



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:20 AM UTC

PDB ID : 1RTJ / pdb_00001rtj
Title : MECHANISM OF INHIBITION OF HIV-1 REVERSE TRANSCRIPTASE
BY NON-NUCLEOSIDE INHIBITORS
Authors : Ren, J.; Esnouf, R.; Ross, C.; Jones, Y.; Stammers, D.; Stuart, D.
Deposited on : 1995-05-03
Resolution : 2.35 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

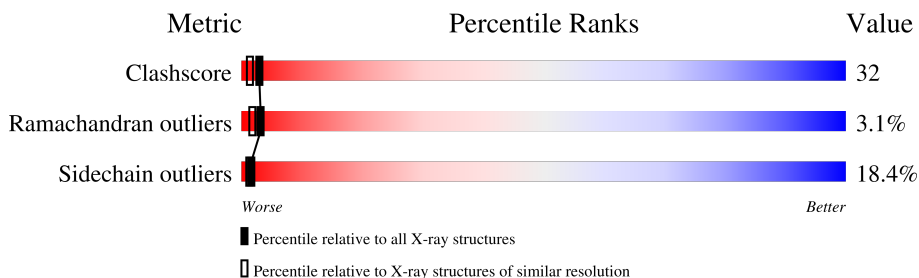
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	 35% 44% 15% . .
2	B	440	 32% 49% 15% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8210 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 HIV-1 REVERSE TRANSCRIPTASE.

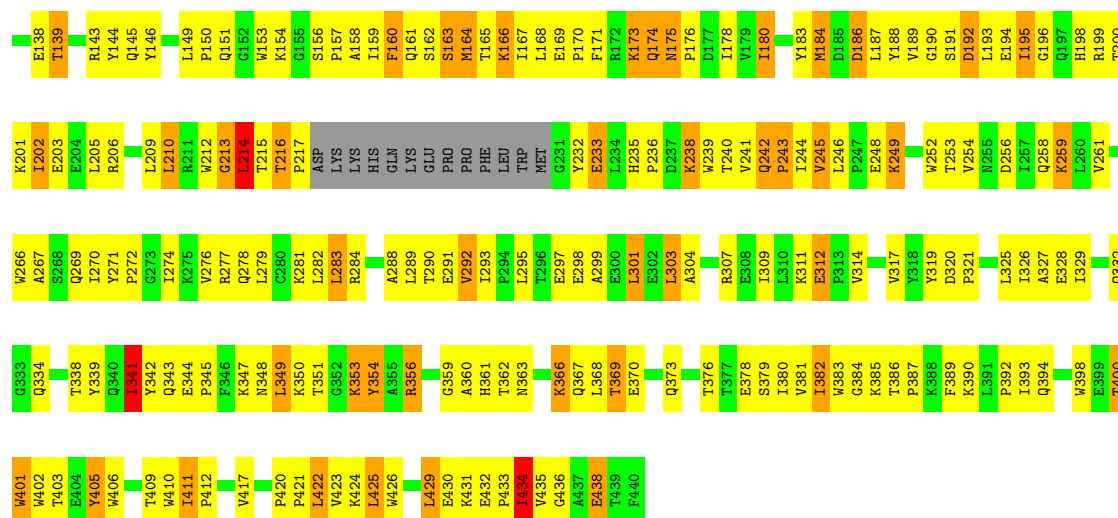
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	543	4435	2869	739	819	8	0	0	0

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	426	3508	2282	580	639	7	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	164	Total	O	0	0
			164	164		
3	B	103	Total	O	0	0
			103	103		



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.50Å 109.40Å 72.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.35	Depositor
% Data completeness (in resolution range)	89.5 (25.00-2.35)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.219 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8210	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

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: CSD

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	0.93	5/4544 (0.1%)	1.41	68/6175 (1.1%)
2	B	0.92	3/3607 (0.1%)	1.34	45/4903 (0.9%)
All	All	0.93	8/8151 (0.1%)	1.38	113/11078 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	1
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	ILE	CA-CB	6.58	1.62	1.54
1	A	419	THR	CA-CB	5.57	1.60	1.53
2	B	411	ILE	CA-CB	5.25	1.58	1.54
2	B	434	ILE	CA-CB	5.25	1.61	1.54
1	A	181	TYR	CA-C	-5.09	1.46	1.52
1	A	314	VAL	CA-CB	5.08	1.59	1.53
1	A	94	ILE	CA-CB	5.08	1.60	1.54
2	B	400	THR	CA-CB	5.01	1.61	1.53

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	SER	N-CA-C	13.52	123.69	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	THR	CA-C-N	11.25	131.96	119.92
1	A	386	THR	C-N-CA	11.25	131.96	119.92
1	A	132	ILE	CA-C-N	10.21	130.28	119.76
1	A	132	ILE	C-N-CA	10.21	130.28	119.76
1	A	356	ARG	N-CA-C	9.48	123.36	110.55
1	A	388	LYS	N-CA-C	-9.26	95.56	110.20
1	A	357	MET	N-CA-C	9.05	122.12	111.71
1	A	419	THR	CA-C-N	9.04	129.69	120.38
1	A	419	THR	C-N-CA	9.04	129.69	120.38
1	A	494	ASN	N-CA-C	-8.25	95.45	108.90
1	A	382	ILE	N-CA-C	8.24	118.27	110.53
1	A	420	PRO	N-CA-C	8.20	120.70	110.70
2	B	382	ILE	N-CA-C	8.14	118.23	110.42
2	B	89	GLU	N-CA-C	-8.04	101.80	111.69
2	B	242	GLN	N-CA-C	7.92	121.81	110.24
2	B	151	GLN	N-CA-C	-7.84	100.19	110.53
2	B	210	LEU	N-CA-C	-7.81	102.71	111.14
1	A	204	GLU	N-CA-C	-7.78	102.49	110.97
1	A	333	GLY	N-CA-C	-7.65	99.58	110.75
2	B	61	PHE	N-CA-C	-7.62	98.12	108.86
1	A	186	ASP	N-CA-C	7.43	121.32	108.76
2	B	18	GLY	CA-C-N	7.38	127.14	119.76
2	B	18	GLY	C-N-CA	7.38	127.14	119.76
2	B	45	GLY	N-CA-C	7.36	125.31	115.59
2	B	202	ILE	N-CA-C	-7.34	103.63	110.53
1	A	156	SER	CA-C-N	-7.25	111.42	118.97
1	A	156	SER	C-N-CA	-7.25	111.42	118.97
1	A	18	GLY	CA-C-N	7.21	127.19	119.76
1	A	18	GLY	C-N-CA	7.21	127.19	119.76
1	A	325	LEU	N-CA-C	-7.16	97.22	108.90
1	A	218	ASP	N-CA-C	7.14	122.55	113.55
2	B	303	LEU	N-CA-C	-7.13	103.43	111.14
2	B	96	HIS	CA-C-N	7.10	128.72	119.84
2	B	96	HIS	C-N-CA	7.10	128.72	119.84
2	B	87	PHE	N-CA-C	7.08	119.23	109.54
1	A	398	TRP	N-CA-C	-7.00	103.34	110.97
2	B	312	GLU	N-CA-C	6.99	114.51	108.22
1	A	139	THR	N-CA-C	-6.94	95.05	108.45
2	B	341	ILE	N-CA-C	-6.92	98.40	108.71
2	B	70	LYS	N-CA-C	-6.89	98.61	109.50
1	A	141	GLY	N-CA-C	-6.84	103.32	112.14
1	A	70	LYS	N-CA-C	-6.83	98.96	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	349	LEU	N-CA-C	-6.62	104.00	111.14
1	A	396	GLU	N-CA-C	-6.56	104.16	111.71
1	A	538	ALA	N-CA-C	6.51	118.93	110.53
2	B	171	PHE	N-CA-C	-6.50	104.28	112.93
1	A	22	LYS	N-CA-C	6.34	118.49	110.24
1	A	503	LEU	N-CA-C	-6.26	104.54	111.36
2	B	184	MET	CB-CA-C	-6.26	109.34	116.54
1	A	540	LYS	N-CA-C	-6.25	101.27	110.52
1	A	508	ALA	N-CA-C	6.18	120.82	113.16
1	A	37	ILE	CB-CA-C	-6.13	104.00	112.04
1	A	520	GLN	N-CA-C	-6.11	104.53	111.07
1	A	375	ILE	N-CA-C	-6.09	104.40	110.30
2	B	366	LYS	N-CA-C	-6.07	104.35	110.97
2	B	438	GLU	N-CA-C	6.06	123.72	110.80
1	A	394	GLN	N-CA-C	-6.05	102.51	110.43
2	B	233	GLU	N-CA-C	-6.03	99.90	109.07
1	A	207	GLN	N-CA-C	-6.02	104.05	111.40
1	A	323	LYS	N-CA-C	6.01	119.34	109.85
1	A	210	LEU	N-CA-C	-5.98	105.24	112.54
2	B	417	VAL	N-CA-C	5.88	117.18	108.65
2	B	69	THR	N-CA-C	-5.86	105.45	113.30
2	B	93	GLY	N-CA-C	-5.85	99.31	113.18
1	A	362	THR	N-CA-C	5.79	115.66	108.19
1	A	493	VAL	CB-CA-C	-5.74	101.50	110.69
1	A	408	ALA	N-CA-C	-5.67	101.24	110.20
2	B	186	ASP	N-CA-C	5.66	118.47	109.81
2	B	259	LYS	N-CA-C	-5.66	104.75	111.03
2	B	232	TYR	N-CA-C	5.64	117.63	108.26
1	A	319	TYR	N-CA-C	5.61	117.83	109.25
1	A	368	LEU	N-CA-C	-5.57	105.11	111.07
1	A	13	LYS	CA-C-N	5.56	126.79	119.84
1	A	13	LYS	C-N-CA	5.56	126.79	119.84
2	B	58	THR	CA-C-N	5.55	125.48	119.76
2	B	58	THR	C-N-CA	5.55	125.48	119.76
1	A	155	GLY	N-CA-C	5.55	122.18	113.86
1	A	277	ARG	N-CA-C	5.51	117.72	111.11
1	A	252	TRP	N-CA-C	5.51	117.21	108.67
1	A	520	GLN	CB-CA-C	-5.49	102.26	110.88
1	A	441	TYR	N-CA-C	-5.48	100.18	108.67
2	B	168	LEU	N-CA-C	5.48	120.06	112.45
2	B	434	ILE	N-CA-C	-5.46	105.05	110.62
1	A	44	GLU	N-CA-C	-5.45	106.71	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	TRP	N-CA-C	-5.43	100.85	109.59
1	A	402	TRP	N-CA-C	5.41	117.93	111.71
1	A	311	LYS	N-CA-C	-5.40	105.50	111.71
1	A	362	THR	CB-CA-C	-5.39	102.72	114.10
2	B	175	ASN	CA-C-N	-5.37	114.72	120.47
2	B	175	ASN	C-N-CA	-5.37	114.72	120.47
2	B	238	LYS	N-CA-C	5.34	119.51	112.89
2	B	422	LEU	N-CA-C	5.32	117.16	111.36
1	A	56	TYR	N-CA-C	5.21	117.41	110.53
1	A	390	LYS	N-CA-C	-5.21	99.80	108.34
1	A	200	THR	N-CA-C	-5.19	105.51	111.07
2	B	401	TRP	N-CA-C	5.19	119.16	112.41
1	A	3	SER	CA-C-N	5.18	126.32	119.84
1	A	3	SER	C-N-CA	5.18	126.32	119.84
1	A	144	TYR	N-CA-C	5.18	115.22	108.07
1	A	90	VAL	N-CA-C	-5.16	98.62	109.34
2	B	423	VAL	CB-CA-C	-5.14	105.30	112.04
2	B	160	PHE	N-CA-C	-5.13	107.53	112.97
2	B	46	LYS	N-CA-C	5.12	116.86	111.28
1	A	336	GLN	N-CA-C	-5.07	100.63	108.90
1	A	348	ASN	N-CA-C	5.07	118.08	109.76
1	A	393	ILE	CB-CA-C	-5.07	101.73	110.65
2	B	279	LEU	N-CA-C	-5.05	105.96	112.68
2	B	420	PRO	N-CA-C	-5.05	104.54	110.70
2	B	94	ILE	CA-C-N	5.03	125.50	120.52
2	B	94	ILE	C-N-CA	5.03	125.50	120.52
1	A	488	ASP	N-CA-C	5.02	119.38	113.16
1	A	276	VAL	N-CA-C	5.00	119.74	109.34

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	TYR	Sidechain
1	A	146	TYR	Sidechain
1	A	319	TYR	Sidechain
2	B	56	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4435	0	4483	287	0
2	B	3508	0	3541	233	0
3	A	164	0	0	7	0
3	B	103	0	0	5	0
All	All	8210	0	8024	513	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 32.

All (513) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.40	1.00
1:A:342:TYR:HB3	1:A:348:ASN:HB3	1.47	0.97
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.47	0.96
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.52	0.92
1:A:14:PRO:HG2	3:A:1024:HOH:O	1.73	0.89
2:B:303:LEU:HD13	2:B:307:ARG:HH21	1.38	0.89
1:A:335:GLY:O	1:A:356:ARG:HB2	1.73	0.88
1:A:515:SER:OG	1:A:518:VAL:HG23	1.73	0.88
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.55	0.88
2:B:122:GLU:HA	2:B:125:ARG:HD2	1.57	0.86
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.11	0.86
1:A:502:ALA:O	1:A:506:ILE:HG13	1.76	0.84
1:A:112:GLY:HA2	1:A:185:ASP:HB3	1.59	0.82
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.60	0.82
1:A:208:HIS:CE1	1:A:212:TRP:HE1	1.98	0.82
1:A:542:ILE:HG13	2:B:283:LEU:HD23	1.60	0.81
1:A:229:TRP:HB3	1:A:232:TYR:HB2	1.61	0.81
1:A:377:THR:O	1:A:381:VAL:HG23	1.81	0.80
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.13	0.78
1:A:229:TRP:CE3	1:A:229:TRP:HA	2.19	0.78
2:B:421:PRO:O	2:B:425:LEU:HD22	1.85	0.77
2:B:92:LEU:HD13	2:B:161:GLN:HB3	1.66	0.76
1:A:229:TRP:HA	1:A:229:TRP:HE3	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ASN:HA	1:A:522:ILE:HD12	1.67	0.76
1:A:21:VAL:HG22	1:A:59:PRO:HD3	1.66	0.75
1:A:208:HIS:O	1:A:211:ARG:HB2	1.87	0.75
1:A:356:ARG:NH2	1:A:367:GLN:O	2.21	0.74
1:A:181:TYR:CD1	2:B:138:GLU:HB3	2.22	0.74
2:B:379:SER:CB	2:B:387:PRO:HD3	2.19	0.73
1:A:239:TRP:HZ2	1:A:349:LEU:O	1.71	0.73
1:A:309:ILE:O	1:A:312:GLU:HB3	1.88	0.73
2:B:178:ILE:HG12	2:B:191:SER:CB	2.16	0.73
2:B:266:TRP:HZ3	2:B:426:TRP:CG	2.06	0.73
2:B:215:THR:C	2:B:217:PRO:HD3	2.12	0.73
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.07	0.73
2:B:60:VAL:HG21	2:B:130:PHE:HD2	1.54	0.72
1:A:8:VAL:O	1:A:121:ASP:HB2	1.89	0.72
1:A:241:VAL:HG21	1:A:314:VAL:HG23	1.72	0.72
1:A:465:LYS:HG3	1:A:466:VAL:N	2.05	0.71
1:A:244:ILE:HG23	1:A:310:LEU:HD13	1.70	0.71
2:B:254:VAL:HG22	2:B:293:ILE:HD11	1.71	0.71
2:B:328:GLU:O	2:B:339:TYR:HA	1.90	0.71
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.26	0.71
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.72	0.71
1:A:244:ILE:HD11	1:A:263:LYS:HE3	1.71	0.71
2:B:344:GLU:HG3	2:B:345:PRO:HD2	1.71	0.71
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.72	0.71
1:A:34:LEU:HD22	1:A:73:LYS:HG3	1.72	0.71
1:A:340:GLN:CB	1:A:351:THR:HG22	2.20	0.71
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.89	0.71
1:A:28:GLU:CD	1:A:32:LYS:HE3	2.16	0.70
1:A:356:ARG:HE	1:A:367:GLN:HG2	1.56	0.70
2:B:122:GLU:HG3	2:B:125:ARG:NH1	2.07	0.70
1:A:542:ILE:CG1	2:B:283:LEU:HD23	2.22	0.70
2:B:5:ILE:HG13	2:B:6:GLU:N	2.06	0.69
1:A:63:ILE:HD12	1:A:65:LYS:HE3	1.74	0.69
1:A:474:ASN:O	1:A:478:GLU:HG3	1.92	0.69
2:B:125:ARG:HG2	2:B:146:TYR:O	1.93	0.68
2:B:426:TRP:O	2:B:429:LEU:HB2	1.93	0.68
2:B:175:ASN:ND2	2:B:201:LYS:HE2	2.08	0.68
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.75	0.68
1:A:27:THR:HB	1:A:30:LYS:HG3	1.76	0.68
1:A:33:ALA:HB1	1:A:71:TRP:HB2	1.75	0.67
1:A:164:MET:HE1	1:A:214:LEU:HD23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:SER:O	2:B:167:ILE:HG13	1.95	0.67
1:A:517:LEU:O	1:A:521:ILE:HG13	1.95	0.67
2:B:266:TRP:CZ3	2:B:426:TRP:CG	2.83	0.67
1:A:362:THR:HG22	1:A:363:ASN:H	1.58	0.67
1:A:240:THR:HG22	1:A:315:HIS:HD2	1.59	0.66
2:B:158:ALA:O	2:B:161:GLN:HB2	1.96	0.66
1:A:164:MET:HG3	1:A:168:LEU:HD22	1.79	0.65
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.78	0.64
1:A:114:ALA:HB1	1:A:214:LEU:HG	1.77	0.64
1:A:224:GLU:HG2	1:A:225:PRO:HD2	1.78	0.64
2:B:281:LYS:HD3	2:B:284:ARG:NH2	2.12	0.64
1:A:66:LYS:H	1:A:66:LYS:HD3	1.62	0.64
1:A:202:ILE:CG2	1:A:206:ARG:HH21	2.10	0.64
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.28	0.64
1:A:277:ARG:O	1:A:281:LYS:HG3	1.97	0.64
1:A:393:ILE:HG23	1:A:423:VAL:HG22	1.77	0.64
2:B:104:LYS:CB	2:B:192:ASP:HA	2.25	0.64
1:A:31:ILE:HD12	1:A:135:ILE:HD12	1.81	0.63
1:A:278:GLN:O	1:A:282:LEU:HD13	1.99	0.63
1:A:20:LYS:HD2	1:A:55:PRO:O	1.99	0.63
2:B:435:VAL:HG23	2:B:436:GLY:H	1.64	0.63
1:A:219:LYS:HE3	1:A:219:LYS:HA	1.80	0.63
1:A:78:ARG:HG3	1:A:79:GLU:N	2.11	0.63
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.80	0.62
1:A:7:THR:HG21	1:A:122:GLU:OE2	1.98	0.62
1:A:26:LEU:HD12	1:A:133:PRO:HD2	1.81	0.62
2:B:369:THR:O	2:B:373:GLN:HG3	1.99	0.62
2:B:434:ILE:HG13	2:B:435:VAL:HG22	1.82	0.62
1:A:253:THR:HG22	1:A:255:ASN:HB2	1.81	0.62
1:A:280:CSD:O	1:A:283:LEU:HB2	1.99	0.62
2:B:277:ARG:O	2:B:281:LYS:HG2	2.01	0.61
2:B:303:LEU:O	2:B:307:ARG:HG3	2.00	0.61
2:B:434:ILE:HG13	2:B:435:VAL:N	2.14	0.61
1:A:241:VAL:CG2	1:A:314:VAL:HG23	2.30	0.61
1:A:393:ILE:HD12	1:A:414:TRP:CZ3	2.36	0.61
2:B:78:ARG:O	2:B:82:LYS:HG3	1.99	0.61
1:A:252:TRP:CD1	1:A:295:LEU:HD21	2.36	0.61
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.35	0.61
1:A:438:GLU:CD	1:A:461:ARG:HD2	2.26	0.61
2:B:50:ILE:HG13	2:B:143:ARG:HB3	1.83	0.61
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:HD3	1:A:321:PRO:HG2	1.82	0.61
1:A:400:THR:HG22	1:A:425:LEU:HD11	1.82	0.61
2:B:101:LYS:HE3	2:B:382:ILE:HA	1.83	0.61
2:B:175:ASN:HD21	2:B:201:LYS:HE2	1.65	0.61
1:A:373:GLN:HG2	3:B:1237:HOH:O	2.01	0.60
2:B:180:ILE:HG13	2:B:189:VAL:HG22	1.83	0.60
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.82	0.60
1:A:231:GLY:HA2	1:A:242:GLN:HB2	1.82	0.60
2:B:244:ILE:HG23	2:B:429:LEU:HB3	1.83	0.60
1:A:125:ARG:HG2	1:A:146:TYR:O	2.01	0.60
1:A:254:VAL:O	1:A:258:GLN:HG3	2.01	0.60
1:A:401:TRP:CZ3	1:A:409:THR:HG21	2.36	0.60
1:A:3:SER:HB3	1:A:4:PRO:HD2	1.84	0.60
1:A:98:ALA:HB1	1:A:349:LEU:HB3	1.84	0.59
2:B:31:ILE:O	2:B:35:VAL:HG23	2.01	0.59
2:B:301:LEU:O	2:B:301:LEU:HG	2.02	0.59
2:B:278:GLN:O	2:B:299:ALA:HB2	2.01	0.59
1:A:297:GLU:HG2	1:A:298:GLU:N	2.17	0.59
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.32	0.59
1:A:357:MET:O	1:A:358:ARG:HB3	2.02	0.59
1:A:113:ASP:HB2	3:A:1045:HOH:O	2.03	0.58
1:A:96:HIS:CD2	1:A:98:ALA:HB3	2.38	0.58
1:A:329:ILE:HD12	1:A:391:LEU:HD21	1.85	0.58
2:B:97:PRO:O	2:B:99:GLY:N	2.33	0.58
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.85	0.58
1:A:491:LEU:HD22	1:A:529:GLU:HG3	1.85	0.58
2:B:292:VAL:C	2:B:293:ILE:HG13	2.29	0.58
1:A:27:THR:HG22	1:A:29:GLU:H	1.67	0.58
1:A:233:GLU:HB2	1:A:240:THR:OG1	2.03	0.58
2:B:64:LYS:HE3	2:B:71:TRP:CE2	2.39	0.58
2:B:301:LEU:O	2:B:304:ALA:HB3	2.03	0.58
1:A:122:GLU:H	1:A:122:GLU:CD	2.12	0.58
1:A:164:MET:CE	1:A:214:LEU:HD23	2.33	0.58
2:B:64:LYS:HE3	2:B:71:TRP:NE1	2.19	0.58
2:B:114:ALA:HB2	2:B:214:LEU:HG	1.85	0.58
1:A:12:LEU:HD22	1:A:83:ARG:O	2.04	0.57
1:A:340:GLN:HA	1:A:351:THR:HA	1.86	0.57
2:B:379:SER:HB2	2:B:387:PRO:HD3	1.84	0.57
1:A:235:HIS:HB2	1:A:238:LYS:O	2.04	0.57
1:A:511:ASP:HA	1:A:522:ILE:HG21	1.85	0.57
2:B:282:LEU:HD11	2:B:295:LEU:HD23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:GLU:HG3	2:B:390:LYS:HB2	1.87	0.57
1:A:31:ILE:HD12	1:A:135:ILE:CD1	2.34	0.57
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.39	0.57
2:B:41:MET:HE2	2:B:47:ILE:HD13	1.87	0.57
1:A:233:GLU:HB2	1:A:240:THR:HG1	1.68	0.57
2:B:254:VAL:O	2:B:258:GLN:HG3	2.05	0.57
1:A:317:VAL:HG12	1:A:349:LEU:HD23	1.87	0.56
1:A:95:PRO:HD3	1:A:183:TYR:CE2	2.40	0.56
1:A:7:THR:CG2	1:A:121:ASP:HA	2.36	0.56
1:A:401:TRP:HZ3	1:A:409:THR:HG21	1.70	0.56
1:A:235:HIS:HB3	1:A:236:PRO:CD	2.26	0.56
2:B:108:VAL:HG13	2:B:188:TYR:CE1	2.41	0.56
2:B:134:SER:CB	2:B:139:THR:HG23	2.36	0.56
2:B:366:LYS:O	2:B:370:GLU:HG3	2.05	0.56
1:A:28:GLU:HB3	3:A:1026:HOH:O	2.05	0.56
2:B:3:SER:O	2:B:119:PRO:HD3	2.05	0.55
1:A:27:THR:O	1:A:31:ILE:HG13	2.05	0.55
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.53	0.55
1:A:149:LEU:HD21	1:A:159:ILE:HG21	1.88	0.55
1:A:22:LYS:HG2	1:A:23:GLN:N	2.22	0.55
1:A:295:LEU:HD23	1:A:295:LEU:N	2.21	0.55
2:B:105:SER:O	2:B:190:GLY:HA2	2.07	0.55
1:A:200:THR:O	1:A:203:GLU:HB3	2.07	0.55
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.42	0.55
1:A:33:ALA:O	1:A:37:ILE:HG13	2.07	0.54
2:B:111:VAL:HG21	2:B:164:MET:CE	2.38	0.54
2:B:270:ILE:O	2:B:272:PRO:HD3	2.08	0.54
2:B:380:ILE:O	2:B:384:GLY:N	2.39	0.54
1:A:312:GLU:HG2	1:A:313:PRO:N	2.22	0.54
1:A:366:LYS:NZ	2:B:394:GLN:NE2	2.55	0.54
1:A:63:ILE:HG13	1:A:63:ILE:O	2.07	0.54
2:B:154:LYS:HA	2:B:184:MET:HE1	1.89	0.54
2:B:288:ALA:O	2:B:291:GLU:HB3	2.08	0.54
2:B:235:HIS:HB3	2:B:238:LYS:HG2	1.90	0.54
1:A:54:ASN:HB3	1:A:143:ARG:HH21	1.73	0.54
2:B:356:ARG:HB3	2:B:367:GLN:OE1	2.08	0.53
1:A:26:LEU:HD12	1:A:133:PRO:CD	2.38	0.53
2:B:433:PRO:HG3	2:B:436:GLY:HA2	1.90	0.53
2:B:122:GLU:HG3	2:B:125:ARG:HH11	1.72	0.53
2:B:281:LYS:HD3	2:B:284:ARG:HH21	1.74	0.53
1:A:400:THR:CG2	1:A:425:LEU:HD11	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:TRP:CZ2	1:A:349:LEU:O	2.57	0.53
1:A:380:ILE:HG13	1:A:386:THR:HG22	1.90	0.53
2:B:134:SER:HB3	2:B:139:THR:HG23	1.90	0.53
1:A:490:GLY:O	1:A:528:LYS:HE3	2.09	0.53
1:A:361:HIS:CE1	1:A:510:PRO:HG3	2.43	0.52
1:A:241:VAL:HG21	1:A:270:ILE:HD12	1.91	0.52
1:A:103:LYS:HG3	1:A:190:GLY:C	2.35	0.52
1:A:218:ASP:O	1:A:222:GLN:HG2	2.09	0.52
1:A:218:ASP:O	1:A:219:LYS:HE3	2.09	0.52
2:B:319:TYR:HE1	2:B:325:LEU:HD13	1.74	0.52
1:A:197:GLN:O	1:A:200:THR:HB	2.09	0.52
2:B:118:VAL:HG21	2:B:160:PHE:HD1	1.75	0.52
2:B:200:THR:O	2:B:203:GLU:HB3	2.08	0.52
1:A:500:GLN:O	1:A:503:LEU:HB3	2.10	0.52
2:B:51:GLY:HA3	2:B:53:GLU:OE2	2.10	0.52
2:B:205:LEU:HD13	2:B:209:LEU:HD12	1.91	0.52
2:B:242:GLN:HA	2:B:242:GLN:HE21	1.75	0.52
2:B:281:LYS:HA	2:B:284:ARG:NH2	2.25	0.52
2:B:97:PRO:C	2:B:99:GLY:H	2.17	0.51
1:A:516:GLU:O	1:A:519:ASN:HB2	2.11	0.51
2:B:125:ARG:O	2:B:128:THR:OG1	2.23	0.51
1:A:307:ARG:O	1:A:311:LYS:HG3	2.09	0.51
1:A:517:LEU:HA	1:A:520:GLN:CG	2.41	0.51
1:A:519:ASN:O	1:A:523:GLU:HG2	2.10	0.51
2:B:343:GLN:HG3	2:B:349:LEU:HD11	1.93	0.51
2:B:400:THR:HG22	2:B:401:TRP:CD2	2.45	0.51
2:B:424:LYS:HD2	2:B:424:LYS:O	2.10	0.51
2:B:92:LEU:HD13	2:B:161:GLN:CB	2.37	0.51
2:B:100:LEU:O	2:B:103:LYS:HB2	2.11	0.51
1:A:50:ILE:CG2	1:A:145:GLN:HG2	2.41	0.50
1:A:255:ASN:HB3	1:A:259:LYS:HE2	1.92	0.50
1:A:532:TYR:HE2	1:A:534:ALA:HB2	1.76	0.50
2:B:245:VAL:CG1	2:B:431:LYS:HB2	2.41	0.50
2:B:329:ILE:HA	2:B:338:THR:O	2.11	0.50
2:B:362:THR:HG22	2:B:362:THR:O	2.12	0.50
2:B:311:LYS:O	2:B:312:GLU:HG3	2.12	0.50
2:B:54:ASN:O	2:B:143:ARG:NH2	2.45	0.50
1:A:5:ILE:HG23	1:A:119:PRO:HD2	1.93	0.50
1:A:11:LYS:O	1:A:85:GLN:HB3	2.12	0.50
1:A:35:VAL:HG22	1:A:132:ILE:HG21	1.94	0.50
2:B:326:ILE:HG22	2:B:327:ALA:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:O	1:A:210:LEU:HD23	2.12	0.50
2:B:23:GLN:HG3	2:B:24:TRP:O	2.12	0.50
2:B:130:PHE:CE1	2:B:144:TYR:HB2	2.46	0.50
1:A:67:ASP:HB2	1:A:72:ARG:HH12	1.77	0.50
1:A:229:TRP:O	1:A:230:MET:HG3	2.11	0.50
1:A:111:VAL:HG11	1:A:187:LEU:CD2	2.42	0.49
1:A:149:LEU:HD13	1:A:156:SER:HA	1.93	0.49
1:A:334:GLN:NE2	3:A:1091:HOH:O	2.42	0.49
1:A:362:THR:O	1:A:510:PRO:HA	2.12	0.49
2:B:22:LYS:H	2:B:22:LYS:HD3	1.76	0.49
2:B:94:ILE:HG13	2:B:95:PRO:HD2	1.94	0.49
2:B:17:ASP:O	2:B:83:ARG:HD3	2.12	0.49
2:B:215:THR:O	2:B:217:PRO:HD3	2.12	0.49
1:A:362:THR:CG2	1:A:363:ASN:H	2.20	0.49
1:A:463:ARG:NH1	1:A:488:ASP:O	2.45	0.49
1:A:486:LEU:HB3	1:A:524:GLN:HB3	1.94	0.49
2:B:249:LYS:HG2	2:B:252:TRP:CE2	2.48	0.49
2:B:36:GLU:O	2:B:39:THR:HG22	2.12	0.49
2:B:79:GLU:O	2:B:83:ARG:HG3	2.13	0.49
2:B:162:SER:O	2:B:166:LYS:HG3	2.11	0.49
1:A:7:THR:HG21	1:A:121:ASP:HA	1.95	0.49
1:A:34:LEU:HD23	1:A:37:ILE:HD12	1.95	0.49
1:A:222:GLN:CD	1:A:223:LYS:H	2.21	0.49
1:A:231:GLY:CA	1:A:242:GLN:HB2	2.43	0.49
1:A:78:ARG:CG	1:A:79:GLU:N	2.74	0.49
1:A:240:THR:HG22	1:A:315:HIS:CD2	2.43	0.49
2:B:78:ARG:HH11	2:B:411:ILE:CG2	2.26	0.49
1:A:393:ILE:HD12	1:A:414:TRP:CH2	2.48	0.49
2:B:85:GLN:O	2:B:85:GLN:HG2	2.12	0.49
2:B:169:GLU:O	2:B:173:LYS:N	2.46	0.49
1:A:218:ASP:O	1:A:222:GLN:CG	2.60	0.49
1:A:13:LYS:O	1:A:16:MET:HB2	2.12	0.49
2:B:363:ASN:ND2	2:B:405:TYR:OH	2.41	0.48
1:A:253:THR:O	1:A:257:ILE:HG13	2.12	0.48
1:A:486:LEU:O	1:A:528:LYS:NZ	2.45	0.48
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.94	0.48
2:B:261:VAL:HG22	2:B:276:VAL:HG22	1.96	0.48
2:B:319:TYR:CZ	2:B:321:PRO:HA	2.48	0.48
1:A:13:LYS:HB3	1:A:16:MET:SD	2.53	0.48
2:B:16:MET:HE3	2:B:83:ARG:HG2	1.95	0.48
1:A:73:LYS:NZ	1:A:73:LYS:HB3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:ASN:ND2	2:B:143:ARG:NH1	2.61	0.48
2:B:422:LEU:HB2	3:B:1244:HOH:O	2.12	0.48
1:A:3:SER:CB	1:A:5:ILE:HG22	2.43	0.48
1:A:5:ILE:HG23	1:A:119:PRO:CD	2.44	0.48
1:A:27:THR:HG22	1:A:29:GLU:N	2.28	0.48
1:A:65:LYS:C	1:A:67:ASP:H	2.22	0.48
1:A:122:GLU:HA	1:A:125:ARG:NE	2.29	0.48
1:A:37:ILE:HD11	1:A:71:TRP:O	2.13	0.48
1:A:111:VAL:HG11	1:A:187:LEU:HD22	1.96	0.48
1:A:420:PRO:HA	1:A:421:PRO:C	2.38	0.48
2:B:111:VAL:HG21	2:B:164:MET:HE2	1.96	0.48
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.14	0.48
1:A:303:LEU:HD11	1:A:307:ARG:NH2	2.29	0.48
1:A:536:VAL:HG11	1:A:542:ILE:HG21	1.95	0.48
2:B:424:LYS:HD2	2:B:424:LYS:C	2.39	0.48
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.95	0.48
1:A:305:GLU:O	1:A:308:GLU:HB2	2.13	0.48
2:B:65:LYS:N	2:B:68:SER:HB2	2.29	0.48
2:B:120:LEU:HD12	2:B:150:PRO:HD3	1.96	0.47
1:A:540:LYS:HB2	1:A:542:ILE:CD1	2.44	0.47
2:B:8:VAL:HG13	2:B:159:ILE:HD13	1.96	0.47
2:B:169:GLU:O	2:B:173:LYS:HB2	2.15	0.47
2:B:379:SER:HA	2:B:383:TRP:CE3	2.49	0.47
2:B:398:TRP:O	2:B:402:TRP:HD1	1.98	0.47
2:B:350:LYS:HG2	2:B:351:THR:N	2.29	0.47
2:B:29:GLU:HG3	2:B:71:TRP:CZ2	2.49	0.47
1:A:356:ARG:HH21	1:A:367:GLN:CA	2.28	0.47
1:A:448:ARG:HB3	3:A:1154:HOH:O	2.15	0.47
1:A:164:MET:HE2	1:A:164:MET:HA	1.97	0.47
2:B:120:LEU:C	2:B:120:LEU:HD23	2.40	0.47
2:B:267:ALA:C	2:B:269:GLN:H	2.21	0.47
2:B:435:VAL:HG23	2:B:436:GLY:N	2.29	0.47
1:A:220:LYS:HB3	1:A:221:HIS:CE1	2.50	0.47
1:A:345:PRO:C	1:A:347:LYS:H	2.23	0.47
2:B:153:TRP:HE3	2:B:156:SER:OG	1.98	0.47
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.97	0.47
1:A:448:ARG:HB2	1:A:448:ARG:NH1	2.30	0.47
2:B:191:SER:HB2	2:B:193:LEU:HD23	1.96	0.47
2:B:213:GLY:O	2:B:214:LEU:HB3	2.15	0.47
2:B:239:TRP:CZ3	2:B:378:GLU:HG2	2.50	0.47
2:B:338:THR:HG22	2:B:353:LYS:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.50	0.47
1:A:229:TRP:CB	1:A:232:TYR:HB2	2.40	0.46
1:A:136:ASN:C	1:A:136:ASN:HD22	2.23	0.46
1:A:225:PRO:HG3	1:A:227:PHE:CZ	2.51	0.46
1:A:395:LYS:HD2	1:A:414:TRP:CZ2	2.50	0.46
2:B:252:TRP:CE3	2:B:256:ASP:HB3	2.50	0.46
2:B:379:SER:HA	2:B:383:TRP:HE3	1.80	0.46
1:A:498:ASP:HA	1:A:536:VAL:O	2.16	0.46
2:B:34:LEU:O	2:B:38:CYS:HB2	2.15	0.46
2:B:327:ALA:O	2:B:389:PHE:HA	2.16	0.46
1:A:115:TYR:OH	1:A:151:GLN:HB2	2.14	0.46
1:A:155:GLY:O	1:A:156:SER:C	2.58	0.46
1:A:517:LEU:HA	1:A:520:GLN:HG3	1.98	0.46
2:B:254:VAL:HG12	2:B:258:GLN:NE2	2.30	0.46
2:B:319:TYR:CE1	2:B:325:LEU:HD13	2.50	0.46
2:B:361:HIS:HD1	2:B:361:HIS:C	2.23	0.46
1:A:28:GLU:O	1:A:32:LYS:HG3	2.14	0.46
1:A:500:GLN:O	1:A:503:LEU:CB	2.64	0.46
2:B:379:SER:HB3	2:B:387:PRO:HD3	1.98	0.46
1:A:360:ALA:HA	1:A:514:GLU:HB2	1.98	0.46
2:B:61:PHE:HB2	2:B:74:LEU:HD23	1.98	0.46
2:B:380:ILE:O	2:B:384:GLY:HA2	2.15	0.46
2:B:354:TYR:CD1	2:B:354:TYR:C	2.94	0.46
1:A:489:SER:CB	1:A:493:VAL:HG13	2.46	0.46
2:B:261:VAL:HG22	2:B:276:VAL:CG2	2.46	0.46
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.97	0.46
1:A:328:GLU:O	1:A:339:TYR:HA	2.16	0.45
1:A:380:ILE:CG1	1:A:386:THR:HG22	2.46	0.45
1:A:542:ILE:N	1:A:542:ILE:HD12	2.31	0.45
2:B:196:GLY:O	2:B:200:THR:HG23	2.17	0.45
1:A:469:LEU:HB2	1:A:472:THR:HG21	1.97	0.45
2:B:5:ILE:CG1	2:B:6:GLU:N	2.74	0.45
2:B:183:TYR:HB3	2:B:188:TYR:HE2	1.80	0.45
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.81	0.45
2:B:376:THR:CG2	2:B:386:THR:HG22	2.46	0.45
1:A:401:TRP:HB2	1:A:425:LEU:HD21	1.98	0.45
2:B:253:THR:H	2:B:256:ASP:HB2	1.81	0.45
2:B:406:TRP:CZ2	2:B:412:PRO:HD2	2.52	0.45
1:A:94:ILE:HG22	1:A:95:PRO:O	2.16	0.45
2:B:60:VAL:CG2	2:B:130:PHE:HD2	2.26	0.45
2:B:271:TYR:O	2:B:274:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:GLN:OE1	2:B:334:GLN:HA	2.16	0.45
2:B:369:THR:CG2	2:B:398:TRP:CH2	3.00	0.45
1:A:515:SER:CB	1:A:518:VAL:HG23	2.45	0.45
2:B:118:VAL:HB	2:B:149:LEU:HG	1.97	0.45
2:B:359:GLY:O	2:B:361:HIS:N	2.50	0.45
1:A:225:PRO:HA	1:A:226:PRO:C	2.41	0.45
2:B:120:LEU:HD21	2:B:124:PHE:HB3	1.98	0.45
2:B:259:LYS:HE3	3:B:1217:HOH:O	2.16	0.45
2:B:410:TRP:O	2:B:410:TRP:CE3	2.70	0.44
1:A:267:ALA:O	1:A:269:GLN:N	2.50	0.44
1:A:326:ILE:O	1:A:341:ILE:HG23	2.17	0.44
1:A:478:GLU:O	1:A:481:ALA:HB3	2.17	0.44
1:A:43:LYS:C	1:A:45:GLY:H	2.25	0.44
1:A:254:VAL:HG23	1:A:291:GLU:O	2.16	0.44
2:B:249:LYS:HE3	2:B:249:LYS:HB3	1.66	0.44
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.99	0.44
1:A:431:LYS:HA	1:A:431:LYS:HD3	1.47	0.44
2:B:248:GLU:O	2:B:248:GLU:HG3	2.18	0.44
1:A:73:LYS:HE2	1:A:75:VAL:HG23	1.98	0.44
1:A:323:LYS:HB3	1:A:343:GLN:NE2	2.32	0.44
2:B:174:GLN:HA	2:B:174:GLN:HE21	1.83	0.44
2:B:266:TRP:O	2:B:269:GLN:OE1	2.35	0.44
2:B:433:PRO:CG	2:B:436:GLY:HA2	2.47	0.44
1:A:73:LYS:HE2	1:A:75:VAL:CG2	2.48	0.44
1:A:210:LEU:HD13	1:A:210:LEU:HA	1.65	0.44
1:A:224:GLU:HG2	1:A:225:PRO:CD	2.47	0.44
2:B:65:LYS:HE3	2:B:72:ARG:HG2	2.00	0.44
2:B:195:ILE:O	2:B:199:ARG:HG3	2.18	0.44
1:A:229:TRP:CE3	1:A:229:TRP:CA	2.98	0.44
1:A:483:TYR:CE2	1:A:487:GLN:OE1	2.70	0.44
2:B:235:HIS:N	2:B:236:PRO:HD3	2.32	0.44
1:A:50:ILE:HG21	1:A:145:GLN:HG2	1.98	0.44
1:A:201:LYS:HA	1:A:201:LYS:HD3	1.81	0.44
1:A:386:THR:HA	1:A:387:PRO:HD2	1.62	0.43
2:B:118:VAL:HG21	2:B:160:PHE:CD1	2.52	0.43
2:B:174:GLN:O	2:B:176:PRO:HD3	2.17	0.43
2:B:198:HIS:O	2:B:202:ILE:HG12	2.18	0.43
1:A:34:LEU:HA	1:A:37:ILE:HD12	1.99	0.43
1:A:366:LYS:O	1:A:369:THR:HB	2.18	0.43
2:B:61:PHE:CD1	2:B:403:THR:HG21	2.53	0.43
2:B:176:PRO:HA	3:B:1209:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:VAL:HG21	2:B:130:PHE:CD2	2.43	0.43
2:B:96:HIS:HE1	2:B:100:LEU:HD21	1.83	0.43
2:B:209:LEU:O	2:B:214:LEU:HD13	2.18	0.43
1:A:22:LYS:HG2	1:A:23:GLN:H	1.81	0.43
1:A:540:LYS:HB2	1:A:542:ILE:HD13	2.01	0.43
1:A:28:GLU:HA	1:A:135:ILE:HD11	2.00	0.43
1:A:31:ILE:HD13	1:A:133:PRO:O	2.18	0.43
1:A:80:LEU:HD12	1:A:80:LEU:O	2.19	0.43
1:A:229:TRP:O	1:A:232:TYR:CD2	2.71	0.43
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.00	0.43
2:B:271:TYR:HB3	2:B:309:ILE:CG2	2.49	0.43
1:A:347:LYS:HD2	3:A:1108:HOH:O	2.17	0.43
2:B:87:PHE:CE2	2:B:154:LYS:HE3	2.53	0.43
2:B:379:SER:O	2:B:385:LYS:O	2.37	0.43
2:B:267:ALA:C	2:B:269:GLN:N	2.74	0.43
2:B:325:LEU:HA	2:B:343:GLN:HG2	2.00	0.43
2:B:379:SER:OG	2:B:387:PRO:HG3	2.19	0.43
1:A:231:GLY:O	1:A:242:GLN:N	2.50	0.43
1:A:485:ALA:O	1:A:489:SER:OG	2.32	0.43
2:B:206:ARG:HB3	2:B:206:ARG:NH1	2.34	0.43
1:A:257:ILE:O	1:A:261:VAL:HG23	2.19	0.43
1:A:34:LEU:CD2	1:A:73:LYS:HG3	2.47	0.43
1:A:156:SER:O	1:A:157:PRO:C	2.60	0.43
1:A:497:THR:O	1:A:535:TRP:HA	2.19	0.43
2:B:361:HIS:C	2:B:361:HIS:ND1	2.76	0.43
1:A:65:LYS:HD2	1:A:65:LYS:HA	1.93	0.42
2:B:58:THR:HG23	2:B:76:ASP:O	2.18	0.42
2:B:393:ILE:HD13	2:B:398:TRP:HB2	2.00	0.42
2:B:271:TYR:HB3	2:B:309:ILE:HG21	2.01	0.42
1:A:31:ILE:CD1	1:A:135:ILE:HD12	2.46	0.42
1:A:43:LYS:HD3	1:A:43:LYS:HA	1.77	0.42
2:B:156:SER:O	2:B:158:ALA:N	2.52	0.42
1:A:3:SER:HB2	1:A:5:ILE:HG22	2.00	0.42
1:A:3:SER:HB3	1:A:5:ILE:HG22	2.01	0.42
1:A:118:VAL:HB	1:A:149:LEU:HG	2.02	0.42
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.54	0.42
2:B:363:ASN:ND2	2:B:405:TYR:CZ	2.87	0.42
1:A:3:SER:HB2	1:A:5:ILE:CG2	2.49	0.42
1:A:61:PHE:HE2	1:A:76:ASP:OD2	2.03	0.42
1:A:371:ALA:O	1:A:372:VAL:C	2.63	0.42
2:B:50:ILE:CG2	2:B:145:GLN:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:LEU:HD23	2:B:303:LEU:HA	1.88	0.42
1:A:20:LYS:HB2	1:A:20:LYS:NZ	2.33	0.42
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.54	0.42
1:A:366:LYS:HZ3	2:B:394:GLN:HE21	1.68	0.42
1:A:181:TYR:CE1	2:B:138:GLU:HB3	2.54	0.42
1:A:208:HIS:HE1	1:A:212:TRP:HE1	1.60	0.42
1:A:454:LYS:HA	1:A:467:VAL:O	2.19	0.42
1:A:202:ILE:CG2	1:A:206:ARG:NH2	2.82	0.42
1:A:399:GLU:O	1:A:400:THR:C	2.61	0.42
2:B:242:GLN:NE2	2:B:243:PRO:HD2	2.34	0.42
2:B:380:ILE:O	2:B:384:GLY:CA	2.68	0.42
1:A:89:GLU:OE2	1:A:91:GLN:HB2	2.19	0.42
1:A:279:LEU:HD23	1:A:302:GLU:OE2	2.20	0.42
1:A:521:ILE:O	1:A:525:LEU:HG	2.20	0.42
1:A:389:PHE:HB2	1:A:414:TRP:HB3	2.01	0.41
2:B:26:LEU:HD13	2:B:31:ILE:HD13	2.01	0.41
1:A:341:ILE:N	1:A:350:LYS:O	2.49	0.41
1:A:517:LEU:HA	1:A:520:GLN:HG2	2.01	0.41
1:A:26:LEU:HG	1:A:133:PRO:HG2	2.02	0.41
1:A:379:SER:HA	1:A:383:TRP:CE3	2.54	0.41
2:B:175:ASN:HD21	2:B:201:LYS:CE	2.29	0.41
1:A:8:VAL:HG21	1:A:159:ILE:HG12	2.02	0.41
1:A:504:GLY:O	1:A:507:GLN:N	2.54	0.41
1:A:508:ALA:O	1:A:509:GLN:C	2.63	0.41
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.55	0.41
1:A:64:LYS:HB2	1:A:71:TRP:CH2	2.56	0.41
1:A:253:THR:HB	1:A:256:ASP:OD2	2.19	0.41
1:A:520:GLN:HG2	1:A:520:GLN:H	1.66	0.41
2:B:64:LYS:C	2:B:68:SER:HB2	2.46	0.41
2:B:252:TRP:HE3	2:B:256:ASP:HB3	1.84	0.41
1:A:325:LEU:HD23	1:A:325:LEU:HA	1.96	0.41
1:A:465:LYS:HG3	1:A:466:VAL:H	1.81	0.41
1:A:516:GLU:O	1:A:520:GLN:HG2	2.21	0.41
1:A:538:ALA:C	1:A:540:LYS:H	2.28	0.41
2:B:84:THR:O	2:B:154:LYS:NZ	2.54	0.41
2:B:103:LYS:HD3	2:B:103:LYS:HA	1.79	0.41
2:B:120:LEU:HD22	2:B:125:ARG:HG3	2.02	0.41
2:B:349:LEU:HD23	2:B:349:LEU:HA	1.84	0.41
1:A:220:LYS:HE3	1:A:221:HIS:NE2	2.35	0.41
1:A:238:LYS:HA	1:A:316:GLY:O	2.20	0.41
1:A:358:ARG:O	1:A:358:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:PRO:HB3	1:A:421:PRO:HA	2.01	0.41
1:A:520:GLN:O	1:A:523:GLU:HB2	2.21	0.41
2:B:43:LYS:C	2:B:45:GLY:H	2.28	0.41
1:A:23:GLN:HG3	1:A:133:PRO:HG3	2.03	0.41
1:A:121:ASP:N	3:A:1012:HOH:O	2.54	0.41
2:B:65:LYS:HB2	2:B:68:SER:OG	2.21	0.41
2:B:174:GLN:HE21	2:B:174:GLN:CA	2.32	0.41
2:B:216:THR:N	2:B:217:PRO:HD3	2.36	0.41
1:A:60:VAL:HG23	1:A:75:VAL:HG22	2.02	0.41
1:A:77:PHE:HB2	1:A:152:GLY:O	2.21	0.41
1:A:286:THR:HG22	1:A:293:ILE:HD11	2.02	0.41
1:A:297:GLU:O	1:A:300:GLU:HB2	2.21	0.41
1:A:309:ILE:H	1:A:309:ILE:HG12	1.70	0.41
1:A:379:SER:HA	1:A:383:TRP:HE3	1.84	0.41
2:B:22:LYS:HB2	2:B:22:LYS:HE2	1.93	0.41
2:B:92:LEU:CD1	2:B:161:GLN:HB3	2.44	0.41
2:B:326:ILE:O	2:B:341:ILE:HA	2.21	0.41
2:B:431:LYS:HG2	2:B:432:GLU:N	2.36	0.41
1:A:135:ILE:HG22	1:A:136:ASN:N	2.36	0.41
2:B:320:ASP:HA	2:B:321:PRO:HD2	1.88	0.41
1:A:173:LYS:HE2	1:A:173:LYS:HB3	1.91	0.40
2:B:77:PHE:O	2:B:80:LEU:N	2.51	0.40
2:B:174:GLN:O	2:B:174:GLN:NE2	2.54	0.40
2:B:206:ARG:HG2	2:B:216:THR:HB	2.04	0.40
2:B:342:TYR:HB3	2:B:348:ASN:HA	2.03	0.40
1:A:219:LYS:HA	1:A:219:LYS:CE	2.51	0.40
1:A:438:GLU:CD	1:A:440:PHE:CE1	2.99	0.40
1:A:453:GLY:O	1:A:469:LEU:N	2.49	0.40
1:A:491:LEU:O	1:A:528:LYS:HB3	2.21	0.40
2:B:50:ILE:HG23	2:B:145:GLN:HB2	2.04	0.40
2:B:341:ILE:HD12	2:B:341:ILE:N	2.36	0.40
1:A:5:ILE:CD1	1:A:166:LYS:HD2	2.52	0.40
1:A:417:VAL:O	1:A:417:VAL:HG13	2.20	0.40
2:B:5:ILE:HG12	2:B:119:PRO:HD2	2.02	0.40
1:A:84:THR:O	1:A:85:GLN:O	2.38	0.40
2:B:47:ILE:HB	2:B:145:GLN:O	2.21	0.40
2:B:145:GLN:NE2	3:B:1175:HOH:O	2.54	0.40
2:B:246:LEU:HD12	2:B:307:ARG:HG2	2.03	0.40
1:A:57:ASN:ND2	1:A:58:THR:N	2.70	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	540/560 (96%)	458 (85%)	65 (12%)	17 (3%)	3	2
2	B	422/440 (96%)	365 (86%)	44 (10%)	13 (3%)	3	2
All	All	962/1000 (96%)	823 (86%)	109 (11%)	30 (3%)	3	2

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	85	GLN
2	B	98	ALA
1	A	14	PRO
1	A	268	SER
2	B	114	ALA
2	B	360	ALA
2	B	438	GLU
1	A	66	LYS
1	A	91	GLN
1	A	399	GLU
2	B	65	LYS
2	B	213	GLY
1	A	112	GLY
1	A	229	TRP
1	A	247	PRO
1	A	313	PRO
1	A	505	ILE
2	B	5	ILE
1	A	176	PRO
2	B	4	PRO
2	B	91	GLN
2	B	214	LEU
2	B	430	GLU
1	A	122	GLU

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Mol	Chain	Res	Type
1	A	236	PRO
2	B	356	ARG
1	A	235	HIS
1	A	93	GLY
2	B	381	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	485/499 (97%)	387 (80%)	98 (20%)	1	1
2	B	386/400 (96%)	324 (84%)	62 (16%)	2	2
All	All	871/899 (97%)	711 (82%)	160 (18%)	1	1

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	7	THR
1	A	14	PRO
1	A	16	MET
1	A	20	LYS
1	A	21	VAL
1	A	39	THR
1	A	41	MET
1	A	58	THR
1	A	65	LYS
1	A	66	LYS
1	A	68	SER
1	A	69	THR
1	A	70	LYS
1	A	73	LYS
1	A	78	ARG
1	A	80	LEU
1	A	83	ARG

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Mol	Chain	Res	Type
1	A	88	TRP
1	A	89	GLU
1	A	92	LEU
1	A	97	PRO
1	A	101	LYS
1	A	102	LYS
1	A	109	LEU
1	A	116	PHE
1	A	122	GLU
1	A	135	ILE
1	A	136	ASN
1	A	148	VAL
1	A	161	GLN
1	A	168	LEU
1	A	174	GLN
1	A	182	GLN
1	A	185	ASP
1	A	186	ASP
1	A	187	LEU
1	A	195	ILE
1	A	202	ILE
1	A	205	LEU
1	A	210	LEU
1	A	211	ARG
1	A	219	LYS
1	A	221	HIS
1	A	222	GLN
1	A	228	LEU
1	A	229	TRP
1	A	230	MET
1	A	245	VAL
1	A	253	THR
1	A	263	LYS
1	A	264	LEU
1	A	276	VAL
1	A	279	LEU
1	A	282	LEU
1	A	283	LEU
1	A	289	LEU
1	A	295	LEU
1	A	297	GLU
1	A	303	LEU

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Mol	Chain	Res	Type
1	A	309	ILE
1	A	312	GLU
1	A	314	VAL
1	A	317	VAL
1	A	323	LYS
1	A	325	LEU
1	A	330	GLN
1	A	331	LYS
1	A	332	GLN
1	A	334	GLN
1	A	340	GLN
1	A	348	ASN
1	A	356	ARG
1	A	358	ARG
1	A	362	THR
1	A	368	LEU
1	A	369	THR
1	A	373	GLN
1	A	386	THR
1	A	388	LYS
1	A	393	ILE
1	A	400	THR
1	A	419	THR
1	A	420	PRO
1	A	423	VAL
1	A	424	LYS
1	A	431	LYS
1	A	442	VAL
1	A	459	THR
1	A	465	LYS
1	A	488	ASP
1	A	489	SER
1	A	493	VAL
1	A	496	VAL
1	A	515	SER
1	A	517	LEU
1	A	528	LYS
1	A	533	LEU
2	B	5	ILE
2	B	8	VAL
2	B	10	VAL
2	B	22	LYS

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Mol	Chain	Res	Type
2	B	26	LEU
2	B	29	GLU
2	B	31	ILE
2	B	39	THR
2	B	53	GLU
2	B	69	THR
2	B	70	LYS
2	B	74	LEU
2	B	85	GLN
2	B	91	GLN
2	B	92	LEU
2	B	101	LYS
2	B	109	LEU
2	B	113	ASP
2	B	116	PHE
2	B	139	THR
2	B	163	SER
2	B	164	MET
2	B	165	THR
2	B	166	LYS
2	B	173	LYS
2	B	174	GLN
2	B	180	ILE
2	B	186	ASP
2	B	187	LEU
2	B	192	ASP
2	B	194	GLU
2	B	195	ILE
2	B	210	LEU
2	B	212	TRP
2	B	214	LEU
2	B	216	THR
2	B	233	GLU
2	B	240	THR
2	B	241	VAL
2	B	243	PRO
2	B	245	VAL
2	B	249	LYS
2	B	283	LEU
2	B	289	LEU
2	B	290	THR
2	B	292	VAL

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Mol	Chain	Res	Type
2	B	297	GLU
2	B	301	LEU
2	B	314	VAL
2	B	317	VAL
2	B	341	ILE
2	B	347	LYS
2	B	353	LYS
2	B	354	TYR
2	B	368	LEU
2	B	369	THR
2	B	392	PRO
2	B	405	TYR
2	B	409	THR
2	B	425	LEU
2	B	429	LEU
2	B	434	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	136	ASN
1	A	145	GLN
1	A	175	ASN
1	A	197	GLN
1	A	208	HIS
1	A	235	HIS
1	A	242	GLN
1	A	278	GLN
1	A	315	HIS
1	A	334	GLN
1	A	418	ASN
1	A	474	ASN
1	A	487	GLN
1	A	524	GLN
2	B	57	ASN
2	B	85	GLN
2	B	137	ASN
2	B	145	GLN
2	B	147	ASN
2	B	161	GLN
2	B	174	GLN

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Mol	Chain	Res	Type
2	B	175	ASN
2	B	242	GLN
2	B	269	GLN
2	B	278	GLN
2	B	394	GLN
2	B	418	ASN
2	B	428	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](#)

1 non-standard protein/DNA/RNA residue is 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
1	CSD	A	280	1	4,7,8	2.68	2 (50%)	1,8,10	10.93	1 (100%)

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
1	CSD	A	280	1	-	2/2/6/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	OD1-SG	4.71	1.51	1.47
1	A	280	CSD	CB-SG	2.02	1.90	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	10.93	125.73	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.