O	1:B:29:GLN:HG3	2.11	0.51
1:C:521:GLN:O	1:C:525:GLN:N	2.40	0.51
1:D:419:THR:HB	1:D:420:PRO:HD3	1.92	0.51
1:D:10:ARG:HG3	1:D:250:LEU:HB3	1.93	0.51
1:B:47:THR:O	1:B:51:LYS:HG3	2.10	0.51
1:D:207:GLU:OE1	1:D:242:LYS:HD3	2.09	0.51
1:B:33:GLN:N	1:B:84:TYR:OH	2.43	0.51
1:D:182:GLU:HG2	5:D:761:HOH:O	2.10	0.51
1:A:237:LEU:HG	1:A:241:HIS:CE1	2.45	0.51
1:A:479:SER:OG	1:A:481:VAL:HG12	2.11	0.51
1:C:264:CYS:O	1:C:267:GLN:HG2	2.10	0.51
1:D:20:GLN:HE21	1:D:47:THR:HG21	1.74	0.51
1:A:341:ALA:O	1:A:344:VAL:N	2.41	0.51
1:A:448:THR:O	1:A:452:LEU:HG	2.11	0.51
1:A:236:ASP:O	1:A:240:VAL:HG23	2.11	0.51
1:A:268:ASP:N	1:A:268:ASP:OD1	2.40	0.51
1:A:427:ARG:HG2	1:A:427:ARG:NH1	2.25	0.51
1:B:150:ALA:HB3	1:B:151:PRO:HD3	1.93	0.51
1:B:52:THR:O	1:B:56:ASP:N	2.32	0.51
1:D:6:GLU:OE2	1:D:10:ARG:NE	2.41	0.51
1:D:510:ALA:C	1:D:512:ILE:N	2.66	0.51
1:A:470:GLU:CD	1:A:470:GLU:H	2.19	0.51
1:B:121:THR:O	1:B:124:ALA:HB3	2.11	0.51
1:D:341:ALA:N	1:D:445:MET:HE3	2.19	0.51
1:D:408:VAL:HG12	1:D:409:ARG:N	2.26	0.51
1:D:466:THR:O	1:D:466:THR:OG1	2.12	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLU:O	1:A:393:LEU:C	2.52	0.50
1:A:478:GLU:O	1:A:479:SER:C	2.53	0.50
1:B:177:LEU:HD12	1:B:178:LEU:N	2.27	0.50
1:A:310:GLU:O	1:A:311:ASP:C	2.53	0.50
1:A:539:THR:HG22	1:A:541:GLU:N	2.26	0.50
1:B:140:GLU:O	1:B:144:ARG:HG3	2.11	0.50
1:B:439:LYS:O	1:B:440:PRO:C	2.54	0.50
1:C:50:ALA:O	1:C:52:THR:N	2.45	0.50
1:D:130:GLU:HG2	3:D:602:PRO:OXT	2.11	0.50
1:B:71:GLY:C	1:B:73:GLU:H	2.18	0.50
1:B:324:VAL:O	1:B:325:PHE:C	2.54	0.50
1:B:501:PHE:HZ	1:B:504:GLU:HG3	1.76	0.50
1:D:77:VAL:O	1:D:80:LEU:HG	2.11	0.50
1:A:9:HIS:C	1:A:9:HIS:CD2	2.88	0.50
1:A:87:MET:CE	1:A:105:HIS:CB	2.86	0.50
1:A:226:ASP:HB2	1:A:229:ASP:H	1.76	0.50
1:A:484:ARG:N	1:A:485:PRO:CD	2.70	0.50
1:B:301:LEU:CD1	1:B:336:ARG:HG3	2.40	0.50
1:B:421:THR:HG23	1:B:462:LEU:HD12	1.94	0.50
1:A:153:LEU:HD12	1:A:153:LEU:O	2.12	0.50
1:A:419:THR:HG23	1:A:529:VAL:HG11	1.93	0.50
1:B:198:ARG:O	1:B:201:SER:HB2	2.12	0.50
1:C:89:ASP:C	1:C:92:GLU:HB3	2.36	0.50
1:A:59:HIS:CG	1:A:60:ALA:H	2.29	0.50
1:B:134:TRP:CD1	3:B:602:PRO:HD3	2.47	0.50
1:C:507:THR:HG23	1:C:509:HIS:HE1	1.76	0.50
1:C:511:ASP:N	1:C:511:ASP:OD1	2.45	0.50
1:C:571:GLY:N	1:C:572:PRO:HD2	2.26	0.50
1:B:81:ARG:HG3	1:B:88:ALA:CB	2.42	0.49
1:C:189:LEU:O	1:C:190:ALA:C	2.55	0.49
1:D:5:SER:HA	1:D:63:ASP:HA	1.93	0.49
1:D:9:HIS:O	1:D:9:HIS:ND1	2.45	0.49
1:D:216:ALA:HB2	1:D:330:LEU:HD11	1.94	0.49
1:D:311:ASP:OD1	1:D:312:LYS:N	2.45	0.49
1:B:197:LEU:O	1:B:198:ARG:C	2.54	0.49
1:B:534:HIS:NE2	1:B:579:GLN:HG2	2.27	0.49
1:C:332:GLU:OE1	1:C:336:ARG:NH2	2.44	0.49
1:A:341:ALA:HB3	1:A:344:VAL:HG23	1.94	0.49
1:C:216:ALA:HB3	1:C:342:VAL:HG13	1.94	0.49
1:C:427:ARG:HG2	1:C:427:ARG:NH1	2.27	0.49
1:D:281:PRO:O	1:D:285:LYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:HD13	1:A:73:GLU:OE1	2.12	0.49
1:B:333:TYR:OH	1:B:377:LYS:NZ	2.31	0.49
1:B:369:TYR:HD1	1:B:369:TYR:O	1.96	0.49
1:C:50:ALA:C	1:C:52:THR:N	2.66	0.49
1:C:48:GLU:O	1:C:51:LYS:HB2	2.13	0.49
1:C:144:ARG:HG3	1:C:144:ARG:HH11	1.78	0.49
1:C:406:LEU:HD13	1:C:429:LEU:HB3	1.93	0.49
1:D:131:LYS:CE	3:D:602:PRO:HB2	2.42	0.49
1:D:163:VAL:O	1:D:167:CYS:HB2	2.12	0.49
1:B:56:ASP:O	1:B:58:SER:N	2.46	0.49
1:B:304:LEU:HD11	1:B:333:TYR:HA	1.93	0.49
1:B:416:GLN:H	1:B:416:GLN:CD	2.21	0.49
1:A:415:PRO:HG2	1:A:496:TYR:CD2	2.46	0.49
1:C:32:GLN:HG2	1:C:143:ARG:O	2.12	0.49
1:B:52:THR:HA	1:B:55:ALA:HB3	1.94	0.49
1:B:81:ARG:HB3	1:B:81:ARG:HH11	1.78	0.49
1:D:39:HIS:O	1:D:43:VAL:HG23	2.12	0.49
1:D:470:GLU:OE2	3:D:605:PRO:HG3	2.13	0.49
1:A:222:PHE:CD1	1:A:222:PHE:N	2.77	0.49
1:B:445:MET:O	1:B:446:PRO:C	2.54	0.49
1:C:553:PHE:CE1	1:C:570:GLU:HB2	2.47	0.49
1:A:138:LEU:O	1:A:142:ALA:HB3	2.13	0.48
1:B:195:GLN:O	1:B:196:ARG:C	2.56	0.48
1:B:318:TYR:OH	1:B:357:GLU:OE1	2.26	0.48
1:B:344:VAL:O	1:B:348:LEU:HG	2.12	0.48
1:B:73:GLU:C	1:B:75:CYS:N	2.65	0.48
1:C:380:VAL:O	1:C:384:GLN:HG2	2.13	0.48
1:D:229:ASP:O	1:D:230:VAL:C	2.56	0.48
1:A:221:LYS:C	1:A:222:PHE:HD1	2.21	0.48
1:C:313:GLU:O	1:C:314:VAL:C	2.55	0.48
1:C:380:VAL:O	1:C:383:PRO:HG2	2.13	0.48
1:D:281:PRO:O	1:D:285:LYS:CB	2.61	0.48
1:A:346:LEU:HD12	3:A:602:PRO:CG	2.43	0.48
1:B:3:HIS:CD2	1:B:9:HIS:HB2	2.49	0.48
1:B:52:THR:C	1:B:54:VAL:N	2.71	0.48
1:A:136:LYS:O	1:A:140:GLU:HG2	2.14	0.48
1:A:501:PHE:O	1:A:504:GLU:O	2.32	0.48
1:D:294:LYS:HD2	1:D:338:PRO:CB	2.43	0.48
1:A:31:LEU:HD11	1:A:74:LEU:HD23	1.95	0.48
1:A:473:THR:O	1:A:473:THR:HG22	2.14	0.48
1:B:221:LYS:HG2	1:B:292:ILE:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ASP:OD1	1:B:229:ASP:N	2.45	0.48
1:D:400:TYR:O	1:D:403:GLN:HB2	2.14	0.48
1:A:84:TYR:HB2	1:A:87:MET:HB3	1.96	0.47
1:D:156:TYR:O	1:D:184:MET:HE1	2.14	0.47
1:B:395:GLU:HA	1:B:395:GLU:OE1	2.13	0.47
1:B:271:SER:HB3	1:B:274:LEU:HG	1.96	0.47
1:B:535:LYS:HE2	1:B:583:ALA:HA	1.95	0.47
1:D:423:VAL:O	1:D:427:ARG:HG3	2.14	0.47
1:B:383:PRO:HA	1:B:386:LEU:HG	1.95	0.47
1:A:116:LYS:HE2	1:B:118:GLU:HG2	1.96	0.47
1:A:439:LYS:O	1:A:444:ARG:NH1	2.48	0.47
1:A:501:PHE:CE2	1:A:533:LYS:HD3	2.49	0.47
1:B:404:ASN:O	1:B:407:ILE:HB	2.15	0.47
1:C:407:ILE:CD1	1:C:525:GLN:HG2	2.43	0.47
1:D:436:CYS:O	1:D:439:LYS:HB2	2.14	0.47
1:A:160:TYR:O	1:A:163:VAL:HB	2.14	0.47
1:A:337:HIS:C	1:A:339:GLU:H	2.22	0.47
1:A:345:LEU:O	1:A:346:LEU:C	2.58	0.47
1:B:484:ARG:CB	1:B:485:PRO:CD	2.89	0.47
1:A:304:LEU:HB3	1:A:373:PHE:CZ	2.50	0.47
1:A:531:LEU:HD21	1:A:546:VAL:HG11	1.95	0.47
1:B:73:GLU:O	1:B:74:LEU:C	2.56	0.47
1:C:266:HIS:O	1:C:269:THR:OG1	2.23	0.47
1:C:407:ILE:HG13	1:C:426:SER:CB	2.45	0.47
1:C:566:CYS:C	1:C:568:LEU:N	2.72	0.47
1:D:562:ASP:HB2	5:D:816:HOH:O	2.14	0.47
1:A:43:VAL:O	1:A:43:VAL:HG12	2.14	0.47
1:A:310:GLU:HA	1:A:366:HIS:NE2	2.29	0.47
1:B:5:SER:CB	1:B:62:CYS:O	2.63	0.47
1:B:515:LEU:O	1:B:520:LYS:HE3	2.15	0.47
1:C:261:LYS:HD3	5:C:715:HOH:O	2.14	0.47
1:B:29:GLN:NE2	1:B:146:PRO:C	2.73	0.47
1:B:261:LYS:HB3	5:B:762:HOH:O	2.15	0.47
1:B:542:GLN:O	1:B:546:VAL:HG23	2.14	0.47
1:C:421:THR:O	1:C:425:ILE:HG12	2.15	0.47
1:D:207:GLU:OE1	1:D:242:LYS:CE	2.63	0.47
1:B:140:GLU:OE1	1:B:144:ARG:NH1	2.46	0.47
1:B:171:GLU:HG2	1:B:172:ASP:N	2.29	0.47
1:C:95:GLU:OE2	1:C:96:PRO:HA	2.15	0.47
1:C:182:GLU:OE1	1:C:182:GLU:HA	2.15	0.47
1:C:150:ALA:HB2	1:C:249:LEU:HD22	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:GLU:H	1:C:251:GLU:CD	2.20	0.46
1:C:544:LYS:HE2	1:C:548:GLU:OE2	2.15	0.46
1:D:419:THR:O	1:D:423:VAL:HG23	2.15	0.46
1:D:502:ASP:C	1:D:504:GLU:H	2.23	0.46
1:A:213:TRP:HB2	3:A:602:PRO:O	2.16	0.46
1:B:348:LEU:O	1:B:352:TYR:N	2.45	0.46
1:C:110:PRO:HG3	1:C:144:ARG:HA	1.97	0.46
1:C:415:PRO:HD2	1:C:416:GLN:OE1	2.14	0.46
1:D:61:GLY:O	1:D:64:LYS:HG3	2.15	0.46
1:D:273:LYS:C	1:D:292:ILE:HD11	2.40	0.46
1:A:236:ASP:HB2	1:A:259:LEU:HD13	1.96	0.46
1:A:311:ASP:HB3	1:A:314:VAL:HG23	1.97	0.46
1:B:408:VAL:O	1:B:412:ARG:HG3	2.15	0.46
1:D:470:GLU:HA	1:D:473:THR:CG2	2.45	0.46
1:A:359:CYS:O	1:A:361:ALA:N	2.49	0.46
1:A:415:PRO:HG2	1:A:496:TYR:CG	2.51	0.46
1:B:490:LEU:HA	5:B:738:HOH:O	2.15	0.46
1:D:419:THR:HG21	1:D:526:THR:HG23	1.96	0.46
1:A:167:CYS:O	1:A:168:CYS:C	2.58	0.46
1:B:54:VAL:HB	5:B:760:HOH:O	2.15	0.46
1:B:134:TRP:CG	3:B:602:PRO:HD3	2.50	0.46
1:C:395:GLU:OE1	1:C:395:GLU:HA	2.16	0.46
1:C:419:THR:HB	1:C:420:PRO:CD	2.45	0.46
1:C:507:THR:HG23	1:C:509:HIS:CE1	2.50	0.46
1:D:364:ASP:HB3	1:D:367:ALA:HB3	1.97	0.46
1:A:44:LYS:O	1:A:48:GLU:HG2	2.14	0.46
1:A:452:LEU:CD1	1:A:484:ARG:HD2	2.45	0.46
1:B:301:LEU:HB3	1:B:336:ARG:HH11	1.80	0.46
1:C:187:LYS:O	1:C:190:ALA:HB3	2.16	0.46
1:C:236:ASP:CB	1:C:259:LEU:HD13	2.46	0.46
1:C:416:GLN:HB2	1:C:469:SER:HB2	1.97	0.46
1:C:519:GLU:OE1	1:C:519:GLU:N	2.48	0.46
1:D:433:GLY:O	1:D:437:CYS:HB2	2.16	0.46
1:A:233:ILE:HG23	1:A:259:LEU:HD11	1.98	0.46
1:A:304:LEU:HD11	1:A:333:TYR:HA	1.98	0.46
1:A:386:LEU:CD2	1:A:484:ARG:HH21	2.29	0.46
1:B:171:GLU:H	1:B:171:GLU:CD	2.21	0.46
1:C:441:GLU:HA	1:C:444:ARG:NH1	2.30	0.46
1:A:275:LYS:HD2	1:A:275:LYS:HA	1.68	0.46
1:B:386:LEU:HD21	1:B:484:ARG:HH12	1.81	0.46
1:C:43:VAL:O	1:C:47:THR:OG1	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:TYR:HA	1:C:445:MET:HE3	1.97	0.46
1:C:388:LYS:O	1:C:392:GLU:HG3	2.16	0.46
1:D:131:LYS:HE3	3:D:602:PRO:HB2	1.96	0.46
1:D:141:VAL:O	1:D:145:HIS:HD2	1.99	0.46
1:D:419:THR:HG23	1:D:529:VAL:HG11	1.97	0.46
1:D:467:PRO:HB2	3:D:605:PRO:CD	2.46	0.46
1:A:16:GLU:HB3	3:A:603:PRO:HG3	1.98	0.46
1:B:25:ILE:O	1:B:26:ALA:C	2.59	0.46
1:D:539:THR:HG23	1:D:542:GLN:OE1	2.16	0.46
1:A:68:THR:HA	1:A:98:ARG:HH12	1.81	0.45
1:A:347:ARG:HH21	1:A:485:PRO:CD	2.29	0.45
1:D:550:PHE:O	1:D:554:VAL:HG23	2.17	0.45
1:A:331:TYR:OH	1:A:335:ARG:NH1	2.50	0.45
1:C:160:TYR:O	1:C:164:PHE:HD2	1.99	0.45
1:D:129:ASP:O	1:D:130:GLU:C	2.58	0.45
1:A:384:GLN:O	1:A:388:LYS:HD2	2.16	0.45
1:A:553:PHE:CZ	1:A:567:PHE:CD1	3.04	0.45
1:B:81:ARG:HG3	1:B:88:ALA:HB2	1.97	0.45
1:A:387:ILE:HG13	1:A:448:THR:HG21	1.98	0.45
1:A:415:PRO:HD2	1:A:416:GLN:HE22	1.77	0.45
1:A:515:LEU:HB3	1:A:519:GLU:HB2	1.97	0.45
1:B:390:ASN:ND2	5:B:709:HOH:O	2.44	0.45
1:D:148:PHE:CD1	1:D:149:TYR:O	2.69	0.45
1:C:33:GLN:H	1:C:84:TYR:HH	1.60	0.45
1:D:59:HIS:ND1	1:D:60:ALA:N	2.64	0.45
1:A:258:ASP:O	1:A:259:LEU:C	2.57	0.45
1:A:264:CYS:O	1:A:267:GLN:CG	2.61	0.45
1:A:334:SER:C	1:A:336:ARG:N	2.74	0.45
1:B:419:THR:HB	1:B:420:PRO:HD3	1.99	0.45
1:C:375:LYS:O	1:C:376:LEU:C	2.58	0.45
1:C:544:LYS:HB2	5:C:783:HOH:O	2.17	0.45
1:D:470:GLU:O	1:D:473:THR:HG22	2.17	0.45
1:D:545:THR:O	1:D:548:GLU:N	2.48	0.45
1:A:407:ILE:O	1:A:411:THR:OG1	2.18	0.45
1:B:163:VAL:O	1:B:167:CYS:HB2	2.17	0.45
1:C:152:GLU:OE1	1:C:287:HIS:ND1	2.38	0.45
1:C:473:THR:HG23	5:C:811:HOH:O	2.16	0.45
1:C:542:GLN:NE2	1:C:582:LEU:HA	2.32	0.45
1:B:347:ARG:HG3	1:B:481:VAL:HG12	1.99	0.45
1:C:83:THR:HG22	1:C:83:THR:O	2.17	0.45
1:C:419:THR:HG23	1:C:529:VAL:CG1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:PHE:CZ	1:C:550:PHE:CE1	3.05	0.45
1:D:464:GLU:HB2	5:D:739:HOH:O	2.17	0.45
1:B:551:VAL:O	1:B:552:ALA:C	2.56	0.45
1:C:101:CYS:O	1:C:104:LYS:HB2	2.16	0.45
1:A:132:LYS:O	1:A:136:LYS:HB2	2.15	0.45
1:A:137:TYR:O	1:A:141:VAL:HG23	2.17	0.45
1:A:347:ARG:HH22	1:A:484:ARG:HH12	1.66	0.45
1:A:463:HIS:CD2	1:A:472:VAL:CG1	2.99	0.45
1:C:6:GLU:HG3	1:C:66:LEU:HD11	1.97	0.45
1:D:16:GLU:O	1:D:20:GLN:HG3	2.17	0.45
1:D:151:PRO:HG2	1:D:256:ARG:HD3	1.98	0.45
1:D:262:TYR:CD2	1:D:262:TYR:C	2.95	0.45
1:D:445:MET:O	1:D:446:PRO:C	2.57	0.45
1:B:257:ALA:O	1:B:260:ALA:HB3	2.17	0.44
1:D:131:LYS:CE	3:D:602:PRO:CB	2.94	0.44
1:D:178:LEU:HB2	1:D:179:PRO:HD3	1.99	0.44
1:D:321:ALA:O	1:D:322:LYS:C	2.57	0.44
1:A:9:HIS:HE1	5:A:783:HOH:O	1.99	0.44
1:A:512:ILE:O	1:A:520:LYS:HE3	2.17	0.44
1:B:274:LEU:HA	1:B:274:LEU:HD23	1.69	0.44
1:C:389:LYS:HA	1:C:392:GLU:OE2	2.16	0.44
1:D:9:HIS:NE2	5:D:703:HOH:O	2.36	0.44
1:A:347:ARG:HH21	1:A:485:PRO:HD3	1.82	0.44
1:C:281:PRO:O	1:C:285:LYS:N	2.50	0.44
1:C:301:LEU:HB3	1:C:336:ARG:NH1	2.33	0.44
1:C:569:LEU:HD22	1:C:570:GLU:CG	2.34	0.44
1:D:268:ASP:OD1	1:D:268:ASP:N	2.37	0.44
1:B:66:LEU:HD23	1:B:69:LEU:HD12	2.00	0.44
1:B:236:ASP:O	1:B:240:VAL:HG23	2.18	0.44
1:C:390:ASN:ND2	3:C:604:PRO:OXT	2.51	0.44
1:D:158:ASN:OD1	3:D:602:PRO:HD3	2.17	0.44
1:D:501:PHE:O	1:D:504:GLU:HB2	2.18	0.44
1:A:44:LYS:HA	1:A:47:THR:HB	1.99	0.44
1:A:243:GLU:OE2	1:A:251:GLU:HB3	2.18	0.44
1:C:160:TYR:HA	1:C:184:MET:HE1	1.99	0.44
1:D:233:ILE:HG23	1:D:259:LEU:HD11	1.98	0.44
1:B:396:LYS:HB2	1:B:396:LYS:HE3	1.71	0.44
1:A:4:LYS:HG2	1:A:57:GLU:OE2	2.16	0.44
1:B:237:LEU:CD1	1:B:241:HIS:CE1	3.01	0.44
1:D:382:GLU:CB	1:D:383:PRO:CD	2.87	0.44
1:A:116:LYS:HA	1:A:117:PRO:HD2	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:CG	1:A:218:LEU:N	2.77	0.44
1:A:484:ARG:HH11	1:A:484:ARG:HB3	1.83	0.44
1:C:396:LYS:HB3	1:C:397:HIS:CD2	2.53	0.44
1:C:445:MET:O	1:C:446:PRO:C	2.60	0.44
1:C:512:ILE:HA	1:C:515:LEU:HD12	1.99	0.44
1:D:340:TYR:HA	1:D:445:MET:CE	2.48	0.44
1:B:139:TYR:CE1	1:B:143:ARG:HD2	2.53	0.43
1:B:257:ALA:HA	1:B:260:ALA:HB3	2.00	0.43
1:B:369:TYR:CD1	1:B:369:TYR:C	2.96	0.43
1:B:493:ASP:OD1	1:B:495:THR:HB	2.17	0.43
1:B:539:THR:CG2	1:B:541:GLU:HG2	2.48	0.43
1:D:164:PHE:CE1	1:D:177:LEU:HD21	2.54	0.43
1:A:333:TYR:HE1	1:A:340:TYR:HE2	1.66	0.43
1:C:223:PRO:HB3	1:C:335:ARG:HB2	2.00	0.43
1:C:539:THR:HB	1:C:542:GLN:H	1.82	0.43
1:A:31:LEU:HB2	1:A:39:HIS:NE2	2.33	0.43
1:A:43:VAL:O	1:A:43:VAL:CG1	2.66	0.43
1:A:386:LEU:HD21	1:A:484:ARG:HH21	1.83	0.43
1:B:51:LYS:HB2	1:B:51:LYS:HE2	1.74	0.43
1:B:333:TYR:HD2	1:B:333:TYR:O	2.02	0.43
1:B:380:VAL:O	1:B:384:GLN:HG3	2.17	0.43
1:B:486:CYS:O	1:B:489:ASP:HB2	2.17	0.43
1:B:515:LEU:CD2	1:B:516:PRO:HD2	2.46	0.43
1:C:22:LEU:O	1:C:23:VAL:C	2.60	0.43
1:C:484:ARG:O	1:C:488:SER:HB2	2.18	0.43
1:D:95:GLU:OE2	1:D:96:PRO:HA	2.19	0.43
1:D:217:ARG:NH1	5:D:718:HOH:O	2.51	0.43
1:D:411:THR:HA	1:D:422:LEU:HD22	1.99	0.43
1:A:6:GLU:HA	1:A:6:GLU:OE1	2.19	0.43
1:A:140:GLU:HA	1:A:140:GLU:OE1	2.19	0.43
1:A:452:LEU:HD13	1:A:484:ARG:HD2	2.00	0.43
1:D:61:GLY:HA2	1:D:64:LYS:HE3	2.01	0.43
1:A:250:LEU:O	1:A:254:ASP:HB2	2.18	0.43
1:A:275:LYS:HD2	1:A:278:CYS:HB2	2.01	0.43
1:C:71:GLY:C	1:C:73:GLU:H	2.27	0.43
1:C:161:ASN:ND2	3:C:603:PRO:HA	2.33	0.43
1:C:294:LYS:NZ	1:C:338:PRO:O	2.45	0.43
1:C:408:VAL:HA	1:C:532:LEU:CD1	2.48	0.43
1:C:412:ARG:HB3	1:C:492:LEU:HD13	2.01	0.43
1:C:550:PHE:CD1	1:C:574:LEU:HD21	2.53	0.43
1:A:508:PHE:N	1:A:508:PHE:CD1	2.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:CYS:HB3	1:B:101:CYS:HB3	1.91	0.43
1:C:318:TYR:CZ	1:C:322:LYS:HE2	2.53	0.43
1:D:81:ARG:CG	1:D:88:ALA:HB3	2.43	0.43
1:D:379:LEU:O	1:D:382:GLU:HG3	2.19	0.43
1:A:334:SER:C	1:A:336:ARG:H	2.27	0.43
1:A:310:GLU:C	1:A:311:ASP:O	2.62	0.43
1:B:47:THR:O	1:B:50:ALA:HB3	2.19	0.43
1:B:433:GLY:HA2	1:B:437:CYS:SG	2.58	0.43
1:C:40:VAL:O	1:C:41:LYS:C	2.62	0.43
1:C:109:SER:HA	5:C:766:HOH:O	2.17	0.43
1:D:407:ILE:HG13	1:D:426:SER:CB	2.48	0.43
1:B:48:GLU:OE1	1:B:51:LYS:NZ	2.52	0.43
1:B:93:LYS:H	1:B:93:LYS:HG2	1.51	0.43
1:B:273:LYS:NZ	1:B:294:LYS:O	2.52	0.43
1:B:366:HIS:O	1:B:370:ALA:HB2	2.19	0.43
1:B:396:LYS:HG3	1:B:397:HIS:ND1	2.34	0.43
1:C:417:VAL:HA	5:C:765:HOH:O	2.18	0.43
1:C:563:LYS:O	1:C:564:GLU:C	2.61	0.43
1:D:39:HIS:O	1:D:40:VAL:C	2.62	0.43
1:A:8:ALA:HB2	1:A:53:CYS:HB2	2.01	0.42
1:C:313:GLU:H	1:C:313:GLU:HG3	1.62	0.42
1:A:406:LEU:HD13	1:A:429:LEU:CB	2.49	0.42
1:B:21:GLY:O	1:B:24:LEU:HB3	2.19	0.42
1:B:310:GLU:O	1:B:311:ASP:C	2.63	0.42
1:C:384:GLN:HE22	1:C:445:MET:HE2	1.84	0.42
1:D:283:LEU:C	1:D:285:LYS:N	2.77	0.42
1:D:470:GLU:C	1:D:473:THR:HG22	2.44	0.42
1:B:29:GLN:NE2	1:B:146:PRO:HA	2.33	0.42
1:B:32:GLN:HA	1:B:143:ARG:HB2	2.01	0.42
1:C:36:PHE:O	1:C:40:VAL:HG23	2.19	0.42
1:C:160:TYR:CE1	1:C:164:PHE:HE2	2.37	0.42
1:C:297:VAL:HG13	1:C:335:ARG:O	2.18	0.42
1:C:299:GLU:HG2	1:C:300:ASN:ND2	2.34	0.42
1:C:417:VAL:HG12	1:C:422:LEU:HG	2.01	0.42
1:A:160:TYR:HA	1:A:184:MET:HE1	2.00	0.42
1:A:226:ASP:HB2	1:A:229:ASP:HB2	2.02	0.42
1:B:87:MET:HE3	1:B:102:PHE:HD1	1.84	0.42
1:B:382:GLU:HB2	1:B:383:PRO:CD	2.50	0.42
1:C:10:ARG:O	1:C:11:PHE:C	2.63	0.42
1:C:470:GLU:HB3	5:C:752:HOH:O	2.19	0.42
1:D:5:SER:HB2	1:D:62:CYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:HIS:O	1:D:246:HIS:CG	2.72	0.42
1:B:150:ALA:O	1:B:151:PRO:C	2.62	0.42
1:B:496:TYR:HE2	1:B:536:PRO:HG3	1.84	0.42
1:C:39:HIS:CE1	1:C:139:TYR:HE1	2.37	0.42
1:C:80:LEU:HD11	1:C:87:MET:SD	2.59	0.42
1:D:61:GLY:HA2	1:D:64:LYS:CE	2.49	0.42
1:D:150:ALA:O	1:D:151:PRO:C	2.59	0.42
1:A:207:GLU:HG3	5:A:785:HOH:O	2.18	0.42
1:B:125:GLU:O	1:B:126:PHE:C	2.61	0.42
1:C:419:THR:HG22	1:C:526:THR:HG23	2.02	0.42
1:D:510:ALA:C	1:D:512:ILE:H	2.27	0.42
1:A:36:PHE:O	1:A:40:VAL:HG23	2.20	0.42
1:A:223:PRO:HA	1:A:335:ARG:HB2	2.02	0.42
1:A:369:TYR:CD1	1:A:369:TYR:C	2.98	0.42
1:A:419:THR:HG23	1:A:529:VAL:CG1	2.49	0.42
1:A:539:THR:HB	1:A:542:GLN:HB2	2.01	0.42
1:B:110:PRO:HG3	1:B:144:ARG:HA	2.01	0.42
1:C:49:PHE:C	1:C:49:PHE:CD2	2.97	0.42
1:D:177:LEU:O	1:D:178:LEU:C	2.62	0.42
1:D:194:ARG:HD2	1:D:198:ARG:NH2	2.35	0.42
1:D:563:LYS:HB2	5:D:772:HOH:O	2.20	0.42
1:A:299:GLU:H	1:A:299:GLU:HG2	1.58	0.42
1:B:535:LYS:CE	1:B:583:ALA:HA	2.49	0.42
1:C:250:LEU:O	1:C:251:GLU:C	2.61	0.42
1:D:78:ALA:C	1:D:80:LEU:H	2.27	0.42
1:A:59:HIS:CD2	1:A:60:ALA:H	2.38	0.42
1:A:182:GLU:O	1:A:183:THR:C	2.62	0.42
1:B:341:ALA:HB1	1:B:449:GLU:HB2	2.01	0.42
1:D:11:PHE:CD1	1:D:11:PHE:C	2.97	0.42
1:D:107:ASP:C	1:D:107:ASP:OD1	2.63	0.42
1:D:242:LYS:HB2	1:D:242:LYS:HE3	1.83	0.42
1:B:341:ALA:HB3	1:B:344:VAL:HG23	2.02	0.42
1:C:164:PHE:CE1	1:C:177:LEU:HD22	2.55	0.42
1:C:230:VAL:O	1:C:231:THR:C	2.63	0.42
1:D:77:VAL:O	1:D:77:VAL:HG12	2.20	0.42
1:D:112:LEU:HB3	1:D:113:PRO:HD2	2.02	0.42
1:D:246:HIS:O	1:D:246:HIS:ND1	2.53	0.42
1:D:538:ALA:HA	5:D:784:HOH:O	2.19	0.42
1:D:550:PHE:HE2	1:D:574:LEU:HD21	1.81	0.42
1:B:391:CYS:O	1:B:395:GLU:HG2	2.19	0.41
1:D:369:TYR:O	1:D:370:ALA:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:CYS:HA	1:D:439:LYS:HD2	2.01	0.41
1:A:35:PRO:O	1:A:38:GLU:HB2	2.20	0.41
1:A:225:ALA:HB2	1:A:270:LEU:HA	2.02	0.41
1:B:387:ILE:HD13	1:B:387:ILE:N	2.34	0.41
1:B:516:PRO:O	1:B:517:ASP:C	2.63	0.41
1:C:6:GLU:HA	1:C:6:GLU:OE1	2.20	0.41
1:A:163:VAL:C	1:A:165:GLN:H	2.27	0.41
1:C:196:ARG:HA	1:C:196:ARG:HD2	1.74	0.41
1:C:344:VAL:O	1:C:345:LEU:C	2.62	0.41
1:C:391:CYS:O	1:C:395:GLU:HG2	2.20	0.41
1:D:299:GLU:HA	5:D:728:HOH:O	2.19	0.41
1:D:565:GLY:O	1:D:569:LEU:HD12	2.20	0.41
1:A:254:ASP:O	1:A:257:ALA:HB3	2.19	0.41
1:A:371:THR:HG22	1:A:371:THR:O	2.20	0.41
1:B:237:LEU:HD11	1:B:241:HIS:NE2	2.36	0.41
1:B:303:PRO:HD3	3:B:603:PRO:HA	2.01	0.41
1:C:499:LYS:HD2	1:C:499:LYS:HA	1.86	0.41
1:D:36:PHE:O	1:D:40:VAL:HG23	2.21	0.41
1:D:103:LEU:HD11	1:D:246:HIS:O	2.20	0.41
1:D:116:LYS:HA	1:D:117:PRO:HD2	1.83	0.41
1:D:229:ASP:O	1:D:233:ILE:HG13	2.21	0.41
1:A:304:LEU:HD23	1:A:308:PHE:CD2	2.55	0.41
1:A:438:ALA:HB3	5:A:751:HOH:O	2.21	0.41
1:B:301:LEU:HD13	1:B:336:ARG:NH1	2.36	0.41
1:C:364:ASP:O	1:C:365:PRO:C	2.62	0.41
1:C:429:LEU:HD23	1:C:429:LEU:HA	1.68	0.41
1:C:544:LYS:HG2	5:C:733:HOH:O	2.20	0.41
1:D:440:PRO:O	1:D:441:GLU:C	2.63	0.41
1:D:440:PRO:O	1:D:444:ARG:HG3	2.20	0.41
1:D:512:ILE:O	1:D:520:LYS:HE3	2.20	0.41
1:A:337:HIS:C	1:A:339:GLU:N	2.77	0.41
1:A:347:ARG:HH21	1:A:485:PRO:CG	2.34	0.41
1:B:530:GLU:O	1:B:531:LEU:C	2.64	0.41
1:C:22:LEU:O	1:C:26:ALA:N	2.45	0.41
1:D:6:GLU:HG3	1:D:66:LEU:HD11	2.02	0.41
1:D:374:ASP:OD1	1:D:374:ASP:N	2.53	0.41
1:D:403:GLN:HG2	1:D:427:ARG:HA	2.02	0.41
1:A:21:GLY:HA3	1:A:154:LEU:HD21	2.03	0.41
1:A:155:TYR:CD2	1:A:155:TYR:C	2.98	0.41
1:A:553:PHE:CZ	1:A:567:PHE:HD1	2.39	0.41
1:B:52:THR:C	1:B:54:VAL:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:PHE:HD2	1:B:574:LEU:HD11	1.86	0.41
1:C:340:TYR:CZ	1:C:380:VAL:HG21	2.55	0.41
1:C:4:LYS:HB2	1:C:57:GLU:CD	2.46	0.41
1:C:412:ARG:CB	1:C:492:LEU:HD13	2.50	0.41
1:A:16:GLU:CG	3:A:603:PRO:HG3	2.50	0.41
1:A:341:ALA:O	1:A:342:VAL:C	2.64	0.41
1:A:359:CYS:C	1:A:361:ALA:N	2.78	0.41
1:A:492:LEU:HD12	1:A:492:LEU:N	2.34	0.41
1:B:6:GLU:OE2	1:B:10:ARG:NE	2.54	0.41
1:B:414:ALA:O	1:B:417:VAL:HG23	2.20	0.41
1:C:130:GLU:HG2	3:C:603:PRO:HB2	2.02	0.41
1:C:218:LEU:HD23	1:C:218:LEU:HA	1.67	0.41
1:C:390:ASN:CB	3:C:604:PRO:HB3	2.50	0.41
1:C:505:SER:HB2	1:C:530:GLU:HG3	2.01	0.41
1:D:17:GLU:OE1	3:D:602:PRO:HB2	2.20	0.41
1:D:393:LEU:HD12	1:D:393:LEU:HA	1.86	0.41
1:D:404:ASN:OD1	1:D:525:GLN:HG2	2.21	0.41
1:A:535:LYS:HA	1:A:536:PRO:HD2	1.79	0.41
1:B:232:LYS:HD3	1:B:236:ASP:OD1	2.21	0.41
1:C:129:ASP:HB3	1:C:132:LYS:HB3	2.03	0.41
1:C:428:SER:O	1:C:429:LEU:C	2.63	0.41
1:C:429:LEU:HD23	1:C:455:ILE:HD13	2.03	0.41
1:D:48:GLU:O	1:D:49:PHE:C	2.63	0.41
1:D:71:GLY:HA3	1:D:98:ARG:HH11	1.84	0.41
1:D:563:LYS:H	1:D:563:LYS:HG3	1.73	0.41
1:A:214:SER:CB	1:A:234:VAL:HG22	2.51	0.40
1:B:160:TYR:O	1:B:164:PHE:HD2	2.04	0.40
1:B:512:ILE:HD13	1:B:554:VAL:HG11	2.02	0.40
1:C:87:MET:CE	1:C:105:HIS:HB2	2.42	0.40
1:D:237:LEU:HD12	1:D:237:LEU:HA	1.82	0.40
1:D:342:VAL:HG21	3:D:603:PRO:HD2	2.03	0.40
1:A:83:THR:HB	1:A:84:TYR:CE2	2.57	0.40
1:A:332:GLU:O	1:A:336:ARG:HD2	2.21	0.40
1:A:334:SER:OG	1:A:345:LEU:HD13	2.21	0.40
1:B:9:HIS:CE1	1:B:13:ASP:OD2	2.74	0.40
1:B:436:CYS:O	1:B:439:LYS:HB2	2.21	0.40
1:C:81:ARG:HD3	1:C:88:ALA:CB	2.51	0.40
1:C:165:GLN:OE1	1:C:165:GLN:HA	2.20	0.40
1:C:535:LYS:HG3	1:C:582:LEU:HD13	2.04	0.40
1:A:353:GLU:HG2	5:A:704:HOH:O	2.22	0.40
1:A:484:ARG:HB3	1:A:484:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:SER:HB3	1:C:274:LEU:HD12	2.03	0.40
1:D:13:ASP:OD1	1:D:254:ASP:OD2	2.39	0.40
1:A:436:CYS:O	1:A:438:ALA:N	2.54	0.40
1:B:33:GLN:HB2	1:B:84:TYR:CZ	2.56	0.40
1:B:52:THR:O	1:B:55:ALA:N	2.55	0.40
1:C:50:ALA:O	1:C:51:LYS:C	2.63	0.40
1:C:232:LYS:O	1:C:232:LYS:HD3	2.21	0.40
1:D:196:ARG:HH12	1:D:200:ALA:HB2	1.86	0.40
1:A:116:LYS:NZ	1:B:116:LYS:HG2	2.37	0.40
1:A:289:ILE:O	1:A:292:ILE:HG22	2.21	0.40
1:A:414:ALA:HB1	1:A:417:VAL:HG23	2.04	0.40
1:A:440:PRO:O	1:A:441:GLU:C	2.63	0.40
1:A:456:LEU:HA	1:A:456:LEU:HD23	1.82	0.40
1:B:224:LYS:HE3	1:B:268:ASP:O	2.21	0.40
1:B:257:ALA:O	1:B:261:LYS:N	2.38	0.40
1:B:416:GLN:NE2	1:B:496:TYR:HB2	2.37	0.40
1:B:533:LYS:O	1:B:536:PRO:HD3	2.21	0.40
1:C:223:PRO:CB	1:C:335:ARG:HB2	2.51	0.40
1:C:402:PHE:O	1:C:405:ALA:HB3	2.22	0.40
1:D:443:GLU:C	1:D:446:PRO:HD2	2.47	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LYS:NZ	1:D:313:GLU:OE2[1_545]	2.05	0.15
1:C:312:LYS:NZ	1:D:361:ALA:O[1_546]	2.15	0.05

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	579/583 (99%)	518 (90%)	58 (10%)	3 (0%)	24	43
1	B	579/583 (99%)	523 (90%)	54 (9%)	2 (0%)	36	55
1	C	579/583 (99%)	515 (89%)	62 (11%)	2 (0%)	36	55
1	D	580/583 (100%)	517 (89%)	60 (10%)	3 (0%)	24	43
All	All	2317/2332 (99%)	2073 (90%)	234 (10%)	10 (0%)	30	49

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	499	LYS
1	A	269	THR
1	B	441	GLU
1	D	79	THR
1	A	360	CYS
1	D	92	GLU
1	D	500	PRO
1	C	382	GLU
1	A	485	PRO
1	C	468	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	515/517 (100%)	468 (91%)	47 (9%)	9	19
1	B	515/517 (100%)	471 (92%)	44 (8%)	10	22
1	C	515/517 (100%)	474 (92%)	41 (8%)	11	24
1	D	516/517 (100%)	480 (93%)	36 (7%)	14	29
All	All	2061/2068 (100%)	1893 (92%)	168 (8%)	11	23

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE

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Mol	Chain	Res	Type
1	A	68	THR
1	A	91	CYS
1	A	94	GLN
1	A	97	GLU
1	A	98	ARG
1	A	104	LYS
1	A	115	LEU
1	A	153	LEU
1	A	204	LYS
1	A	215	VAL
1	A	217	ARG
1	A	218	LEU
1	A	221	LYS
1	A	224	LYS
1	A	234	VAL
1	A	239	LYS
1	A	268	ASP
1	A	275	LYS
1	A	297	VAL
1	A	299	GLU
1	A	304	LEU
1	A	312	LYS
1	A	314	VAL
1	A	328	SER
1	A	347	ARG
1	A	375	LYS
1	A	386	LEU
1	A	392	GLU
1	A	431	LYS
1	A	439	LYS
1	A	441	GLU
1	A	465	LYS
1	A	466	THR
1	A	479	SER
1	A	483	ARG
1	A	491	THR
1	A	492	LEU
1	A	495	THR
1	A	497	VAL
1	A	501	PHE
1	A	507	THR
1	A	523	LYS

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Mol	Chain	Res	Type
1	A	541	GLU
1	A	545	THR
1	A	578	THR
1	A	582	LEU
1	B	3	HIS
1	B	4	LYS
1	B	7	ILE
1	B	38	GLU
1	B	49	PHE
1	B	80	LEU
1	B	92	GLU
1	B	97	GLU
1	B	136	LYS
1	B	161	ASN
1	B	173	LYS
1	B	180	LYS
1	B	194	ARG
1	B	202	ILE
1	B	215	VAL
1	B	221	LYS
1	B	229	ASP
1	B	268	ASP
1	B	272	SER
1	B	275	LYS
1	B	310	GLU
1	B	311	ASP
1	B	313	GLU
1	B	319	GLN
1	B	331	TYR
1	B	343	SER
1	B	351	GLU
1	B	355	THR
1	B	356	LEU
1	B	380	VAL
1	B	387	ILE
1	B	408	VAL
1	B	417	VAL
1	B	439	LYS
1	B	450	ASP
1	B	472	VAL
1	B	474	LYS
1	B	481	VAL

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Mol	Chain	Res	Type
1	B	495	THR
1	B	511	ASP
1	B	512	ILE
1	B	517	ASP
1	B	541	GLU
1	B	544	LYS
1	C	34	CYS
1	C	38	GLU
1	C	43	VAL
1	C	47	THR
1	C	51	LYS
1	C	52	THR
1	C	53	CYS
1	C	54	VAL
1	C	72	ASP
1	C	93	LYS
1	C	105	HIS
1	C	116	LYS
1	C	131	LYS
1	C	163	VAL
1	C	177	LEU
1	C	183	THR
1	C	221	LYS
1	C	233	ILE
1	C	234	VAL
1	C	235	THR
1	C	268	ASP
1	C	297	VAL
1	C	312	LYS
1	C	336	ARG
1	C	350	LYS
1	C	356	LEU
1	C	379	LEU
1	C	407	ILE
1	C	409	ARG
1	C	424	GLU
1	C	461	VAL
1	C	474	LYS
1	C	484	ARG
1	C	495	THR
1	C	499	LYS
1	C	501	PHE

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Mol	Chain	Res	Type
1	C	519	GLU
1	C	524	LYS
1	C	537	LYS
1	C	556	LYS
1	C	578	THR
1	D	13	ASP
1	D	17	GLU
1	D	44	LYS
1	D	47	THR
1	D	76	LYS
1	D	77	VAL
1	D	104	LYS
1	D	130	GLU
1	D	131	LYS
1	D	178	LEU
1	D	204	LYS
1	D	233	ILE
1	D	239	LYS
1	D	256	ARG
1	D	268	ASP
1	D	271	SER
1	D	292	ILE
1	D	293	ASP
1	D	300	ASN
1	D	312	LYS
1	D	314	VAL
1	D	374	ASP
1	D	386	LEU
1	D	388	LYS
1	D	417	VAL
1	D	424	GLU
1	D	471	LYS
1	D	477	THR
1	D	480	LEU
1	D	491	THR
1	D	498	PRO
1	D	501	PHE
1	D	507	THR
1	D	518	THR
1	D	564	GLU
1	D	582	LEU

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	94	GLN
1	A	105	HIS
1	A	203	GLN
1	A	241	HIS
1	A	317	ASN
1	A	463	HIS
1	A	509	HIS
1	A	534	HIS
1	B	29	GLN
1	B	33	GLN
1	B	67	HIS
1	B	319	GLN
1	B	463	HIS
1	C	300	ASN
1	C	397	HIS
1	C	482	ASN
1	D	3	HIS
1	D	20	GLN
1	D	99	ASN
1	D	145	HIS
1	D	463	HIS
1	D	579	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](#)

16 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	PRO	D	602	-	8,8,8	0.96	0	10,10,10	1.91	2 (20%)
2	PGE	B	601	-	9,9,9	0.57	0	8,8,8	0.77	0
3	PRO	B	602	-	8,8,8	0.93	0	10,10,10	1.27	1 (10%)
3	PRO	C	605	-	8,8,8	0.75	0	10,10,10	1.46	2 (20%)
3	PRO	D	603	-	8,8,8	0.96	1 (12%)	10,10,10	1.68	2 (20%)
3	PRO	D	605	-	8,8,8	0.85	0	10,10,10	1.29	1 (10%)
2	PGE	C	601	-	9,9,9	0.59	0	8,8,8	0.67	0
3	PRO	C	604	-	8,8,8	1.05	1 (12%)	10,10,10	1.57	1 (10%)
3	PRO	A	602	-	8,8,8	1.10	1 (12%)	10,10,10	1.95	2 (20%)
2	PGE	A	601	-	9,9,9	0.61	0	8,8,8	0.29	0
3	PRO	B	603	-	8,8,8	0.87	0	10,10,10	1.54	3 (30%)
3	PRO	A	603	-	8,8,8	0.68	0	10,10,10	1.45	2 (20%)
3	PRO	C	603	-	8,8,8	0.93	1 (12%)	10,10,10	1.18	1 (10%)
3	PRO	D	604	-	8,8,8	0.91	1 (12%)	10,10,10	1.27	1 (10%)
4	PEG	D	601	-	6,6,6	0.45	0	5,5,5	0.34	0
4	PEG	C	602	-	6,6,6	0.48	0	5,5,5	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PRO	D	602	-	-	4/4/11/11	0/1/1/1
2	PGE	B	601	-	-	5/7/7/7	-
3	PRO	B	602	-	-	2/4/11/11	0/1/1/1
3	PRO	C	605	-	-	2/4/11/11	0/1/1/1
3	PRO	D	603	-	-	4/4/11/11	0/1/1/1
3	PRO	D	605	-	-	4/4/11/11	0/1/1/1
2	PGE	C	601	-	-	3/7/7/7	-
3	PRO	C	604	-	-	4/4/11/11	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PRO	A	602	-	-	4/4/11/11	0/1/1/1
2	PGE	A	601	-	-	4/7/7/7	-
3	PRO	B	603	-	-	4/4/11/11	0/1/1/1
3	PRO	A	603	-	-	4/4/11/11	0/1/1/1
3	PRO	C	603	-	-	2/4/11/11	0/1/1/1
3	PRO	D	604	-	-	4/4/11/11	0/1/1/1
4	PEG	D	601	-	-	2/4/4/4	-
4	PEG	C	602	-	-	3/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	PRO	OXT-C	-2.79	1.21	1.30
3	C	604	PRO	OXT-C	-2.57	1.22	1.30
3	D	603	PRO	OXT-C	-2.05	1.24	1.30
3	C	603	PRO	OXT-C	-2.04	1.24	1.30
3	D	604	PRO	OXT-C	-2.02	1.24	1.30

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	PRO	OXT-C-O	-4.80	113.20	124.08
3	D	602	PRO	OXT-C-O	-4.16	114.64	124.08
3	C	604	PRO	OXT-C-O	-3.43	116.31	124.08
3	D	603	PRO	OXT-C-O	-3.43	116.31	124.08
3	D	602	PRO	OXT-C-CA	3.11	124.05	113.51
3	B	603	PRO	OXT-C-O	-2.92	117.46	124.08
3	A	602	PRO	OXT-C-CA	2.82	123.04	113.51
3	A	603	PRO	OXT-C-CA	2.81	123.03	113.51
3	C	605	PRO	OXT-C-CA	2.63	122.42	113.51
3	D	603	PRO	OXT-C-CA	2.61	122.34	113.51
3	C	605	PRO	OXT-C-O	-2.53	118.33	124.08
3	B	603	PRO	OXT-C-CA	2.41	121.65	113.51
3	C	603	PRO	CB-CA-C	-2.32	106.74	112.72
3	B	602	PRO	OXT-C-CA	2.29	121.26	113.51
3	A	603	PRO	OXT-C-O	-2.19	119.12	124.08
3	D	605	PRO	OXT-C-O	-2.12	119.27	124.08
3	B	603	PRO	C-CA-N	2.08	114.94	106.84
3	D	604	PRO	OXT-C-O	-2.01	119.51	124.08

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	PRO	O-C-CA-N
3	A	602	PRO	OXT-C-CA-N
3	A	602	PRO	O-C-CA-CB
3	A	602	PRO	OXT-C-CA-CB
3	A	603	PRO	O-C-CA-N
3	A	603	PRO	OXT-C-CA-N
3	A	603	PRO	O-C-CA-CB
3	A	603	PRO	OXT-C-CA-CB
3	C	603	PRO	O-C-CA-N
3	C	603	PRO	OXT-C-CA-N
3	C	604	PRO	O-C-CA-N
3	C	604	PRO	OXT-C-CA-N
3	C	604	PRO	O-C-CA-CB
3	C	604	PRO	OXT-C-CA-CB
3	C	605	PRO	O-C-CA-N
3	C	605	PRO	OXT-C-CA-N
3	D	602	PRO	O-C-CA-N
3	D	602	PRO	OXT-C-CA-N
3	D	603	PRO	O-C-CA-N
3	D	603	PRO	OXT-C-CA-N
3	D	603	PRO	O-C-CA-CB
3	D	603	PRO	OXT-C-CA-CB
3	D	604	PRO	O-C-CA-N
3	D	604	PRO	OXT-C-CA-N
3	D	604	PRO	O-C-CA-CB
3	D	604	PRO	OXT-C-CA-CB
3	D	605	PRO	O-C-CA-N
3	D	605	PRO	OXT-C-CA-N
4	D	601	PEG	O2-C3-C4-O4
2	A	601	PGE	O1-C1-C2-O2
2	A	601	PGE	O3-C5-C6-O4
2	C	601	PGE	O3-C5-C6-O4
4	C	602	PEG	O1-C1-C2-O2
2	B	601	PGE	O3-C5-C6-O4
2	B	601	PGE	O2-C3-C4-O3
3	B	603	PRO	OXT-C-CA-CB
2	C	601	PGE	C6-C5-O3-C4
4	C	602	PEG	C4-C3-O2-C2
2	A	601	PGE	C3-C4-O3-C5
2	C	601	PGE	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
2	B	601	PGE	C4-C3-O2-C2
2	B	601	PGE	O1-C1-C2-O2
4	C	602	PEG	O2-C3-C4-O4
3	B	603	PRO	O-C-CA-CB
3	D	602	PRO	O-C-CA-CB
3	D	602	PRO	OXT-C-CA-CB
3	D	605	PRO	O-C-CA-CB
3	D	605	PRO	OXT-C-CA-CB
3	B	602	PRO	O-C-CA-N
3	B	602	PRO	OXT-C-CA-N
3	B	603	PRO	O-C-CA-N
3	B	603	PRO	OXT-C-CA-N
2	A	601	PGE	O2-C3-C4-O3
4	D	601	PEG	O1-C1-C2-O2
2	B	601	PGE	C3-C4-O3-C5

There are no ring outliers.

14 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	PRO	9	0
2	B	601	PGE	1	0
3	B	602	PRO	5	0
3	D	603	PRO	2	0
3	D	605	PRO	3	0
3	C	604	PRO	3	0
3	A	602	PRO	9	0
2	A	601	PGE	1	0
3	B	603	PRO	1	0
3	A	603	PRO	3	0
3	C	603	PRO	3	0
3	D	604	PRO	1	0
4	D	601	PEG	2	0
4	C	602	PEG	1	0

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	581/583 (99%)	-0.43	2 (0%) 90 87	33, 62, 96, 118	0
1	B	581/583 (99%)	-0.46	1 (0%) 91 89	33, 60, 104, 138	0
1	C	581/583 (99%)	-0.42	1 (0%) 91 89	36, 62, 106, 154	0
1	D	581/583 (99%)	-0.48	0 100 100	32, 60, 97, 133	1 (0%)
All	All	2324/2332 (99%)	-0.45	4 (0%) 91 89	32, 61, 102, 154	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	PHE	2.4
1	C	70	PHE	2.3
1	A	31	LEU	2.3
1	A	89	ASP	2.2

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	PRO	B	603	8/8	0.81	0.10	80,86,91,92	0
3	PRO	D	604	8/8	0.85	0.08	66,77,83,86	0
3	PRO	D	603	8/8	0.86	0.13	74,86,104,105	0
3	PRO	C	605	8/8	0.87	0.07	78,88,91,91	0
3	PRO	A	603	8/8	0.88	0.07	81,82,90,92	0
2	PGE	C	601	10/10	0.90	0.07	52,61,68,75	0
3	PRO	B	602	8/8	0.90	0.10	75,88,94,97	0
3	PRO	D	605	8/8	0.90	0.07	80,83,100,100	0
3	PRO	A	602	8/8	0.91	0.11	78,84,88,92	0
3	PRO	C	604	8/8	0.92	0.11	68,74,81,90	0
3	PRO	C	603	8/8	0.92	0.10	74,84,86,90	0
3	PRO	D	602	8/8	0.92	0.07	61,70,89,100	0
2	PGE	A	601	10/10	0.94	0.11	47,71,85,97	0
2	PGE	B	601	10/10	0.94	0.09	45,55,86,87	0
4	PEG	C	602	7/7	0.94	0.11	55,66,77,83	0
4	PEG	D	601	7/7	0.95	0.07	52,53,62,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.