



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:54 PM UTC

PDB ID : 3ITH / pdb_00003ith
Title : Crystal structure of the HIV-1 reverse transcriptase bound to a 6-vinylpyrimidine inhibitor
Authors : Freisz, S.; Bec, G.; Wolff, P.; Dumas, P.; Radi, M.; Botta, M.
Deposited on : 2009-08-28
Resolution : 2.80 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

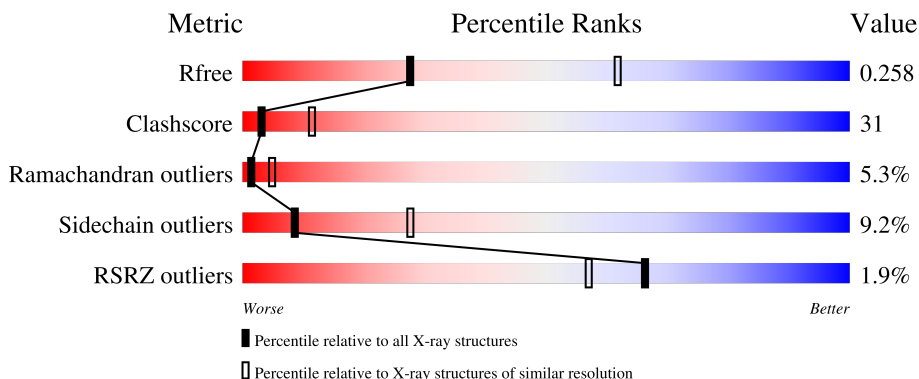
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	560	 2% 42% 46% 9% ..
1	C	560	 2% 46% 44% 9% .
2	B	427	 % 48% 39% 9% ..
2	D	427	 2% 44% 44% 9% .

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	EDM	A	561	-	-	X	-
3	EDM	C	561	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15912 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	556	4521	2927	753	833	8	0	0	0
1	C	556	4521	2927	753	833	8	0	0	0

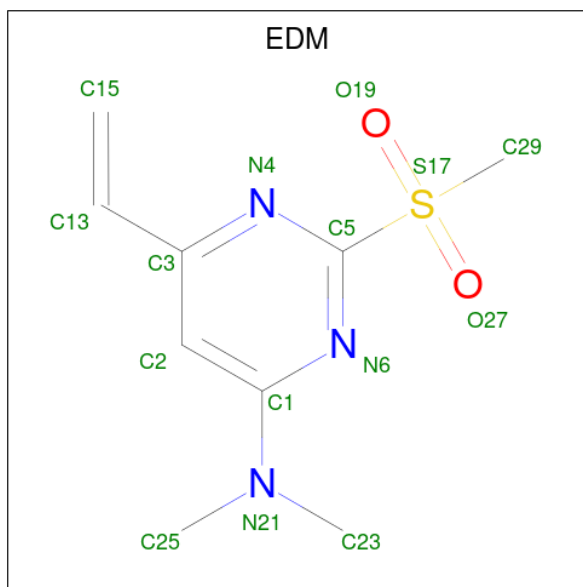
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	478	GLN	GLU	SEE REMARK 999	UNP P03366
C	478	GLN	GLU	SEE REMARK 999	UNP P03366

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	415	3420	2225	565	623	7	0	0	0
2	D	415	3420	2225	565	623	7	0	0	0

- Molecule 3 is 6-ethenyl-N,N-dimethyl-2-(methylsulfonyl)pyrimidin-4-amine (CCD ID: EDM) (formula: C₉H₁₃N₃O₂S).

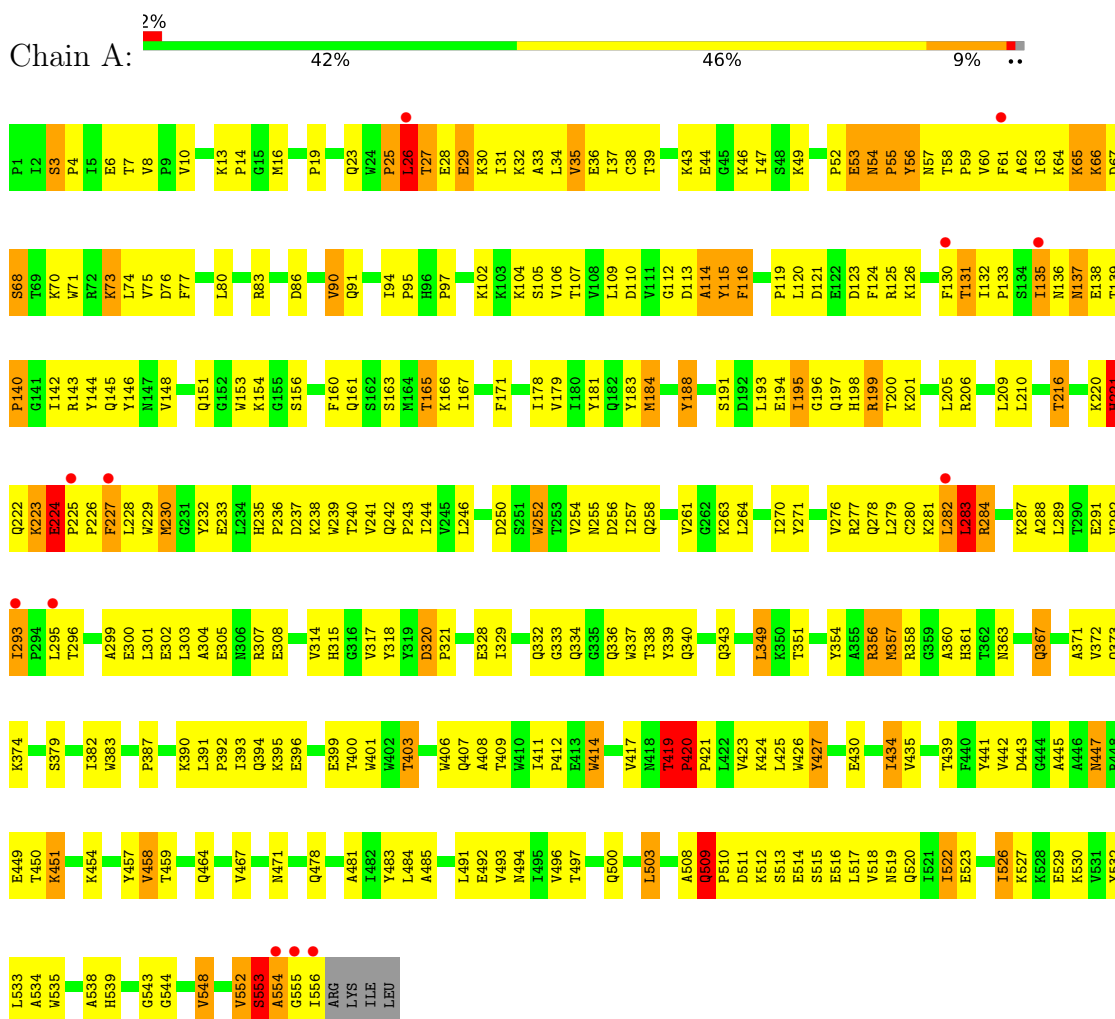


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	Total	C	N	O	S	0	0
			15	9	3	2	1		
3	C	1	Total	C	N	O	S	0	0
			15	9	3	2	1		

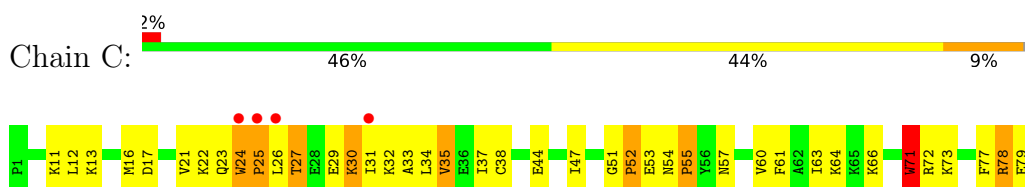
3 Residue-property plots

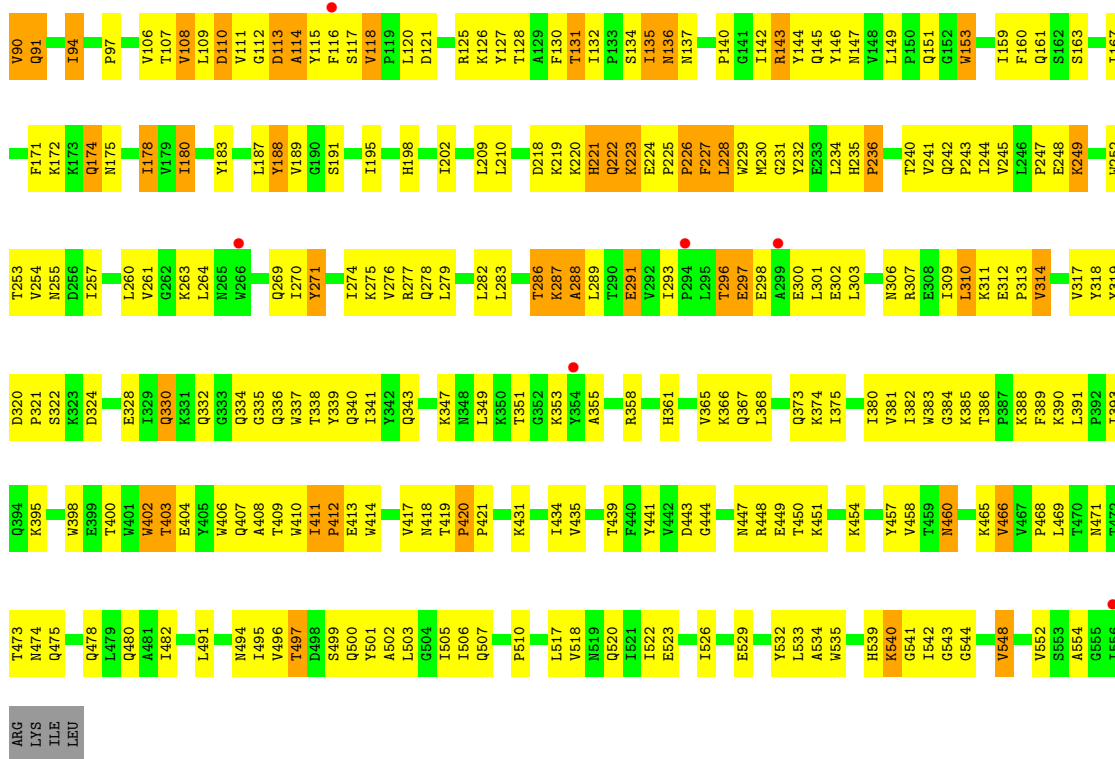
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

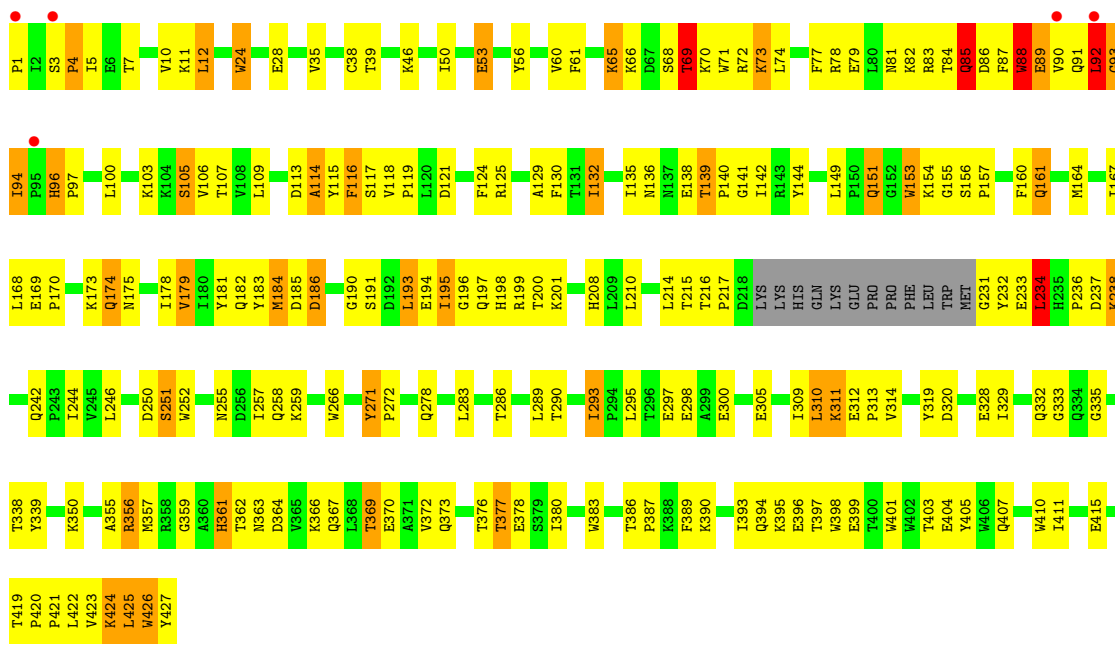


• Molecule 1: Reverse transcriptase/ribonuclease H



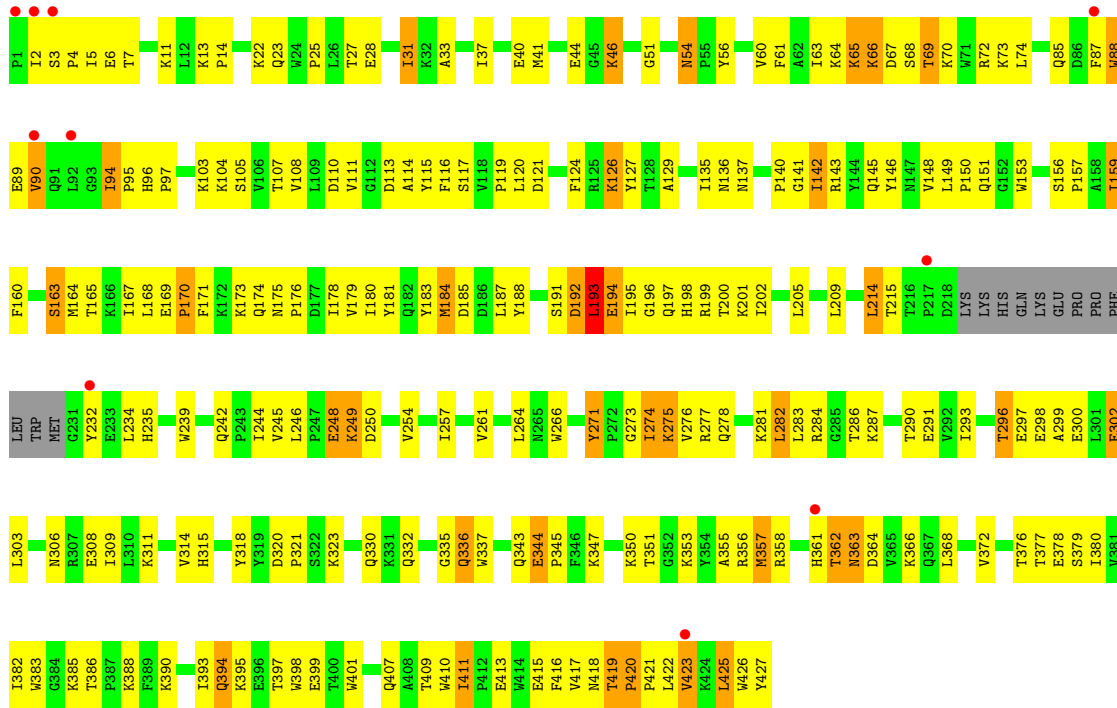


• Molecule 2: p51 RT



• Molecule 2: p51 RT





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.10Å 72.49Å 216.29Å 90.00° 95.89° 90.00°	Depositor
Resolution (Å)	43.90 – 2.80 43.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	85.3 (43.90-2.80) 85.3 (43.90-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.4_57)	Depositor
R, R_{free}	0.212 , 0.270 0.203 , 0.258	Depositor DCC
R_{free} test set	5835 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	79.9	Xtrriage
Anisotropy	0.230	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15912	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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: EDM

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	2/4639 (0.0%)	0.97	19/6302 (0.3%)
1	C	0.56	0/4639	0.96	12/6302 (0.2%)
2	B	0.64	0/3518	1.03	17/4781 (0.4%)
2	D	0.58	0/3518	0.96	12/4781 (0.3%)
All	All	0.60	2/16314 (0.0%)	0.98	60/22166 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	ILE	CA-CB	5.53	1.58	1.54
1	A	467	VAL	CA-CB	-5.35	1.50	1.54

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	54	ASN	CA-C-N	9.07	131.18	119.84
1	C	54	ASN	C-N-CA	9.07	131.18	119.84
1	C	51	GLY	CA-C-N	8.77	130.80	119.84
1	C	51	GLY	C-N-CA	8.77	130.80	119.84
2	D	419	THR	CA-C-N	8.36	129.00	120.38
2	D	419	THR	C-N-CA	8.36	129.00	120.38
2	D	54	ASN	CA-C-N	7.60	128.55	120.12
2	D	54	ASN	C-N-CA	7.60	128.55	120.12
1	A	548	VAL	CB-CA-C	-7.56	102.14	112.04
1	A	53	GLU	N-CA-C	7.17	120.10	110.35
2	B	259	LYS	N-CA-C	-7.14	103.10	111.03
2	B	88	TRP	CB-CA-C	-7.01	108.50	116.63
1	A	3	SER	CA-C-N	6.96	127.93	120.83
1	A	3	SER	C-N-CA	6.96	127.93	120.83
2	B	85	GLN	N-CA-C	6.46	119.84	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	344	GLU	CA-C-N	6.34	127.77	119.84
2	D	344	GLU	C-N-CA	6.34	127.77	119.84
2	B	246	LEU	CA-C-N	6.31	126.33	119.89
2	B	246	LEU	C-N-CA	6.31	126.33	119.89
1	C	271	TYR	CA-C-N	6.25	127.65	119.84
1	C	271	TYR	C-N-CA	6.25	127.65	119.84
1	A	320	ASP	CA-C-N	6.25	126.36	119.87
1	A	320	ASP	C-N-CA	6.25	126.36	119.87
1	A	216	THR	CA-C-N	6.16	126.53	119.93
1	A	216	THR	C-N-CA	6.16	126.53	119.93
2	D	31	ILE	CB-CA-C	-6.14	104.00	112.04
2	B	151	GLN	N-CA-C	6.12	117.95	111.28
1	A	522	ILE	CB-CA-C	-5.97	104.23	111.88
1	A	420	PRO	CA-C-N	-5.96	112.89	120.23
1	A	420	PRO	C-N-CA	-5.96	112.89	120.23
2	B	242	GLN	CA-C-N	5.92	125.68	119.76
2	B	242	GLN	C-N-CA	5.92	125.68	119.76
1	C	548	VAL	CB-CA-C	-5.86	104.13	112.22
2	D	300	GLU	N-CA-C	-5.83	105.67	112.89
1	A	467	VAL	CB-CA-C	-5.80	104.50	110.13
1	C	382	ILE	N-CA-C	5.76	116.54	110.72
2	B	139	THR	CA-C-N	-5.52	114.91	120.21
2	B	139	THR	C-N-CA	-5.52	114.91	120.21
2	B	320	ASP	CA-C-N	5.52	125.17	119.05
2	B	320	ASP	C-N-CA	5.52	125.17	119.05
2	B	153	TRP	N-CA-C	5.51	119.84	113.18
1	A	156	SER	CA-C-N	-5.46	113.02	119.84
1	A	156	SER	C-N-CA	-5.46	113.02	119.84
1	C	411	ILE	CA-C-N	5.45	126.65	119.84
1	C	411	ILE	C-N-CA	5.45	126.65	119.84
2	B	426	TRP	CB-CA-C	-5.41	103.80	111.76
1	A	184	MET	CB-CA-C	-5.32	110.42	116.54
1	A	414	TRP	N-CA-C	5.29	117.03	109.14
2	D	184	MET	CB-CA-C	-5.29	110.04	117.23
2	D	51	GLY	CA-C-N	5.26	125.34	119.87
2	D	51	GLY	C-N-CA	5.26	125.34	119.87
2	B	161	GLN	N-CA-C	5.24	117.67	111.33
2	B	293	ILE	N-CA-C	5.22	113.58	107.89
2	D	6	GLU	N-CA-C	5.20	117.04	110.33
1	A	552	VAL	CB-CA-C	-5.16	106.79	112.68
1	C	228	LEU	N-CA-C	5.14	117.28	108.90
1	C	410	TRP	N-CA-C	5.07	116.77	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	178	ILE	N-CA-C	5.05	116.19	109.37
1	A	156	SER	CB-CA-C	-5.03	100.26	110.17
1	A	401	TRP	N-CA-C	5.02	116.44	110.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4521	0	4586	332	0
1	C	4521	0	4586	293	0
2	B	3420	0	3454	203	0
2	D	3420	0	3454	215	0
3	A	15	0	13	11	0
3	C	15	0	13	8	0
All	All	15912	0	16106	1002	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 31.

All (1002) 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:C:13:LYS:HD2	1:C:16:MET:HE3	1.27	1.11
1:C:419:THR:HB	1:C:420:PRO:HD2	1.14	1.11
2:B:216:THR:HB	2:B:217:PRO:HD2	1.31	1.08
1:C:91:GLN:HE22	2:D:140:PRO:HA	1.20	1.06
1:A:435:VAL:HG13	2:B:290:THR:HG21	1.38	1.01
1:A:454:LYS:HB2	1:A:552:VAL:HG23	1.41	1.01
1:A:420:PRO:HB2	1:A:421:PRO:HD2	1.41	0.99
1:A:25:PRO:HB2	1:A:133:PRO:HG3	1.43	0.99
1:C:358:ARG:HD3	1:C:366:LYS:HD3	1.42	0.98
1:C:13:LYS:HB2	1:C:16:MET:HG3	1.47	0.96
1:C:419:THR:HB	1:C:420:PRO:CD	1.95	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:THR:CB	1:C:420:PRO:HD2	1.96	0.95
2:B:93:GLY:HA2	2:B:161:GLN:OE1	1.67	0.95
2:D:281:LYS:HG2	2:D:284:ARG:CZ	1.98	0.94
1:C:448:ARG:HH12	1:C:475:GLN:HE22	1.04	0.93
1:C:231:GLY:N	3:C:561:EDM:H25B	1.84	0.93
2:D:393:ILE:HD13	2:D:398:TRP:HB2	1.51	0.91
1:C:460:ASN:H	1:C:460:ASN:HD22	1.12	0.91
1:C:38:CYS:HB3	1:C:144:TYR:HE2	1.35	0.91
2:D:63:ILE:HD13	2:D:74:LEU:HD22	1.51	0.91
2:D:275:LYS:HE3	2:D:276:VAL:H	1.35	0.88
1:C:447:ASN:HD22	1:C:450:THR:H	1.23	0.87
2:D:191:SER:OG	2:D:198:HIS:HD2	1.58	0.86
1:A:317:VAL:HG12	1:A:318:TYR:H	1.38	0.86
2:D:90:VAL:HG11	2:D:95:PRO:HD3	1.56	0.86
2:D:104:LYS:H	2:D:192:ASP:HB3	1.39	0.86
1:C:38:CYS:HB3	1:C:144:TYR:CE2	2.11	0.86
1:C:230:MET:C	3:C:561:EDM:H25B	2.01	0.84
2:B:390:LYS:HZ3	2:B:415:GLU:HG3	1.43	0.84
1:A:407:GLN:HE22	2:B:394:GLN:HG2	1.42	0.84
1:C:91:GLN:NE2	2:D:140:PRO:HA	1.93	0.83
2:B:60:VAL:HG21	2:B:130:PHE:HD2	1.41	0.83
2:B:422:LEU:HA	2:B:425:LEU:HD22	1.61	0.83
1:C:338:THR:HG22	1:C:353:LYS:HB3	1.60	0.82
1:A:420:PRO:HB2	1:A:421:PRO:CD	2.10	0.82
1:A:340:GLN:HG3	1:A:351:THR:HG22	1.61	0.82
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.62	0.82
2:B:395:LYS:O	2:B:399:GLU:HG3	1.79	0.82
1:C:183:TYR:CE2	1:C:230:MET:HE3	2.14	0.82
1:A:116:PHE:HE1	1:A:151:GLN:HE21	1.26	0.82
1:A:91:GLN:HE22	2:B:140:PRO:HA	1.45	0.81
2:B:167:ILE:O	2:B:208:HIS:HE1	1.64	0.81
2:D:169:GLU:HB3	2:D:170:PRO:HD3	1.63	0.81
2:B:390:LYS:NZ	2:B:415:GLU:HG3	1.95	0.80
2:B:191:SER:OG	2:B:198:HIS:HD2	1.65	0.80
1:A:254:VAL:HB	1:A:289:LEU:HA	1.64	0.80
1:A:26:LEU:HD11	1:A:137:ASN:OD1	1.82	0.80
1:A:424:LYS:HD2	1:A:425:LEU:H	1.47	0.79
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.64	0.79
2:B:311:LYS:HE3	2:B:311:LYS:HA	1.65	0.79
2:D:116:PHE:HZ	2:D:151:GLN:NE2	1.80	0.79
2:D:249:LYS:HE3	2:D:249:LYS:HA	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ASP:HB3	1:C:117:SER:OG	1.83	0.78
1:A:419:THR:HG23	1:A:420:PRO:HD2	1.65	0.78
2:B:60:VAL:HG21	2:B:130:PHE:CD2	2.18	0.78
1:C:53:GLU:O	1:C:55:PRO:HD3	1.83	0.78
2:D:275:LYS:CE	2:D:276:VAL:H	1.97	0.78
1:C:317:VAL:HG12	1:C:318:TYR:N	1.98	0.77
1:C:57:ASN:HD21	1:C:131:THR:HG23	1.49	0.77
2:D:335:GLY:HA3	2:D:357:MET:HB2	1.66	0.77
1:A:317:VAL:HG12	1:A:318:TYR:N	1.98	0.77
2:D:422:LEU:HA	2:D:425:LEU:HB2	1.66	0.77
1:A:518:VAL:O	1:A:522:ILE:HG12	1.85	0.77
1:A:27:THR:C	1:A:29:GLU:H	1.93	0.76
1:A:109:LEU:HD22	1:A:216:THR:HG21	1.66	0.76
2:D:261:VAL:HG13	2:D:276:VAL:HG11	1.67	0.76
2:B:139:THR:HG23	2:B:140:PRO:O	1.84	0.76
2:B:298:GLU:CD	2:B:298:GLU:H	1.94	0.76
1:C:90:VAL:HG22	1:C:161:GLN:HE22	1.50	0.76
1:C:420:PRO:CB	1:C:421:PRO:CD	2.64	0.76
2:B:426:TRP:O	2:B:427:TYR:HB3	1.86	0.76
1:C:434:ILE:H	1:C:494:ASN:HD21	1.34	0.76
1:A:91:GLN:HE22	2:B:140:PRO:CA	1.99	0.76
1:C:244:ILE:CG2	1:C:263:LYS:HD3	2.16	0.76
1:C:306:ASN:HA	1:C:309:ILE:HD12	1.67	0.76
1:A:91:GLN:NE2	2:B:140:PRO:HA	2.01	0.75
1:A:139:THR:HA	1:A:140:PRO:C	2.10	0.75
2:B:193:LEU:HD11	2:B:201:LYS:HD2	1.68	0.75
1:C:271:TYR:HB2	1:C:274:ILE:HD11	1.66	0.75
2:B:350:LYS:HE2	2:B:378:GLU:OE1	1.86	0.75
2:B:252:TRP:CD1	2:B:295:LEU:HD22	2.21	0.75
2:B:237:ASP:O	2:B:238:LYS:HB2	1.87	0.75
1:A:354:TYR:HB2	1:A:374:LYS:NZ	2.02	0.74
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.22	0.74
2:B:160:PHE:CE2	2:B:164:MET:HE2	2.22	0.74
1:C:469:LEU:HD11	1:C:480:GLN:HG2	1.70	0.73
1:A:49:LYS:HE2	1:A:142:ILE:HD11	1.70	0.73
2:B:160:PHE:HE2	2:B:164:MET:HE2	1.53	0.73
2:B:216:THR:HB	2:B:217:PRO:CD	2.15	0.73
1:C:448:ARG:HH12	1:C:475:GLN:NE2	1.85	0.73
1:C:63:ILE:HG23	1:C:64:LYS:H	1.54	0.73
1:C:420:PRO:HB2	1:C:421:PRO:CD	2.19	0.73
1:C:332:GLN:HB3	1:C:336:GLN:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.71	0.72
1:C:503:LEU:HD11	1:C:507:GLN:HE21	1.55	0.72
2:D:357:MET:HG3	2:D:358:ARG:HD3	1.71	0.72
1:A:419:THR:HG23	1:A:420:PRO:CD	2.19	0.72
1:C:90:VAL:HG23	2:D:141:GLY:H	1.54	0.72
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.72	0.72
1:A:165:THR:HG21	2:B:140:PRO:HG2	1.72	0.71
1:C:180:ILE:HG23	1:C:189:VAL:HG22	1.73	0.71
1:C:518:VAL:O	1:C:522:ILE:HG12	1.90	0.71
1:C:289:LEU:H	1:C:289:LEU:HD23	1.53	0.71
2:D:72:ARG:HG3	2:D:73:LYS:N	2.06	0.71
1:A:240:THR:HA	1:A:315:HIS:HB3	1.72	0.71
2:D:196:GLY:O	2:D:200:THR:HG23	1.91	0.71
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.73	0.71
2:B:170:PRO:O	2:B:174:GLN:HG2	1.91	0.71
1:A:178:ILE:HD11	1:A:201:LYS:HG3	1.72	0.70
1:A:25:PRO:CB	1:A:133:PRO:HG3	2.20	0.70
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.74	0.70
1:A:64:LYS:CD	1:A:71:TRP:HD1	2.03	0.70
1:A:183:TYR:HE2	3:A:561:EDM:H23A	1.56	0.70
2:B:377:THR:HG22	2:B:410:TRP:HZ2	1.57	0.70
1:C:420:PRO:CB	1:C:421:PRO:HD3	2.22	0.69
2:B:154:LYS:HG3	2:B:184:MET:SD	2.31	0.69
2:D:275:LYS:HE3	2:D:276:VAL:N	2.06	0.69
1:A:115:TYR:HD1	1:A:115:TYR:H	1.39	0.69
2:B:1:PRO:O	2:B:117:SER:HA	1.91	0.69
1:A:64:LYS:HB3	1:A:70:LYS:O	1.92	0.69
2:B:191:SER:OG	2:B:198:HIS:CD2	2.45	0.69
1:C:454:LYS:NZ	1:C:554:ALA:HB3	2.07	0.69
1:A:396:GLU:O	1:A:400:THR:HG23	1.92	0.69
1:C:261:VAL:HG13	1:C:276:VAL:HG11	1.74	0.69
1:A:244:ILE:HG23	1:A:263:LYS:HE3	1.73	0.69
1:C:91:GLN:HE22	2:D:140:PRO:CA	2.03	0.69
1:C:263:LYS:HB2	3:C:561:EDM:H15	1.75	0.69
2:D:344:GLU:HG3	2:D:345:PRO:HD2	1.74	0.69
1:A:184:MET:CE	3:A:561:EDM:H23B	2.23	0.69
1:A:224:GLU:CG	1:A:225:PRO:HD2	2.22	0.69
2:B:103:LYS:HE2	2:B:179:VAL:CG2	2.22	0.69
2:B:286:THR:HG22	2:B:286:THR:O	1.92	0.69
1:C:11:LYS:HB2	1:C:85:GLN:HE21	1.57	0.69
1:C:30:LYS:C	1:C:32:LYS:H	2.01	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:114:ALA:HB2	2:D:214:LEU:HG	1.75	0.69
1:A:107:THR:OG1	1:A:198:HIS:HE1	1.76	0.68
1:A:183:TYR:HE2	3:A:561:EDM:C23	2.05	0.68
2:B:46:LYS:HD3	2:B:116:PHE:HB2	1.74	0.68
2:D:113:ASP:OD2	2:D:215:THR:HB	1.94	0.68
2:D:116:PHE:CZ	2:D:151:GLN:NE2	2.62	0.68
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.75	0.67
2:B:153:TRP:CD1	2:B:153:TRP:O	2.46	0.67
2:B:107:THR:OG1	2:B:198:HIS:HE1	1.77	0.67
1:C:420:PRO:HB3	1:C:421:PRO:HD3	1.77	0.67
1:A:116:PHE:HE1	1:A:151:GLN:NE2	1.93	0.67
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.75	0.67
2:D:323:LYS:HB2	2:D:343:GLN:NE2	2.09	0.67
1:A:332:GLN:HG3	1:A:338:THR:HG23	1.76	0.67
1:A:358:ARG:HH22	2:B:396:GLU:HB2	1.60	0.67
1:C:12:LEU:HD11	1:C:127:TYR:CE1	2.30	0.67
2:D:234:LEU:HD12	2:D:234:LEU:O	1.95	0.67
1:C:30:LYS:NZ	1:C:30:LYS:HA	2.10	0.67
2:D:175:ASN:HB3	2:D:178:ILE:HD13	1.76	0.67
2:D:275:LYS:HG3	2:D:277:ARG:H	1.59	0.67
1:C:57:ASN:HD21	1:C:131:THR:CG2	2.06	0.66
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.75	0.66
1:A:317:VAL:CG1	1:A:318:TYR:H	2.08	0.66
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.76	0.66
1:C:11:LYS:O	1:C:85:GLN:HG2	1.95	0.66
1:C:417:VAL:HG22	1:C:419:THR:HG23	1.76	0.66
1:C:448:ARG:NH1	1:C:475:GLN:HE22	1.87	0.66
1:C:12:LEU:HD11	1:C:127:TYR:CZ	2.29	0.66
1:C:230:MET:HA	3:C:561:EDM:H23A	1.78	0.66
1:A:191:SER:HB3	1:A:198:HIS:CD2	2.31	0.66
2:D:271:TYR:O	2:D:274:ILE:HG22	1.96	0.66
1:C:254:VAL:HB	1:C:289:LEU:HA	1.76	0.66
1:C:330:GLN:HE22	1:C:340:GLN:HE22	1.42	0.66
1:C:406:TRP:HH2	2:D:418:ASN:HA	1.62	0.65
2:B:94:ILE:HD13	2:B:94:ILE:H	1.61	0.65
2:D:274:ILE:HG13	2:D:306:ASN:CG	2.21	0.65
2:D:426:TRP:O	2:D:427:TYR:HB2	1.95	0.65
1:A:131:THR:HG22	1:A:143:ARG:HG2	1.78	0.65
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.77	0.65
2:D:214:LEU:H	2:D:214:LEU:HD12	1.60	0.65
1:A:447:ASN:ND2	1:A:450:THR:H	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:SER:HB3	1:A:198:HIS:HD2	1.62	0.65
1:A:552:VAL:HG13	1:A:552:VAL:O	1.95	0.65
1:A:420:PRO:CB	1:A:421:PRO:CD	2.75	0.65
1:A:184:MET:HE2	3:A:561:EDM:H23B	1.79	0.65
1:C:183:TYR:CD2	1:C:230:MET:HE3	2.31	0.65
2:D:107:THR:HA	2:D:232:TYR:O	1.97	0.65
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.26	0.64
1:C:52:PRO:HA	1:C:143:ARG:HD2	1.79	0.64
1:C:94:ILE:CD1	1:C:269:GLN:HG3	2.28	0.64
1:A:278:GLN:HB3	1:A:302:GLU:OE1	1.96	0.64
1:C:63:ILE:HG23	1:C:64:LYS:N	2.12	0.64
1:A:126:LYS:HA	1:A:145:GLN:NE2	2.13	0.64
2:B:138:GLU:CG	2:B:139:THR:H	2.10	0.64
2:B:420:PRO:HB2	2:B:422:LEU:HD23	1.80	0.64
1:C:406:TRP:CH2	2:D:418:ASN:HA	2.32	0.64
2:D:361:HIS:HB2	2:D:366:LYS:HD3	1.79	0.64
2:B:89:GLU:C	2:B:91:GLN:H	2.06	0.63
1:A:16:MET:HE3	1:A:83:ARG:HA	1.79	0.63
1:C:435:VAL:HA	2:D:290:THR:HG21	1.80	0.63
2:D:209:LEU:HB3	2:D:214:LEU:HB2	1.81	0.63
1:A:354:TYR:HB2	1:A:374:LYS:HZ2	1.62	0.63
2:D:308:GLU:OE1	2:D:311:LYS:HD2	1.98	0.63
1:A:35:VAL:O	1:A:39:THR:HG23	1.99	0.63
2:B:85:GLN:OE1	2:B:85:GLN:HA	1.98	0.63
2:B:153:TRP:O	2:B:153:TRP:CG	2.52	0.62
1:C:84:THR:HG21	1:C:153:TRP:HE1	1.64	0.62
1:A:29:GLU:OE2	1:A:29:GLU:HA	1.98	0.62
1:A:34:LEU:C	1:A:36:GLU:H	2.08	0.62
1:C:30:LYS:HE3	1:C:71:TRP:HE1	1.63	0.62
1:A:57:ASN:ND2	1:A:143:ARG:HH21	1.97	0.62
1:A:395:LYS:HD3	1:A:414:TRP:CH2	2.35	0.62
2:B:183:TYR:CD2	2:B:380:ILE:HD13	2.34	0.62
2:D:232:TYR:CE2	2:D:234:LEU:HD23	2.34	0.62
1:A:35:VAL:HG23	1:A:132:ILE:HG21	1.82	0.62
1:A:116:PHE:CE1	1:A:151:GLN:NE2	2.66	0.62
2:B:390:LYS:HZ3	2:B:415:GLU:CG	2.12	0.62
1:C:403:THR:HG22	1:C:404:GLU:N	2.14	0.62
1:C:454:LYS:HZ3	1:C:554:ALA:HB3	1.64	0.62
2:D:257:ILE:O	2:D:261:VAL:HG23	2.00	0.62
1:A:64:LYS:HG2	1:A:71:TRP:HA	1.81	0.62
1:C:47:ILE:HD12	1:C:144:TYR:CD2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:ASN:HD22	1:C:532:TYR:HB3	1.64	0.62
1:C:361:HIS:CE1	1:C:505:ILE:HD13	2.35	0.62
1:A:183:TYR:CE2	3:A:561:EDM:H23A	2.35	0.61
1:A:511:ASP:OD1	1:A:512:LYS:HG3	2.00	0.61
2:D:153:TRP:O	2:D:184:MET:HE1	2.00	0.61
1:A:67:ASP:O	1:A:68:SER:HB3	2.00	0.61
1:C:317:VAL:CG1	1:C:318:TYR:N	2.62	0.61
1:A:57:ASN:HD22	1:A:143:ARG:HH21	1.48	0.61
1:A:419:THR:HG23	1:A:420:PRO:N	2.15	0.61
2:B:24:TRP:CH2	2:B:61:PHE:CD1	2.87	0.61
1:C:263:LYS:HB2	3:C:561:EDM:C15	2.31	0.61
2:B:3:SER:O	2:B:5:ILE:HG13	2.01	0.61
2:B:394:GLN:O	2:B:395:LYS:C	2.44	0.61
1:C:94:ILE:HD12	1:C:269:GLN:HG3	1.83	0.61
1:A:302:GLU:HG3	1:A:303:LEU:N	2.14	0.61
1:C:34:LEU:O	1:C:35:VAL:HB	2.00	0.61
1:C:116:PHE:CE2	1:C:151:GLN:HB2	2.36	0.61
2:D:37:ILE:O	2:D:41:MET:HG3	2.00	0.61
2:D:72:ARG:HG3	2:D:73:LYS:H	1.64	0.61
2:B:167:ILE:O	2:B:208:HIS:CE1	2.52	0.61
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.82	0.61
1:C:317:VAL:HG12	1:C:318:TYR:H	1.65	0.61
2:B:252:TRP:NE1	2:B:295:LEU:HD22	2.16	0.61
2:D:232:TYR:CD2	2:D:234:LEU:HD23	2.35	0.61
2:D:344:GLU:HB3	2:D:347:LYS:HD2	1.82	0.61
1:C:337:TRP:HE1	1:C:367:GLN:NE2	1.99	0.60
2:D:257:ILE:HG22	2:D:283:LEU:HD11	1.82	0.60
1:A:224:GLU:HG2	1:A:225:PRO:HD2	1.83	0.60
1:A:224:GLU:HB3	1:A:226:PRO:HD2	1.82	0.60
1:A:115:TYR:O	1:A:116:PHE:CD1	2.54	0.60
1:C:30:LYS:HE3	1:C:71:TRP:NE1	2.16	0.60
2:D:278:GLN:HB3	2:D:299:ALA:HB2	1.81	0.60
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.31	0.60
1:C:287:LYS:HE3	1:C:288:ALA:H	1.66	0.60
1:C:412:PRO:HG3	2:D:401:TRP:CZ2	2.36	0.60
2:D:273:GLY:O	2:D:309:ILE:HD13	2.01	0.60
1:A:393:ILE:HD12	1:A:423:VAL:HG23	1.82	0.60
2:B:65:LYS:HG3	2:B:66:LYS:H	1.65	0.60
1:C:460:ASN:H	1:C:460:ASN:ND2	1.89	0.60
2:B:116:PHE:HD2	2:B:116:PHE:C	2.10	0.59
2:D:277:ARG:NH1	2:D:281:LYS:HZ3	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.42	0.59
1:C:287:LYS:HE3	1:C:288:ALA:N	2.17	0.59
2:B:116:PHE:C	2:B:116:PHE:CD2	2.80	0.59
1:C:291:GLU:O	1:C:293:ILE:HG13	2.02	0.59
1:C:542:ILE:HD11	2:D:261:VAL:HG11	1.84	0.59
2:D:23:GLN:OE1	2:D:60:VAL:HG12	2.02	0.59
1:A:303:LEU:O	1:A:303:LEU:HD23	2.01	0.59
1:A:556:ILE:HG22	1:A:556:ILE:O	2.02	0.59
1:C:298:GLU:OE2	1:C:301:LEU:HD23	2.03	0.59
2:D:193:LEU:HD13	2:D:197:GLN:HG2	1.85	0.59
2:D:105:SER:HB3	2:D:235:HIS:ND1	2.17	0.59
2:D:330:GLN:NE2	2:D:422:LEU:HD11	2.17	0.59
1:A:424:LYS:CD	1:A:425:LEU:H	2.13	0.59
1:A:91:GLN:HE22	2:B:140:PRO:CB	2.16	0.59
2:B:355:ALA:O	2:B:356:ARG:HB3	2.02	0.59
1:C:297:GLU:HG2	1:C:298:GLU:N	2.17	0.59
2:D:163:SER:O	2:D:167:ILE:HG13	2.03	0.59
1:A:64:LYS:CD	1:A:71:TRP:CD1	2.84	0.58
1:A:161:GLN:O	1:A:165:THR:HG23	2.03	0.58
1:A:252:TRP:CD1	1:A:295:LEU:HD21	2.38	0.58
2:B:377:THR:HG22	2:B:410:TRP:CZ2	2.37	0.58
1:C:107:THR:HG21	1:C:219:LYS:NZ	2.17	0.58
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.39	0.58
1:C:244:ILE:HG21	1:C:263:LYS:HD3	1.86	0.58
2:D:129:ALA:HB1	2:D:143:ARG:HH21	1.68	0.58
1:A:382:ILE:O	2:B:136:ASN:HB2	2.03	0.58
1:A:517:LEU:HD12	1:A:517:LEU:O	2.02	0.58
1:C:226:PRO:O	1:C:227:PHE:HB3	2.02	0.58
2:B:66:LYS:HA	2:B:407:GLN:OE1	2.03	0.58
1:C:235:HIS:HB3	1:C:236:PRO:HD2	1.84	0.58
2:D:33:ALA:O	2:D:37:ILE:HG13	2.03	0.58
2:D:281:LYS:HG2	2:D:284:ARG:NH2	2.19	0.58
1:A:91:GLN:HE22	2:B:140:PRO:HB3	1.69	0.58
1:A:194:GLU:O	1:A:196:GLY:N	2.37	0.58
1:C:244:ILE:HG23	1:C:263:LYS:HD3	1.86	0.58
2:D:88:TRP:HE3	2:D:89:GLU:N	2.01	0.58
2:D:314:VAL:HG12	2:D:315:HIS:N	2.18	0.58
2:B:81:ASN:O	2:B:84:THR:HG22	2.04	0.58
2:D:151:GLN:HB3	2:D:185:ASP:OD2	2.04	0.58
2:D:357:MET:HE3	2:D:357:MET:O	2.04	0.58
1:A:75:VAL:HG11	1:A:77:PHE:CZ	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.85	0.58
1:A:459:THR:O	2:B:286:THR:HG21	2.04	0.58
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.39	0.58
1:C:226:PRO:O	1:C:227:PHE:CB	2.51	0.57
2:B:216:THR:CB	2:B:217:PRO:HD2	2.20	0.57
1:A:447:ASN:HD21	1:A:449:GLU:HB2	1.69	0.57
2:B:138:GLU:HG2	2:B:139:THR:H	1.68	0.57
1:C:491:LEU:HB3	1:C:529:GLU:HG3	1.87	0.57
2:D:419:THR:HG21	2:D:423:VAL:HG23	1.86	0.57
1:A:116:PHE:C	1:A:148:VAL:HG21	2.30	0.57
2:B:153:TRP:O	2:B:155:GLY:N	2.37	0.57
1:C:106:VAL:HG12	1:C:227:PHE:CZ	2.40	0.57
2:D:115:TYR:CE1	2:D:156:SER:HB3	2.40	0.57
1:A:361:HIS:HD2	1:A:513:SER:OG	1.87	0.57
1:A:363:ASN:OD1	1:A:363:ASN:C	2.47	0.57
1:C:320:ASP:C	1:C:322:SER:H	2.13	0.57
1:C:420:PRO:HB2	1:C:421:PRO:HD2	1.87	0.57
2:B:424:LYS:HA	2:B:427:TYR:CE2	2.39	0.57
1:C:134:SER:HB3	1:C:140:PRO:O	2.04	0.57
1:C:191:SER:OG	1:C:198:HIS:HD2	1.87	0.57
1:C:224:GLU:N	1:C:225:PRO:CD	2.68	0.57
2:B:56:TYR:O	2:B:129:ALA:HB3	2.04	0.56
2:B:107:THR:OG1	2:B:198:HIS:CE1	2.57	0.56
1:C:106:VAL:HG12	1:C:227:PHE:HZ	1.70	0.56
1:C:317:VAL:HG21	1:C:347:LYS:HB3	1.86	0.56
1:C:417:VAL:O	1:C:417:VAL:HG13	2.04	0.56
2:B:355:ALA:O	2:B:356:ARG:CB	2.53	0.56
2:D:191:SER:OG	2:D:198:HIS:CD2	2.48	0.56
1:A:73:LYS:HE3	1:A:151:GLN:OE1	2.05	0.56
1:A:426:TRP:O	1:A:427:TYR:HB3	2.04	0.56
1:A:441:TYR:O	1:A:548:VAL:HG21	2.05	0.56
1:C:174:GLN:C	1:C:175:ASN:HD22	2.13	0.56
1:C:335:GLY:O	1:C:355:ALA:HA	2.06	0.56
1:C:341:ILE:HD11	1:C:375:ILE:HG23	1.85	0.56
1:C:398:TRP:NE1	1:C:402:TRP:HD1	2.02	0.56
2:D:63:ILE:CD1	2:D:74:LEU:HD22	2.30	0.56
1:A:8:VAL:CG1	2:B:53:GLU:HG3	2.36	0.56
1:A:523:GLU:OE1	1:A:527:LYS:HE2	2.05	0.56
2:B:319:TYR:CD1	2:B:383:TRP:CD1	2.94	0.56
1:C:309:ILE:C	1:C:311:LYS:H	2.12	0.56
1:A:115:TYR:O	1:A:116:PHE:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:SER:H	2:B:157:PRO:HD2	1.70	0.56
1:A:301:LEU:O	1:A:304:ALA:HB3	2.06	0.56
2:B:195:ILE:HG23	2:B:196:GLY:H	1.71	0.56
1:C:30:LYS:HA	1:C:30:LYS:HZ2	1.71	0.56
1:C:282:LEU:HD21	1:C:296:THR:HG23	1.86	0.56
1:A:8:VAL:CG1	2:B:53:GLU:CG	2.84	0.56
1:A:171:PHE:CZ	1:A:205:LEU:HB2	2.40	0.56
2:D:350:LYS:HE3	2:D:378:GLU:OE1	2.06	0.56
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.87	0.55
2:D:278:GLN:HB2	2:D:302:GLU:OE1	2.07	0.55
2:D:278:GLN:HB3	2:D:299:ALA:CB	2.36	0.55
1:C:298:GLU:HA	1:C:298:GLU:OE1	2.06	0.55
1:A:237:ASP:O	1:A:238:LYS:HG2	2.06	0.55
1:A:442:VAL:CG2	1:A:481:ALA:HB1	2.36	0.55
2:B:424:LYS:HA	2:B:427:TYR:HE2	1.72	0.55
1:C:539:HIS:O	1:C:541:GLY:N	2.40	0.55
1:A:112:GLY:O	1:A:113:ASP:HB2	2.06	0.55
2:B:295:LEU:HG	2:B:300:GLU:HG3	1.88	0.55
1:C:66:LYS:HB2	1:C:71:TRP:CZ3	2.40	0.55
1:C:391:LEU:O	1:C:417:VAL:HG12	2.06	0.55
1:A:105:SER:HB2	1:A:198:HIS:CD2	2.41	0.55
1:A:132:ILE:HB	1:A:142:ILE:CG2	2.37	0.55
1:A:354:TYR:CD2	1:A:371:ALA:HB2	2.42	0.55
1:C:94:ILE:HG23	1:C:269:GLN:HE21	1.71	0.55
1:C:112:GLY:C	1:C:114:ALA:H	2.15	0.55
2:D:296:THR:HG22	2:D:298:GLU:H	1.71	0.55
1:A:91:GLN:CD	2:B:140:PRO:HA	2.31	0.55
1:A:515:SER:HB3	1:A:518:VAL:HG23	1.88	0.55
1:C:317:VAL:CG1	1:C:318:TYR:H	2.19	0.55
2:D:88:TRP:CE3	2:D:89:GLU:N	2.74	0.55
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.88	0.55
1:A:53:GLU:O	1:A:54:ASN:HB2	2.06	0.55
1:C:77:PHE:O	1:C:78:ARG:C	2.50	0.55
1:C:97:PRO:HG3	1:C:232:TYR:CD1	2.41	0.55
1:C:460:ASN:HD22	1:C:460:ASN:N	1.92	0.55
1:A:64:LYS:HD2	1:A:71:TRP:CD1	2.42	0.54
1:A:543:GLY:HA3	2:B:283:LEU:O	2.06	0.54
1:C:395:LYS:HD3	1:C:414:TRP:CH2	2.42	0.54
1:C:303:LEU:O	1:C:307:ARG:HG3	2.07	0.54
2:D:296:THR:O	2:D:299:ALA:N	2.40	0.54
1:A:63:ILE:HG12	1:A:65:LYS:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLN:O	1:A:243:PRO:C	2.48	0.54
2:B:113:ASP:C	2:B:114:ALA:O	2.48	0.54
2:D:111:VAL:HG11	2:D:187:LEU:HD22	1.90	0.54
2:D:393:ILE:HG21	2:D:398:TRP:HB2	1.89	0.54
1:A:393:ILE:HD12	1:A:423:VAL:CG2	2.38	0.54
1:C:57:ASN:HD22	1:C:143:ARG:HH22	1.56	0.54
1:C:223:LYS:C	1:C:225:PRO:HD2	2.33	0.54
2:B:60:VAL:CG2	2:B:130:PHE:CD2	2.91	0.54
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.43	0.54
2:D:65:LYS:HD2	2:D:409:THR:HG23	1.89	0.54
2:D:214:LEU:HD12	2:D:214:LEU:N	2.23	0.54
1:A:454:LYS:O	1:A:552:VAL:HG21	2.08	0.54
1:C:135:ILE:O	1:C:135:ILE:HG12	2.08	0.54
1:C:278:GLN:HB2	1:C:302:GLU:CD	2.33	0.54
1:A:97:PRO:HD3	1:A:232:TYR:CZ	2.43	0.53
1:A:115:TYR:O	1:A:116:PHE:HD1	1.91	0.53
1:A:116:PHE:O	1:A:148:VAL:HG21	2.09	0.53
1:A:224:GLU:CB	1:A:225:PRO:HD2	2.38	0.53
1:C:97:PRO:HG3	1:C:232:TYR:CG	2.42	0.53
1:C:270:ILE:CG2	1:C:314:VAL:HG11	2.38	0.53
2:D:183:TYR:CD2	2:D:380:ILE:HD13	2.44	0.53
2:D:214:LEU:H	2:D:214:LEU:CD1	2.20	0.53
1:A:289:LEU:HD23	1:A:289:LEU:H	1.74	0.53
1:A:503:LEU:HD23	2:B:421:PRO:HG2	1.91	0.53
2:B:106:VAL:O	2:B:234:LEU:HB2	2.08	0.53
1:C:443:ASP:OD1	1:C:444:GLY:N	2.40	0.53
1:A:104:LYS:HD3	1:A:104:LYS:N	2.22	0.53
1:C:319:TYR:OH	1:C:385:LYS:HE2	2.08	0.53
1:C:503:LEU:HD12	1:C:503:LEU:O	2.09	0.53
1:A:30:LYS:HD2	1:A:62:ALA:O	2.08	0.53
1:C:441:TYR:CD2	1:C:544:GLY:HA3	2.42	0.53
1:A:233:GLU:O	1:A:239:TRP:HA	2.09	0.53
1:A:382:ILE:HG22	1:A:383:TRP:CG	2.44	0.53
1:C:282:LEU:HD22	1:C:293:ILE:CG2	2.39	0.53
1:A:91:GLN:NE2	2:B:140:PRO:HB3	2.24	0.53
1:A:229:TRP:CH2	1:A:230:MET:HE2	2.43	0.53
2:B:237:ASP:O	2:B:238:LYS:CB	2.57	0.53
1:C:361:HIS:HE1	1:C:505:ILE:HD13	1.73	0.53
1:A:538:ALA:HB1	1:A:539:HIS:ND1	2.23	0.52
2:D:160:PHE:O	2:D:160:PHE:CD2	2.63	0.52
1:A:115:TYR:O	1:A:116:PHE:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:THR:OG1	1:C:198:HIS:HE1	1.91	0.52
1:C:202:ILE:HG21	1:C:219:LYS:HZ3	1.73	0.52
1:C:389:PHE:O	1:C:414:TRP:HA	2.10	0.52
2:D:110:ASP:C	2:D:110:ASP:OD1	2.52	0.52
2:D:254:VAL:HG23	2:D:293:ILE:HD13	1.91	0.52
1:A:419:THR:CG2	1:A:420:PRO:HD2	2.38	0.52
1:C:303:LEU:O	1:C:303:LEU:HD23	2.09	0.52
1:A:27:THR:O	1:A:29:GLU:N	2.41	0.52
2:B:426:TRP:O	2:B:427:TYR:CB	2.55	0.52
1:C:502:ALA:O	1:C:506:ILE:HG12	2.10	0.52
2:D:296:THR:HG22	2:D:298:GLU:N	2.24	0.52
2:B:97:PRO:HG3	2:B:181:TYR:HB2	1.92	0.52
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.91	0.52
2:B:156:SER:N	2:B:157:PRO:HD2	2.24	0.52
2:B:366:LYS:HG2	2:B:370:GLU:OE2	2.10	0.52
1:C:116:PHE:HE1	1:C:146:TYR:HE2	1.58	0.52
1:C:482:ILE:HD11	1:C:497:THR:HG21	1.91	0.52
1:A:544:GLY:O	1:A:548:VAL:HG23	2.10	0.52
2:B:91:GLN:O	2:B:92:LEU:C	2.53	0.52
1:C:468:PRO:O	1:C:468:PRO:HG2	2.09	0.52
1:C:282:LEU:HD22	1:C:293:ILE:HG21	1.92	0.52
2:D:395:LYS:HG3	2:D:416:PHE:CE2	2.45	0.52
1:A:44:GLU:HB3	1:A:46:LYS:HE3	1.90	0.52
1:A:276:VAL:C	1:A:278:GLN:H	2.18	0.52
1:A:279:LEU:HB3	1:A:299:ALA:HB1	1.91	0.52
2:B:138:GLU:CG	2:B:139:THR:N	2.72	0.52
2:B:195:ILE:HG23	2:B:196:GLY:N	2.25	0.52
1:A:406:TRP:CE3	1:A:407:GLN:HG3	2.45	0.52
2:B:257:ILE:HG22	2:B:283:LEU:HD11	1.92	0.52
1:C:126:LYS:HG3	1:C:127:TYR:H	1.75	0.52
1:C:202:ILE:HG21	1:C:219:LYS:NZ	2.24	0.52
1:A:10:VAL:HG12	1:A:124:PHE:CD1	2.45	0.51
1:A:120:LEU:HD12	1:A:121:ASP:H	1.75	0.51
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.45	0.51
1:C:110:ASP:OD1	1:C:111:VAL:N	2.43	0.51
1:C:393:ILE:O	1:C:414:TRP:HZ3	1.94	0.51
1:C:496:VAL:HG22	1:C:534:ALA:HB3	1.91	0.51
2:D:7:THR:CG2	2:D:119:PRO:HG2	2.40	0.51
2:D:171:PHE:CE2	2:D:205:LEU:HB2	2.45	0.51
1:C:126:LYS:HG3	1:C:127:TYR:N	2.25	0.51
1:C:441:TYR:CG	1:C:544:GLY:HA3	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:422:LEU:HA	2:D:425:LEU:HD22	1.92	0.51
2:B:103:LYS:O	2:B:236:PRO:HG2	2.10	0.51
1:C:188:TYR:HB2	1:C:229:TRP:CD1	2.45	0.51
1:C:408:ALA:HB1	2:D:364:ASP:HB3	1.91	0.51
2:D:160:PHE:O	2:D:160:PHE:CG	2.63	0.51
2:D:395:LYS:O	2:D:399:GLU:HG3	2.10	0.51
1:A:183:TYR:CD2	1:A:230:MET:HG2	2.46	0.51
1:A:420:PRO:CB	1:A:421:PRO:HD2	2.27	0.51
2:B:164:MET:HE3	2:B:182:GLN:HE22	1.75	0.51
2:B:169:GLU:HB3	2:B:170:PRO:CD	2.37	0.51
2:B:419:THR:HG22	2:B:420:PRO:O	2.10	0.51
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.75	0.51
1:A:263:LYS:CA	3:A:561:EDM:C15	2.89	0.51
1:A:337:TRP:NE1	1:A:367:GLN:HG2	2.26	0.51
2:B:60:VAL:HG12	2:B:61:PHE:N	2.24	0.51
2:B:173:LYS:C	2:B:175:ASN:H	2.18	0.51
2:D:72:ARG:NH1	2:D:110:ASP:OD2	2.44	0.51
1:A:424:LYS:HD2	1:A:425:LEU:N	2.22	0.51
2:B:118:VAL:HB	2:B:149:LEU:HG	1.92	0.51
1:C:337:TRP:HE1	1:C:367:GLN:HE21	1.58	0.51
1:A:65:LYS:HB3	1:A:67:ASP:OD1	2.10	0.51
2:D:248:GLU:CD	2:D:248:GLU:N	2.68	0.51
1:C:109:LEU:HD23	1:C:219:LYS:HD3	1.92	0.51
1:C:447:ASN:HD22	1:C:450:THR:N	2.02	0.51
2:D:7:THR:HG22	2:D:119:PRO:HG2	1.91	0.51
2:D:275:LYS:HE3	2:D:275:LYS:HA	1.93	0.51
2:B:164:MET:HE3	2:B:182:GLN:NE2	2.26	0.50
1:A:135:ILE:HG22	1:A:136:ASN:N	2.26	0.50
1:A:206:ARG:HH11	1:A:206:ARG:HG2	1.76	0.50
1:A:250:ASP:C	1:A:252:TRP:H	2.19	0.50
2:B:232:TYR:HB3	2:B:234:LEU:HD23	1.93	0.50
1:C:30:LYS:C	1:C:32:LYS:N	2.66	0.50
1:C:406:TRP:CZ3	1:C:407:GLN:CG	2.95	0.50
2:D:63:ILE:HD13	2:D:74:LEU:CD2	2.34	0.50
2:D:296:THR:HG23	2:D:298:GLU:OE1	2.10	0.50
2:D:323:LYS:HB2	2:D:343:GLN:HE21	1.75	0.50
1:C:465:LYS:O	1:C:466:VAL:HG23	2.11	0.50
2:D:120:LEU:O	2:D:121:ASP:C	2.53	0.50
2:D:357:MET:HE1	2:D:362:THR:OG1	2.10	0.50
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.40	0.50
1:A:131:THR:CG2	1:A:143:ARG:HG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:C	1:A:283:LEU:H	2.19	0.50
2:D:332:GLN:HB2	2:D:336:GLN:HB3	1.92	0.50
2:D:420:PRO:CB	2:D:421:PRO:HD2	2.41	0.50
1:A:237:ASP:O	1:A:238:LYS:CG	2.59	0.50
2:B:393:ILE:HG21	2:B:398:TRP:HB2	1.94	0.50
1:A:29:GLU:O	1:A:30:LYS:HB3	2.12	0.50
1:A:194:GLU:O	1:A:195:ILE:C	2.53	0.50
1:A:382:ILE:HG22	1:A:383:TRP:CD2	2.47	0.50
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.41	0.50
1:C:257:ILE:O	1:C:261:VAL:HG23	2.11	0.50
1:C:482:ILE:HD11	1:C:497:THR:CG2	2.42	0.50
2:D:296:THR:C	2:D:298:GLU:N	2.69	0.50
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.92	0.50
2:B:350:LYS:CE	2:B:378:GLU:OE1	2.58	0.50
2:D:363:ASN:OD1	2:D:363:ASN:C	2.54	0.50
1:A:354:TYR:HB2	1:A:374:LYS:HZ3	1.74	0.50
1:C:320:ASP:O	1:C:322:SER:N	2.45	0.50
1:C:341:ILE:HG21	1:C:383:TRP:CH2	2.46	0.50
1:C:94:ILE:HD13	1:C:94:ILE:O	2.11	0.50
1:C:447:ASN:HB3	1:C:450:THR:OG1	2.12	0.50
1:A:91:GLN:OE1	2:B:140:PRO:HA	2.12	0.49
1:A:320:ASP:C	1:A:320:ASP:OD1	2.55	0.49
2:B:24:TRP:HH2	2:B:61:PHE:CD1	2.29	0.49
1:C:90:VAL:HG22	1:C:161:GLN:NE2	2.22	0.49
2:B:24:TRP:HH2	2:B:61:PHE:CE1	2.30	0.49
2:B:153:TRP:C	2:B:155:GLY:H	2.19	0.49
1:C:13:LYS:CB	1:C:16:MET:HG3	2.33	0.49
1:C:263:LYS:HE2	3:C:561:EDM:O27	2.12	0.49
1:A:403:THR:O	1:A:403:THR:CG2	2.60	0.49
1:C:135:ILE:O	1:C:136:ASN:C	2.56	0.49
1:C:373:GLN:NE2	2:D:397:THR:HG23	2.26	0.49
2:D:244:ILE:HD13	2:D:266:TRP:HZ3	1.77	0.49
1:A:442:VAL:HG22	1:A:481:ALA:HB1	1.94	0.49
1:C:500:GLN:O	1:C:501:TYR:C	2.55	0.49
1:C:29:GLU:O	1:C:29:GLU:HG2	2.13	0.49
1:C:61:PHE:O	1:C:73:LYS:HB2	2.12	0.49
1:C:132:ILE:HB	1:C:142:ILE:HB	1.94	0.49
1:C:174:GLN:O	1:C:175:ASN:ND2	2.39	0.49
2:B:72:ARG:HG2	2:B:73:LYS:O	2.13	0.49
2:D:3:SER:C	2:D:5:ILE:H	2.21	0.49
2:D:281:LYS:HG2	2:D:284:ARG:NH1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LYS:O	1:C:32:LYS:N	2.46	0.49
1:C:406:TRP:CZ3	1:C:407:GLN:HG2	2.47	0.49
2:D:107:THR:OG1	2:D:198:HIS:HE1	1.95	0.49
1:A:252:TRP:NE1	1:A:295:LEU:HD21	2.28	0.49
1:A:263:LYS:HA	3:A:561:EDM:C15	2.43	0.49
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.43	0.49
1:A:430:GLU:HB2	1:A:532:TYR:HB2	1.95	0.49
2:B:233:GLU:O	2:B:234:LEU:O	2.31	0.49
2:D:2:ILE:O	2:D:4:PRO:HD3	2.13	0.49
1:A:34:LEU:HD21	1:A:62:ALA:CB	2.43	0.48
2:B:390:LYS:NZ	2:B:415:GLU:CG	2.72	0.48
1:C:336:GLN:OE1	1:C:355:ALA:HB2	2.13	0.48
1:A:287:LYS:HZ3	1:A:287:LYS:HB2	1.79	0.48
1:C:57:ASN:HD22	1:C:143:ARG:NH2	2.10	0.48
1:C:247:PRO:HG2	1:C:252:TRP:HH2	1.78	0.48
1:C:324:ASP:OD2	1:C:388:LYS:HE3	2.13	0.48
1:C:340:GLN:HG3	1:C:351:THR:HG22	1.96	0.48
2:D:188:TYR:CE1	2:D:380:ILE:HG21	2.48	0.48
1:A:31:ILE:HD12	1:A:133:PRO:HG2	1.95	0.48
2:B:77:PHE:O	2:B:78:ARG:C	2.55	0.48
1:C:225:PRO:HB2	1:C:226:PRO:CD	2.42	0.48
2:D:296:THR:CG2	2:D:298:GLU:HB2	2.44	0.48
1:A:131:THR:HG23	1:A:143:ARG:HE	1.78	0.48
1:C:143:ARG:HH11	1:C:143:ARG:HB3	1.78	0.48
2:D:175:ASN:OD1	2:D:201:LYS:HE2	2.14	0.48
1:A:263:LYS:N	3:A:561:EDM:C15	2.76	0.48
1:C:60:VAL:CG2	1:C:130:PHE:HB2	2.43	0.48
2:D:277:ARG:NH1	2:D:281:LYS:NZ	2.62	0.48
1:A:263:LYS:HG3	3:A:561:EDM:O27	2.14	0.48
2:D:129:ALA:HB1	2:D:143:ARG:NH2	2.28	0.48
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.96	0.48
1:C:439:THR:H	1:C:460:ASN:ND2	2.11	0.48
2:D:242:GLN:O	2:D:242:GLN:HG3	2.13	0.48
2:D:282:LEU:HD21	2:D:296:THR:HB	1.96	0.48
1:A:95:PRO:HB2	1:A:230:MET:HE1	1.95	0.48
1:A:442:VAL:HG22	1:A:481:ALA:CB	2.44	0.48
1:A:484:LEU:O	1:A:485:ALA:C	2.57	0.48
2:B:24:TRP:CZ3	2:B:61:PHE:CD1	3.02	0.48
1:C:94:ILE:HG23	1:C:269:GLN:HG3	1.96	0.48
1:C:391:LEU:C	1:C:417:VAL:HG12	2.39	0.48
1:A:33:ALA:O	1:A:37:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.96	0.48
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.49	0.48
1:C:116:PHE:CZ	1:C:151:GLN:HB2	2.48	0.48
2:D:178:ILE:N	2:D:178:ILE:HD12	2.29	0.48
1:A:54:ASN:HB3	1:A:55:PRO:HB3	1.96	0.48
1:A:97:PRO:HG3	1:A:232:TYR:CD1	2.49	0.48
1:A:407:GLN:NE2	2:B:394:GLN:HG2	2.22	0.48
1:C:22:LYS:HD2	1:C:22:LYS:N	2.29	0.48
1:A:235:HIS:O	1:A:236:PRO:C	2.56	0.47
1:A:503:LEU:O	1:A:503:LEU:HG	2.11	0.47
2:B:109:LEU:O	2:B:186:ASP:HA	2.13	0.47
1:C:218:ASP:OD1	1:C:220:LYS:HB2	2.14	0.47
1:C:439:THR:H	1:C:460:ASN:HD21	1.62	0.47
2:D:173:LYS:C	2:D:175:ASN:H	2.21	0.47
2:D:286:THR:O	2:D:286:THR:HG22	2.14	0.47
1:A:454:LYS:NZ	1:A:554:ALA:HB3	2.29	0.47
1:C:223:LYS:O	1:C:223:LYS:HG2	2.13	0.47
1:C:230:MET:CA	3:C:561:EDM:H23A	2.43	0.47
2:D:336:GLN:C	2:D:337:TRP:CD1	2.91	0.47
1:A:34:LEU:C	1:A:36:GLU:N	2.72	0.47
1:A:458:VAL:HB	1:A:548:VAL:HG22	1.95	0.47
1:A:481:ALA:HA	1:A:484:LEU:HD12	1.97	0.47
1:A:509:GLN:N	1:A:510:PRO:CD	2.77	0.47
2:B:81:ASN:HA	2:B:84:THR:HG22	1.96	0.47
1:A:60:VAL:HG11	1:A:130:PHE:HD2	1.79	0.47
1:A:258:GLN:O	1:A:261:VAL:HG22	2.14	0.47
1:C:26:LEU:HD22	1:C:27:THR:HG22	1.96	0.47
1:C:240:THR:HG22	1:C:241:VAL:N	2.29	0.47
2:D:394:GLN:O	2:D:395:LYS:C	2.57	0.47
1:A:230:MET:HE3	1:A:232:TYR:HE2	1.79	0.47
2:B:124:PHE:CE2	2:B:153:TRP:CZ2	3.03	0.47
2:D:11:LYS:O	2:D:85:GLN:HB2	2.13	0.47
2:D:89:GLU:O	2:D:90:VAL:HG23	2.14	0.47
2:D:320:ASP:OD1	2:D:320:ASP:C	2.57	0.47
1:A:230:MET:HE3	1:A:232:TYR:CE2	2.50	0.47
1:A:257:ILE:HD12	1:A:293:ILE:HG23	1.97	0.47
1:A:553:SER:C	1:A:555:GLY:N	2.72	0.47
2:D:422:LEU:HD12	2:D:422:LEU:O	2.15	0.47
1:A:35:VAL:O	1:A:39:THR:CG2	2.63	0.47
1:A:255:ASN:O	1:A:258:GLN:N	2.48	0.47
1:A:337:TRP:HE1	1:A:367:GLN:HG2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:SER:C	1:A:555:GLY:H	2.23	0.47
2:B:93:GLY:CA	2:B:161:GLN:OE1	2.53	0.47
1:C:278:GLN:HB2	1:C:302:GLU:OE2	2.15	0.47
1:C:332:GLN:HG3	1:C:332:GLN:O	2.14	0.47
2:D:350:LYS:HG2	2:D:351:THR:N	2.29	0.47
2:D:94:ILE:HG23	2:D:95:PRO:CD	2.45	0.47
1:A:328:GLU:O	1:A:339:TYR:HA	2.14	0.47
1:C:253:THR:O	1:C:257:ILE:HG13	2.14	0.47
2:D:353:LYS:NZ	2:D:427:TYR:CD2	2.82	0.47
1:A:270:ILE:N	1:A:270:ILE:HD12	2.30	0.47
1:C:406:TRP:CE3	2:D:419:THR:HB	2.49	0.47
1:C:478:GLN:HA	1:C:478:GLN:OE1	2.14	0.47
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.51	0.46
2:D:67:ASP:O	2:D:68:SER:HB3	2.15	0.46
1:A:65:LYS:HG2	1:A:66:LYS:N	2.30	0.46
1:A:271:TYR:CE1	1:A:314:VAL:HG23	2.50	0.46
1:A:360:ALA:HA	1:A:514:GLU:HG2	1.97	0.46
2:B:84:THR:HA	2:B:87:PHE:CZ	2.50	0.46
2:B:115:TYR:HE2	2:B:185:ASP:OD1	1.98	0.46
1:C:271:TYR:CB	1:C:274:ILE:HD11	2.42	0.46
1:C:439:THR:HG22	1:C:441:TYR:CE1	2.50	0.46
1:A:295:LEU:HB3	1:A:300:GLU:HB2	1.96	0.46
1:A:491:LEU:HD13	1:A:529:GLU:HG3	1.96	0.46
2:D:148:VAL:O	2:D:149:LEU:C	2.58	0.46
1:A:8:VAL:HG12	2:B:53:GLU:HG2	1.96	0.46
1:C:107:THR:HG21	1:C:219:LYS:HZ3	1.78	0.46
1:C:260:LEU:O	1:C:264:LEU:HD12	2.16	0.46
1:C:450:THR:O	1:C:451:LYS:HB2	2.15	0.46
1:C:451:LYS:HB3	1:C:471:ASN:HA	1.96	0.46
1:A:76:ASP:HB2	1:A:289:LEU:HD21	1.97	0.46
1:A:132:ILE:O	1:A:142:ILE:HG22	2.14	0.46
1:A:183:TYR:CD2	1:A:230:MET:CG	2.99	0.46
2:D:97:PRO:HD2	2:D:181:TYR:CD1	2.51	0.46
1:A:417:VAL:O	1:A:417:VAL:HG13	2.16	0.46
1:C:151:GLN:HA	1:C:151:GLN:OE1	2.15	0.46
2:D:116:PHE:N	2:D:116:PHE:CD1	2.83	0.46
2:D:169:GLU:HB3	2:D:170:PRO:CD	2.38	0.46
2:D:195:ILE:HD11	2:D:199:ARG:HH11	1.81	0.46
2:D:276:VAL:O	2:D:276:VAL:HG12	2.16	0.46
2:D:421:PRO:O	2:D:425:LEU:HD22	2.14	0.46
1:A:97:PRO:HG3	1:A:232:TYR:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:LEU:HD12	1:A:517:LEU:C	2.37	0.46
1:C:94:ILE:HD13	1:C:269:GLN:HG3	1.96	0.46
1:C:473:THR:O	1:C:474:ASN:C	2.59	0.46
1:A:8:VAL:CG1	2:B:53:GLU:HG2	2.45	0.46
1:A:76:ASP:OD1	1:A:289:LEU:HD22	2.16	0.46
1:A:252:TRP:HA	1:A:252:TRP:CE3	2.50	0.46
1:A:503:LEU:HD12	1:A:533:LEU:CD2	2.45	0.46
2:B:88:TRP:HB3	2:B:89:GLU:H	1.38	0.46
1:C:419:THR:O	1:C:420:PRO:C	2.59	0.46
1:A:65:LYS:HG2	1:A:66:LYS:H	1.80	0.46
1:A:132:ILE:HB	1:A:142:ILE:HG22	1.98	0.46
1:C:312:GLU:CB	1:C:313:PRO:HD2	2.46	0.46
1:C:393:ILE:O	1:C:414:TRP:CZ3	2.69	0.46
2:D:124:PHE:CE2	2:D:153:TRP:CZ2	3.04	0.46
2:D:244:ILE:HD13	2:D:266:TRP:CZ3	2.51	0.46
2:D:274:ILE:HG13	2:D:306:ASN:ND2	2.31	0.46
1:A:205:LEU:O	1:A:209:LEU:HG	2.16	0.46
1:A:235:HIS:O	1:A:237:ASP:N	2.49	0.46
1:A:407:GLN:HE22	2:B:394:GLN:CG	2.23	0.46
1:A:451:LYS:HG2	1:A:471:ASN:HA	1.98	0.46
2:D:183:TYR:OH	2:D:386:THR:HG23	2.17	0.46
1:A:280:CYS:HB3	1:A:284:ARG:HH21	1.81	0.45
1:A:30:LYS:C	1:A:32:LYS:N	2.73	0.45
2:B:84:THR:HG21	2:B:153:TRP:HE1	1.81	0.45
1:C:125:ARG:NH1	1:C:147:ASN:OD1	2.49	0.45
2:D:88:TRP:O	2:D:89:GLU:C	2.58	0.45
2:D:296:THR:C	2:D:298:GLU:H	2.25	0.45
2:D:308:GLU:O	2:D:311:LYS:HB2	2.16	0.45
1:A:198:HIS:O	1:A:200:THR:N	2.49	0.45
2:B:237:ASP:C	2:B:238:LYS:HD3	2.41	0.45
1:C:174:GLN:C	1:C:175:ASN:ND2	2.74	0.45
2:D:382:ILE:HG22	2:D:383:TRP:CE2	2.51	0.45
1:A:223:LYS:HB2	1:A:227:PHE:CE2	2.52	0.45
2:B:94:ILE:C	2:B:96:HIS:H	2.24	0.45
2:B:197:GLN:O	2:B:200:THR:HB	2.16	0.45
1:C:117:SER:O	1:C:118:VAL:HB	2.16	0.45
2:B:3:SER:HA	2:B:4:PRO:HD3	1.84	0.45
1:C:63:ILE:CG2	1:C:64:LYS:H	2.27	0.45
1:C:243:PRO:HB3	1:C:311:LYS:O	2.17	0.45
1:A:356:ARG:O	1:A:357:MET:HB2	2.17	0.45
1:A:478:GLN:HA	1:A:478:GLN:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ASN:OD1	1:A:532:TYR:HB3	2.16	0.45
1:A:522:ILE:O	1:A:526:ILE:HG22	2.16	0.45
1:C:178:ILE:HG23	1:C:191:SER:HB3	1.98	0.45
1:C:332:GLN:HB3	1:C:336:GLN:CB	2.43	0.45
1:C:381:VAL:HG22	2:D:25:PRO:HB3	1.97	0.45
2:D:27:THR:O	2:D:31:ILE:HG13	2.15	0.45
1:A:64:LYS:HD3	1:A:71:TRP:HD1	1.80	0.45
1:A:244:ILE:CG2	1:A:263:LYS:HE3	2.45	0.45
3:A:561:EDM:H2	3:A:561:EDM:H23	1.77	0.45
1:C:242:GLN:O	1:C:243:PRO:C	2.59	0.45
1:A:47:ILE:HD12	1:A:144:TYR:CG	2.52	0.45
1:A:77:PHE:CD1	1:A:80:LEU:HD23	2.51	0.45
2:B:89:GLU:C	2:B:91:GLN:N	2.71	0.45
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.52	0.45
2:D:13:LYS:O	2:D:14:PRO:C	2.60	0.45
2:D:41:MET:HE2	2:D:41:MET:HB3	1.81	0.45
1:A:23:GLN:C	1:A:25:PRO:HD3	2.42	0.45
1:C:520:GLN:O	1:C:523:GLU:HG2	2.16	0.45
2:B:12:LEU:HD23	2:B:124:PHE:HE1	1.82	0.44
2:B:94:ILE:O	2:B:96:HIS:N	2.44	0.44
2:B:118:VAL:HG12	2:B:119:PRO:O	2.17	0.44
2:B:191:SER:HB2	2:B:193:LEU:HG	1.99	0.44
2:B:231:GLY:O	2:B:232:TYR:HB2	2.16	0.44
2:B:393:ILE:HG12	2:B:394:GLN:H	1.82	0.44
2:D:69:THR:HG23	2:D:70:LYS:H	1.82	0.44
2:D:193:LEU:HB3	2:D:194:GLU:H	1.46	0.44
2:B:357:MET:HG3	2:B:361:HIS:CG	2.52	0.44
1:C:307:ARG:HH11	1:C:307:ARG:HG2	1.83	0.44
1:A:90:VAL:HG12	2:B:141:GLY:HA3	1.99	0.44
1:A:90:VAL:HG12	2:B:141:GLY:CA	2.47	0.44
2:B:255:ASN:O	2:B:258:GLN:N	2.50	0.44
1:C:417:VAL:HG22	1:C:419:THR:CG2	2.46	0.44
2:D:65:LYS:HG2	2:D:407:GLN:O	2.17	0.44
1:A:25:PRO:HB2	1:A:26:LEU:H	1.60	0.44
1:C:411:ILE:HA	1:C:412:PRO:HD3	1.80	0.44
2:D:193:LEU:CD1	2:D:197:GLN:HG2	2.45	0.44
2:B:60:VAL:CG2	2:B:130:PHE:HD2	2.20	0.44
2:D:164:MET:O	2:D:165:THR:C	2.61	0.44
1:A:30:LYS:C	1:A:32:LYS:H	2.24	0.44
1:C:108:VAL:O	1:C:108:VAL:HG12	2.18	0.44
1:C:343:GLN:HG3	1:C:349:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:THR:O	2:B:380:ILE:HG13	2.18	0.44
1:C:112:GLY:C	1:C:114:ALA:N	2.74	0.44
1:C:539:HIS:N	1:C:539:HIS:CD2	2.86	0.44
2:D:156:SER:O	2:D:157:PRO:C	2.59	0.44
2:D:368:LEU:O	2:D:372:VAL:HG23	2.18	0.44
1:A:67:ASP:O	1:A:68:SER:CB	2.65	0.44
1:A:305:GLU:O	1:A:308:GLU:HB3	2.17	0.44
1:A:457:TYR:C	1:A:457:TYR:CD2	2.96	0.44
1:A:548:VAL:O	1:A:552:VAL:HG12	2.18	0.44
2:B:69:THR:HB	2:B:70:LYS:H	1.50	0.44
2:B:401:TRP:HE3	2:B:404:GLU:HG3	1.83	0.44
1:C:128:THR:OG1	1:C:146:TYR:HB2	2.17	0.44
1:C:283:LEU:O	1:C:286:THR:HG23	2.17	0.44
1:C:503:LEU:CD2	1:C:535:TRP:HB2	2.44	0.44
2:D:116:PHE:HE1	2:D:151:GLN:HG3	1.83	0.44
2:B:366:LYS:HE2	2:B:370:GLU:OE2	2.17	0.44
1:C:457:TYR:C	1:C:457:TYR:CD2	2.95	0.44
1:A:282:LEU:HD21	1:A:296:THR:HG23	2.00	0.43
1:A:497:THR:O	1:A:535:TRP:HA	2.18	0.43
2:D:136:ASN:O	2:D:137:ASN:HB2	2.18	0.43
2:D:336:GLN:HG3	2:D:355:ALA:HB2	1.98	0.43
1:A:30:LYS:HD3	1:A:64:LYS:HZ2	1.83	0.43
2:B:79:GLU:O	2:B:83:ARG:HB2	2.18	0.43
1:C:23:GLN:HE22	1:C:60:VAL:HG23	1.83	0.43
2:D:40:GLU:O	2:D:44:GLU:HG3	2.19	0.43
1:A:191:SER:OG	1:A:193:LEU:HG	2.18	0.43
1:A:333:GLY:H	1:A:336:GLN:HB2	1.83	0.43
1:A:442:VAL:O	1:A:443:ASP:HB2	2.17	0.43
1:C:188:TYR:CD1	1:C:188:TYR:C	2.95	0.43
2:D:296:THR:CG2	2:D:298:GLU:H	2.31	0.43
1:A:13:LYS:O	1:A:14:PRO:C	2.60	0.43
1:A:183:TYR:HE2	3:A:561:EDM:H23B	1.83	0.43
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.98	0.43
1:C:21:VAL:HG12	1:C:22:LYS:N	2.34	0.43
1:C:248:GLU:O	1:C:249:LYS:HB3	2.19	0.43
2:D:56:TYR:O	2:D:129:ALA:HB3	2.18	0.43
1:A:394:GLN:O	1:A:395:LYS:C	2.61	0.43
1:A:516:GLU:OE2	1:A:520:GLN:HG3	2.18	0.43
2:B:130:PHE:CE1	2:B:144:TYR:HB2	2.53	0.43
1:C:17:ASP:O	1:C:83:ARG:HD3	2.18	0.43
2:D:64:LYS:O	2:D:407:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:LYS:NZ	2:D:127:TYR:CE1	2.85	0.43
1:A:181:TYR:CE1	2:B:138:GLU:HB2	2.53	0.43
1:A:206:ARG:HG3	1:A:216:THR:HB	2.00	0.43
1:C:248:GLU:O	1:C:249:LYS:CB	2.66	0.43
2:D:54:ASN:C	2:D:54:ASN:OD1	2.60	0.43
2:D:115:TYR:C	2:D:117:SER:H	2.27	0.43
2:D:200:THR:C	2:D:202:ILE:N	2.75	0.43
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.53	0.43
1:A:165:THR:CG2	2:B:140:PRO:HG2	2.44	0.43
2:B:124:PHE:O	2:B:125:ARG:C	2.62	0.43
2:B:168:LEU:O	2:B:169:GLU:C	2.62	0.43
2:B:183:TYR:OH	2:B:386:THR:HG23	2.19	0.43
1:C:63:ILE:CG2	1:C:64:LYS:N	2.82	0.43
1:A:33:ALA:HB1	1:A:71:TRP:HB3	2.01	0.43
2:B:309:ILE:C	2:B:311:LYS:H	2.26	0.43
1:C:33:ALA:O	1:C:37:ILE:HB	2.18	0.43
1:C:286:THR:HG22	1:C:291:GLU:OE2	2.19	0.43
1:C:451:LYS:HB2	1:C:451:LYS:HE3	1.77	0.43
1:C:478:GLN:HG3	1:C:499:SER:HB2	2.01	0.43
2:D:87:PHE:C	2:D:89:GLU:H	2.27	0.43
2:D:159:ILE:HG22	2:D:160:PHE:N	2.30	0.43
2:D:287:LYS:HD3	2:D:291:GLU:OE2	2.19	0.43
2:D:419:THR:HA	2:D:420:PRO:HD3	1.59	0.43
1:A:123:ASP:O	1:A:126:LYS:HE3	2.18	0.43
1:A:179:VAL:O	1:A:179:VAL:HG23	2.18	0.43
1:A:442:VAL:HG22	1:A:443:ASP:N	2.33	0.43
2:D:116:PHE:N	2:D:116:PHE:HD1	2.15	0.43
1:A:198:HIS:C	1:A:200:THR:N	2.77	0.43
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.49	0.43
2:B:82:LYS:O	2:B:82:LYS:HG3	2.18	0.43
2:B:244:ILE:O	2:B:310:LEU:HB3	2.19	0.43
1:C:52:PRO:HA	1:C:143:ARG:CD	2.45	0.43
2:D:357:MET:HE3	2:D:357:MET:C	2.44	0.43
2:B:24:TRP:HZ3	2:B:61:PHE:CG	2.36	0.42
2:B:93:GLY:HA2	2:B:161:GLN:CD	2.40	0.42
1:C:451:LYS:O	1:C:471:ASN:N	2.50	0.42
2:D:281:LYS:O	2:D:284:ARG:HD2	2.19	0.42
1:A:392:PRO:O	1:A:423:VAL:HG22	2.19	0.42
2:B:357:MET:HG2	2:B:367:GLN:HG2	2.00	0.42
1:C:227:PHE:C	1:C:228:LEU:HD12	2.44	0.42
1:C:330:GLN:HE21	1:C:330:GLN:HB2	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:LEU:HD12	1:C:503:LEU:C	2.44	0.42
2:D:314:VAL:CG1	2:D:315:HIS:N	2.82	0.42
1:A:7:THR:HG22	1:A:119:PRO:HG2	2.02	0.42
2:B:91:GLN:O	2:B:93:GLY:N	2.52	0.42
1:C:26:LEU:HD23	1:C:27:THR:N	2.34	0.42
1:C:341:ILE:HG21	1:C:383:TRP:CZ3	2.54	0.42
1:C:368:LEU:HD12	1:C:368:LEU:HA	1.78	0.42
2:B:81:ASN:C	2:B:83:ARG:H	2.27	0.42
1:C:120:LEU:O	1:C:121:ASP:C	2.63	0.42
1:C:230:MET:HA	3:C:561:EDM:C23	2.48	0.42
2:D:191:SER:C	2:D:193:LEU:H	2.27	0.42
1:A:3:SER:HA	1:A:4:PRO:HD3	1.73	0.42
1:A:221:HIS:HB2	1:A:222:GLN:H	1.59	0.42
1:A:302:GLU:HG3	1:A:303:LEU:H	1.85	0.42
1:C:417:VAL:O	1:C:419:THR:N	2.53	0.42
2:D:89:GLU:CD	2:D:90:VAL:N	2.78	0.42
1:A:139:THR:CA	1:A:140:PRO:C	2.88	0.42
1:A:360:ALA:O	1:A:514:GLU:HG2	2.20	0.42
1:A:447:ASN:ND2	1:A:450:THR:HG23	2.35	0.42
1:A:280:CYS:HB3	1:A:284:ARG:NH2	2.34	0.42
1:C:30:LYS:HA	1:C:30:LYS:HZ3	1.84	0.42
1:C:115:TYR:HE1	1:C:160:PHE:CD2	2.37	0.42
1:C:227:PHE:HD2	1:C:234:LEU:O	2.03	0.42
1:C:298:GLU:C	1:C:300:GLU:N	2.77	0.42
2:D:103:LYS:HD3	2:D:192:ASP:CG	2.44	0.42
2:B:312:GLU:HA	2:B:313:PRO:HD2	1.90	0.42
1:C:117:SER:O	1:C:118:VAL:O	2.38	0.42
1:C:221:HIS:O	1:C:222:GLN:HB3	2.20	0.42
1:C:230:MET:HE2	1:C:230:MET:HB3	1.67	0.42
1:C:254:VAL:HB	1:C:289:LEU:CA	2.48	0.42
1:C:301:LEU:HD12	1:C:301:LEU:O	2.20	0.42
2:D:88:TRP:HE3	2:D:88:TRP:C	2.26	0.42
2:D:410:TRP:C	2:D:411:ILE:HG12	2.45	0.42
1:A:23:GLN:O	1:A:25:PRO:HD3	2.20	0.42
1:A:39:THR:O	1:A:43:LYS:HG3	2.19	0.42
1:A:283:LEU:HB3	1:A:284:ARG:H	1.61	0.42
1:A:419:THR:CB	1:A:420:PRO:CD	2.98	0.42
1:C:113:ASP:O	1:C:114:ALA:O	2.38	0.42
1:C:195:ILE:O	1:C:195:ILE:HG22	2.19	0.42
1:C:380:ILE:O	1:C:384:GLY:HA2	2.20	0.42
1:C:510:PRO:HG2	1:C:522:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:PHE:CZ	2:D:74:LEU:HD23	2.55	0.42
2:B:295:LEU:HD12	2:B:295:LEU:HA	1.91	0.42
1:C:34:LEU:O	1:C:35:VAL:CB	2.66	0.42
2:D:28:GLU:HG3	2:D:135:ILE:HD11	2.01	0.42
2:D:173:LYS:C	2:D:175:ASN:N	2.77	0.42
1:A:60:VAL:HG11	1:A:130:PHE:CD2	2.55	0.41
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.60	0.41
2:B:94:ILE:HD13	2:B:94:ILE:N	2.33	0.41
2:B:373:GLN:O	2:B:377:THR:HG23	2.20	0.41
1:C:297:GLU:CG	1:C:298:GLU:N	2.81	0.41
2:D:146:TYR:CE2	2:D:150:PRO:HB3	2.55	0.41
2:D:379:SER:HB3	2:D:385:LYS:O	2.20	0.41
1:A:135:ILE:HD12	1:A:135:ILE:N	2.36	0.41
1:A:246:LEU:CD1	1:A:264:LEU:HD21	2.50	0.41
1:A:516:GLU:O	1:A:519:ASN:HB2	2.20	0.41
2:B:197:GLN:O	2:B:200:THR:N	2.53	0.41
2:B:290:THR:O	2:B:290:THR:HG22	2.19	0.41
2:B:297:GLU:O	2:B:298:GLU:C	2.63	0.41
1:C:274:ILE:HD13	1:C:310:LEU:HD21	2.02	0.41
1:C:328:GLU:O	1:C:339:TYR:HA	2.20	0.41
1:C:406:TRP:CZ3	1:C:407:GLN:HG3	2.55	0.41
1:A:23:GLN:HE22	1:A:60:VAL:HG22	1.86	0.41
1:A:419:THR:OG1	1:A:420:PRO:HD3	2.19	0.41
1:C:522:ILE:O	1:C:526:ILE:HG13	2.19	0.41
1:A:13:LYS:HD3	1:A:16:MET:HE2	2.01	0.41
1:A:246:LEU:HB2	1:A:307:ARG:HG2	2.03	0.41
1:A:255:ASN:O	1:A:256:ASP:C	2.64	0.41
1:A:492:GLU:HA	1:A:530:LYS:O	2.20	0.41
2:B:11:LYS:O	2:B:87:PHE:CE2	2.74	0.41
2:B:194:GLU:O	2:B:195:ILE:C	2.62	0.41
2:B:271:TYR:HA	2:B:272:PRO:HD2	1.94	0.41
2:D:202:ILE:HD13	2:D:202:ILE:HA	1.93	0.41
2:D:209:LEU:HD22	2:D:214:LEU:HD22	2.03	0.41
2:D:390:LYS:NZ	2:D:415:GLU:OE2	2.54	0.41
1:A:10:VAL:HG12	1:A:10:VAL:O	2.20	0.41
2:B:105:SER:O	2:B:190:GLY:HA2	2.21	0.41
1:C:447:ASN:ND2	1:C:450:THR:HG23	2.35	0.41
2:D:135:ILE:H	2:D:135:ILE:HG13	1.68	0.41
2:D:274:ILE:HG23	2:D:274:ILE:O	2.21	0.41
1:A:74:LEU:O	1:A:75:VAL:C	2.63	0.41
1:A:136:ASN:C	1:A:138:GLU:H	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:GLU:HA	1:A:399:GLU:HB2	2.03	0.41
1:A:419:THR:CG2	1:A:420:PRO:CD	2.92	0.41
1:A:442:VAL:CG2	1:A:481:ALA:CB	2.98	0.41
1:A:445:ALA:HB3	1:A:552:VAL:HG22	2.02	0.41
1:A:508:ALA:O	1:A:509:GLN:CB	2.69	0.41
1:C:163:SER:O	1:C:167:ILE:HG13	2.21	0.41
2:D:146:TYR:CD2	2:D:150:PRO:HB3	2.55	0.41
2:D:357:MET:SD	2:D:362:THR:HG23	2.61	0.41
1:A:194:GLU:HG3	1:A:197:GLN:HG3	2.02	0.41
1:A:373:GLN:NE2	2:B:397:THR:OG1	2.54	0.41
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.55	0.41
2:B:113:ASP:O	2:B:114:ALA:O	2.38	0.41
2:B:250:ASP:O	2:B:251:SER:HB2	2.20	0.41
1:C:307:ARG:HG2	1:C:307:ARG:NH1	2.35	0.41
2:D:142:ILE:H	2:D:142:ILE:HG12	1.41	0.41
2:D:234:LEU:CD2	2:D:377:THR:HG21	2.51	0.41
1:A:120:LEU:O	1:A:121:ASP:C	2.63	0.41
1:A:358:ARG:NH2	2:B:396:GLU:HB2	2.30	0.41
1:A:493:VAL:CG2	1:A:494:ASN:N	2.84	0.41
1:C:406:TRP:CH2	1:C:407:GLN:HG3	2.56	0.41
2:D:239:TRP:CH2	2:D:378:GLU:HA	2.56	0.41
2:D:320:ASP:HA	2:D:321:PRO:HD3	1.81	0.41
2:D:376:THR:O	2:D:380:ILE:HG13	2.20	0.41
2:D:390:LYS:HB3	2:D:417:VAL:HG11	2.02	0.41
1:A:31:ILE:O	1:A:31:ILE:HG22	2.20	0.41
1:A:113:ASP:O	1:A:114:ALA:HB3	2.21	0.41
1:A:252:TRP:HA	1:A:252:TRP:HE3	1.86	0.41
1:A:379:SER:CB	1:A:387:PRO:HD3	2.51	0.41
1:A:419:THR:O	1:A:420:PRO:O	2.38	0.41
2:B:7:THR:HB	2:B:121:ASP:HA	2.02	0.41
2:B:65:LYS:HD2	2:B:65:LYS:HA	1.89	0.41
2:B:271:TYR:N	2:B:271:TYR:CD1	2.89	0.41
2:B:333:GLY:O	2:B:335:GLY:N	2.47	0.41
1:C:209:LEU:HD23	1:C:209:LEU:HA	1.93	0.41
1:C:306:ASN:N	1:C:306:ASN:HD22	2.17	0.41
1:C:411:ILE:HG22	1:C:414:TRP:CD1	2.55	0.41
2:D:96:HIS:HA	2:D:97:PRO:HD2	1.82	0.41
2:D:108:VAL:HG22	2:D:188:TYR:CD2	2.55	0.41
1:A:132:ILE:HA	1:A:133:PRO:HD2	1.96	0.41
1:A:257:ILE:HD12	1:A:293:ILE:CG2	2.51	0.41
2:B:237:ASP:OD2	2:B:238:LYS:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:CYS:CB	1:C:144:TYR:HE2	2.20	0.41
1:C:149:LEU:HD21	1:C:159:ILE:HG21	2.03	0.41
1:C:517:LEU:HD12	1:C:517:LEU:HA	1.90	0.41
2:D:104:LYS:O	2:D:235:HIS:HB3	2.20	0.41
2:D:422:LEU:HD12	2:D:426:TRP:HD1	1.86	0.41
1:A:120:LEU:HD12	1:A:121:ASP:N	2.35	0.40
1:A:198:HIS:O	1:A:199:ARG:C	2.64	0.40
2:B:78:ARG:NH1	2:B:411:ILE:HG22	2.37	0.40
1:C:275:LYS:HG3	1:C:277:ARG:NH2	2.36	0.40
2:D:173:LYS:O	2:D:176:PRO:HD3	2.20	0.40
2:D:246:LEU:CD2	2:D:264:LEU:HD21	2.51	0.40
2:D:420:PRO:CB	2:D:421:PRO:CD	2.99	0.40
1:A:23:GLN:NE2	1:A:60:VAL:HG22	2.35	0.40
1:A:86:ASP:HA	1:A:154:LYS:NZ	2.36	0.40
1:A:110:ASP:HB2	1:A:221:HIS:HE1	1.86	0.40
1:A:382:ILE:HG22	1:A:383:TRP:CD1	2.57	0.40
2:B:153:TRP:C	2:B:155:GLY:N	2.79	0.40
2:B:289:LEU:HD23	2:B:289:LEU:HA	1.92	0.40
2:B:328:GLU:O	2:B:339:TYR:HA	2.21	0.40
1:C:419:THR:O	1:C:420:PRO:O	2.39	0.40
2:D:54:ASN:HD22	2:D:145:GLN:HE21	1.69	0.40
2:D:89:GLU:O	2:D:90:VAL:CG2	2.69	0.40
2:D:356:ARG:O	2:D:358:ARG:N	2.54	0.40
1:A:291:GLU:O	1:A:292:VAL:C	2.64	0.40
2:B:309:ILE:C	2:B:311:LYS:N	2.78	0.40
1:C:24:TRP:HA	1:C:25:PRO:HD2	1.98	0.40
1:C:286:THR:CG2	1:C:293:ILE:HD11	2.51	0.40
1:C:291:GLU:O	1:C:291:GLU:HG2	2.22	0.40
2:D:46:LYS:HE2	2:D:116:PHE:HB3	2.04	0.40
2:D:168:LEU:O	2:D:169:GLU:C	2.64	0.40
1:A:56:TYR:O	1:A:143:ARG:NH2	2.55	0.40
1:A:125:ARG:HB3	1:A:146:TYR:O	2.21	0.40
1:A:163:SER:O	1:A:167:ILE:HG13	2.21	0.40
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.77	0.40
2:B:61:PHE:CE2	2:B:403:THR:HG22	2.56	0.40
2:B:79:GLU:CG	2:B:83:ARG:HH21	2.34	0.40
2:B:183:TYR:CE2	2:B:380:ILE:HD13	2.57	0.40
1:C:260:LEU:HD23	1:C:279:LEU:HD21	2.04	0.40
1:C:465:LYS:C	1:C:466:VAL:HG23	2.45	0.40
2:D:3:SER:C	2:D:5:ILE:N	2.79	0.40
2:D:87:PHE:O	2:D:89:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TYR:CD1	1:A:188:TYR:C	2.99	0.40
1:A:194:GLU:CG	1:A:197:GLN:HG3	2.52	0.40
1:A:360:ALA:HA	1:A:514:GLU:CG	2.50	0.40
2:B:114:ALA:O	2:B:116:PHE:N	2.52	0.40
1:C:131:THR:HG22	1:C:143:ARG:HG2	2.03	0.40
1:C:171:PHE:O	1:C:172:LYS:C	2.64	0.40
1:C:465:LYS:O	1:C:466:VAL:CG2	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	554/560 (99%)	456 (82%)	61 (11%)	37 (7%)	1	3
1	C	554/560 (99%)	437 (79%)	85 (15%)	32 (6%)	1	4
2	B	411/427 (96%)	332 (81%)	57 (14%)	22 (5%)	1	4
2	D	411/427 (96%)	356 (87%)	44 (11%)	11 (3%)	4	15
All	All	1930/1974 (98%)	1581 (82%)	247 (13%)	102 (5%)	1	5

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	52	PRO
1	A	55	PRO
1	A	65	LYS
1	A	140	PRO
1	A	220	LYS
1	A	221	HIS
1	A	356	ARG

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Mol	Chain	Res	Type
1	A	420	PRO
2	B	65	LYS
2	B	69	THR
2	B	86	ASP
2	B	90	VAL
2	B	114	ALA
2	B	234	LEU
2	B	251	SER
2	B	356	ARG
1	C	31	ILE
1	C	35	VAL
1	C	71	TRP
1	C	114	ALA
1	C	153	TRP
1	C	222	GLN
1	C	418	ASN
1	C	420	PRO
2	D	66	LYS
2	D	69	THR
2	D	214	LEU
2	D	357	MET
1	A	25	PRO
1	A	28	GLU
1	A	61	PHE
1	A	68	SER
1	A	116	PHE
1	A	135	ILE
1	A	195	ILE
1	A	223	LYS
1	A	288	ALA
1	A	334	GLN
1	A	553	SER
2	B	12	LEU
2	B	68	SER
2	B	71	TRP
2	B	92	LEU
2	B	93	GLY
2	B	215	THR
2	B	359	GLY
2	B	361	HIS
2	B	363	ASN
1	C	27	THR

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Mol	Chain	Res	Type
1	C	227	PHE
1	C	249	LYS
1	C	286	THR
1	C	296	THR
1	C	540	LYS
1	C	543	GLY
2	D	90	VAL
1	A	26	LEU
1	A	56	TYR
1	A	427	TYR
1	A	509	GLN
1	A	554	ALA
2	B	96	HIS
2	B	238	LYS
1	C	55	PRO
1	C	78	ARG
1	C	118	VAL
1	C	136	ASN
1	C	221	HIS
1	C	288	ALA
1	C	412	PRO
2	D	297	GLU
1	A	277	ARG
1	A	283	LEU
1	A	284	ARG
1	A	357	MET
1	A	419	THR
2	B	184	MET
1	C	310	LEU
2	D	174	GLN
2	D	193	LEU
1	A	114	ALA
1	A	137	ASN
1	A	199	ARG
1	A	282	LEU
2	B	4	PRO
1	C	113	ASP
1	C	291	GLU
1	C	334	GLN
2	D	65	LYS
1	A	224	GLU
1	A	412	PRO

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Mol	Chain	Res	Type
2	B	100	LEU
1	C	52	PRO
2	D	420	PRO
1	A	54	ASN
1	C	226	PRO
1	C	236	PRO
2	D	170	PRO
1	C	25	PRO
1	C	321	PRO
1	C	466	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	496/500 (99%)	459 (92%)	37 (8%)	12	37
1	C	496/500 (99%)	448 (90%)	48 (10%)	8	25
2	B	377/389 (97%)	336 (89%)	41 (11%)	6	21
2	D	377/389 (97%)	342 (91%)	35 (9%)	8	27
All	All	1746/1778 (98%)	1585 (91%)	161 (9%)	8	27

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	26	LEU
1	A	27	THR
1	A	29	GLU
1	A	66	LYS
1	A	73	LYS
1	A	90	VAL
1	A	94	ILE
1	A	102	LYS
1	A	106	VAL
1	A	115	TYR

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Mol	Chain	Res	Type
1	A	131	THR
1	A	165	THR
1	A	166	LYS
1	A	188	TYR
1	A	210	LEU
1	A	221	HIS
1	A	224	GLU
1	A	227	PHE
1	A	228	LEU
1	A	230	MET
1	A	252	TRP
1	A	283	LEU
1	A	349	LEU
1	A	367	GLN
1	A	403	THR
1	A	409	THR
1	A	419	THR
1	A	434	ILE
1	A	447	ASN
1	A	451	LYS
1	A	458	VAL
1	A	500	GLN
1	A	503	LEU
1	A	509	GLN
1	A	526	ILE
1	A	553	SER
2	B	10	VAL
2	B	24	TRP
2	B	35	VAL
2	B	39	THR
2	B	50	ILE
2	B	53	GLU
2	B	69	THR
2	B	73	LYS
2	B	85	GLN
2	B	88	TRP
2	B	89	GLU
2	B	92	LEU
2	B	94	ILE
2	B	105	SER
2	B	116	PHE
2	B	132	ILE

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Mol	Chain	Res	Type
2	B	142	ILE
2	B	151	GLN
2	B	174	GLN
2	B	179	VAL
2	B	186	ASP
2	B	193	LEU
2	B	195	ILE
2	B	210	LEU
2	B	214	LEU
2	B	234	LEU
2	B	271	TYR
2	B	278	GLN
2	B	293	ILE
2	B	305	GLU
2	B	310	LEU
2	B	311	LYS
2	B	314	VAL
2	B	329	ILE
2	B	362	THR
2	B	369	THR
2	B	372	VAL
2	B	377	THR
2	B	423	VAL
2	B	424	LYS
2	B	425	LEU
1	C	24	TRP
1	C	30	LYS
1	C	44	GLU
1	C	71	TRP
1	C	72	ARG
1	C	79	GLU
1	C	90	VAL
1	C	91	GLN
1	C	94	ILE
1	C	108	VAL
1	C	110	ASP
1	C	131	THR
1	C	135	ILE
1	C	137	ASN
1	C	143	ARG
1	C	145	GLN
1	C	174	GLN

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Mol	Chain	Res	Type
1	C	178	ILE
1	C	180	ILE
1	C	187	LEU
1	C	188	TYR
1	C	210	LEU
1	C	223	LYS
1	C	245	VAL
1	C	255	ASN
1	C	287	LYS
1	C	297	GLU
1	C	314	VAL
1	C	330	GLN
1	C	365	VAL
1	C	374	LYS
1	C	386	THR
1	C	390	LYS
1	C	400	THR
1	C	402	TRP
1	C	403	THR
1	C	409	THR
1	C	413	GLU
1	C	431	LYS
1	C	449	GLU
1	C	458	VAL
1	C	460	ASN
1	C	495	ILE
1	C	497	THR
1	C	533	LEU
1	C	540	LYS
1	C	548	VAL
1	C	552	VAL
2	D	22	LYS
2	D	46	LYS
2	D	66	LYS
2	D	88	TRP
2	D	94	ILE
2	D	126	LYS
2	D	142	ILE
2	D	159	ILE
2	D	163	SER
2	D	179	VAL
2	D	180	ILE

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Mol	Chain	Res	Type
2	D	192	ASP
2	D	193	LEU
2	D	194	GLU
2	D	245	VAL
2	D	248	GLU
2	D	249	LYS
2	D	250	ASP
2	D	271	TYR
2	D	274	ILE
2	D	275	LYS
2	D	282	LEU
2	D	296	THR
2	D	302	GLU
2	D	303	LEU
2	D	318	TYR
2	D	336	GLN
2	D	362	THR
2	D	363	ASN
2	D	388	LYS
2	D	394	GLN
2	D	411	ILE
2	D	413	GLU
2	D	423	VAL
2	D	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	91	GLN
1	A	136	ASN
1	A	145	GLN
1	A	161	GLN
1	A	175	ASN
1	A	198	HIS
1	A	242	GLN
1	A	255	ASN
1	A	306	ASN
1	A	315	HIS
1	A	334	GLN
1	A	361	HIS
1	A	373	GLN

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Mol	Chain	Res	Type
1	A	407	GLN
1	A	447	ASN
2	B	57	ASN
2	B	91	GLN
2	B	137	ASN
2	B	182	GLN
2	B	197	GLN
2	B	198	HIS
2	B	208	HIS
2	B	235	HIS
2	B	242	GLN
2	B	306	ASN
2	B	418	ASN
1	C	23	GLN
1	C	57	ASN
1	C	85	GLN
1	C	161	GLN
1	C	175	ASN
1	C	182	GLN
1	C	198	HIS
1	C	255	ASN
1	C	315	HIS
1	C	330	GLN
1	C	361	HIS
1	C	367	GLN
1	C	373	GLN
1	C	407	GLN
1	C	447	ASN
1	C	460	ASN
1	C	475	GLN
1	C	494	ASN
1	C	507	GLN
1	C	539	HIS
1	C	547	GLN
2	D	91	GLN
2	D	137	ASN
2	D	145	GLN
2	D	151	GLN
2	D	198	HIS
2	D	208	HIS
2	D	255	ASN
2	D	269	GLN

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Mol	Chain	Res	Type
2	D	278	GLN
2	D	306	ASN
2	D	315	HIS
2	D	330	GLN
2	D	340	GLN
2	D	361	HIS
2	D	418	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	EDM	C	561	-	15,15,15	2.36	4 (26%)	18,22,22	4.37	9 (50%)
3	EDM	A	561	-	15,15,15	2.28	2 (13%)	18,22,22	4.04	8 (44%)

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	EDM	C	561	-	-	6/12/12/12	0/1/1/1
3	EDM	A	561	-	-	5/12/12/12	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	561	EDM	C5-S17	-7.49	1.75	1.80
3	A	561	EDM	C5-S17	-7.43	1.75	1.80
3	A	561	EDM	O19-S17	2.76	1.50	1.44
3	C	561	EDM	O19-S17	2.51	1.50	1.44
3	C	561	EDM	C5-N4	2.03	1.34	1.32
3	C	561	EDM	C5-N6	2.03	1.34	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	561	EDM	N4-C5-N6	-12.80	119.87	130.48
3	A	561	EDM	N4-C5-N6	-11.88	120.63	130.48
3	C	561	EDM	C29-S17-C5	7.41	110.03	104.39
3	C	561	EDM	N6-C1-N21	7.23	120.89	116.91
3	A	561	EDM	C29-S17-C5	7.17	109.85	104.39
3	A	561	EDM	N6-C1-N21	5.95	120.19	116.91
3	A	561	EDM	O19-S17-O27	-5.12	109.30	117.99
3	C	561	EDM	O19-S17-O27	-5.08	109.38	117.99
3	C	561	EDM	S17-C5-N4	3.21	120.15	115.07
3	C	561	EDM	S17-C5-N6	3.11	119.98	115.07
3	A	561	EDM	S17-C5-N6	2.99	119.80	115.07
3	C	561	EDM	O27-S17-C5	2.89	110.04	107.42
3	A	561	EDM	S17-C5-N4	2.80	119.49	115.07
3	A	561	EDM	O27-S17-C5	2.52	109.70	107.42
3	C	561	EDM	C2-C1-N6	-2.15	119.19	123.34
3	C	561	EDM	O19-S17-C5	2.12	109.34	107.42
3	A	561	EDM	C2-C1-N6	-2.07	119.35	123.34

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	561	EDM	N6-C5-S17-C29
3	A	561	EDM	C15-C13-C3-C2

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Mol	Chain	Res	Type	Atoms
3	C	561	EDM	C15-C13-C3-C2
3	C	561	EDM	N6-C1-N21-C23
3	A	561	EDM	N6-C5-S17-C29
3	A	561	EDM	N6-C5-S17-O27
3	A	561	EDM	N4-C5-S17-C29
3	A	561	EDM	N4-C5-S17-O27
3	C	561	EDM	N6-C5-S17-O27
3	C	561	EDM	N4-C5-S17-C29
3	C	561	EDM	N6-C1-N21-C25

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	561	EDM	8	0
3	A	561	EDM	11	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	556/560 (99%)	-0.07	12 (2%) 62 52	56, 84, 151, 171	0
1	C	556/560 (99%)	-0.02	10 (1%) 67 58	55, 91, 156, 177	0
2	B	415/427 (97%)	-0.23	5 (1%) 76 68	49, 75, 119, 145	0
2	D	415/427 (97%)	-0.05	10 (2%) 59 49	55, 86, 129, 157	0
All	All	1942/1974 (98%)	-0.08	37 (1%) 66 57	49, 84, 144, 177	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	PRO	3.8
1	C	556	ILE	3.8
1	C	26	LEU	3.4
1	A	135	ILE	3.4
2	D	3	SER	3.3
2	B	92	LEU	3.2
1	C	299	ALA	3.1
1	C	116	PHE	2.9
2	B	95	PRO	2.9
1	A	227	PHE	2.8
2	D	423	VAL	2.7
1	A	26	LEU	2.7
1	A	130	PHE	2.7
2	D	92	LEU	2.7
1	A	282	LEU	2.7
2	B	1	PRO	2.6
1	C	24	TRP	2.6
2	D	1	PRO	2.6
1	A	295	LEU	2.6
1	A	556	ILE	2.6
1	C	25	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	293	ILE	2.5
1	A	61	PHE	2.5
1	C	266	TRP	2.4
2	D	2	ILE	2.4
2	B	3	SER	2.4
2	D	90	VAL	2.3
1	A	554	ALA	2.3
2	D	217	PRO	2.2
2	D	361	HIS	2.2
1	C	354	TYR	2.2
2	D	87	PHE	2.2
2	D	232	TYR	2.1
1	C	294	PRO	2.1
1	A	555	GLY	2.1
1	C	31	ILE	2.1
2	B	90	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDM	A	561	15/15	0.53	0.21	118,132,136,150	0
3	EDM	C	561	15/15	0.74	0.20	114,131,137,145	0

6.5 Other polymers [i](#)

There are no such residues in this entry.