



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 08:24 AM GMT

PDB ID : 3IS9
Title : Crystal structure of the HIV-1 reverse transcriptase (RT) in complex with the alkenyldiarylmethane (ADAM) Non-nucleoside RT Inhibitor dimethyl 3,3'-(6-methoxy-6-oxohex-1-ene-1,1-diyl)bis(5-cyano-6-methoxybenzoate).
Authors : Ho, W.C.; Bauman, J.D.; Das, K.; Arnold, E.
Deposited on : 2009-08-25
Resolution : 2.55 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

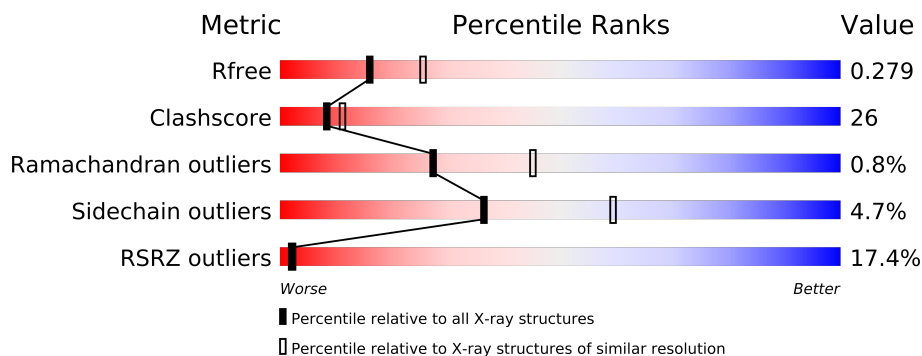
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



The reported resolution of this entry is 2.55 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}	66092	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	558	
2	B	428	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	AC7	A	556	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8103 atoms, of which 0 are hydrogen and 0 are deuterium.

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/ribonucleaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4501	2913	748	833	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P03366
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered	UNP P03366
A	173	ALA	LYS	engineered	UNP P03366
A	280	SER	CYS	engineered	UNP P03366

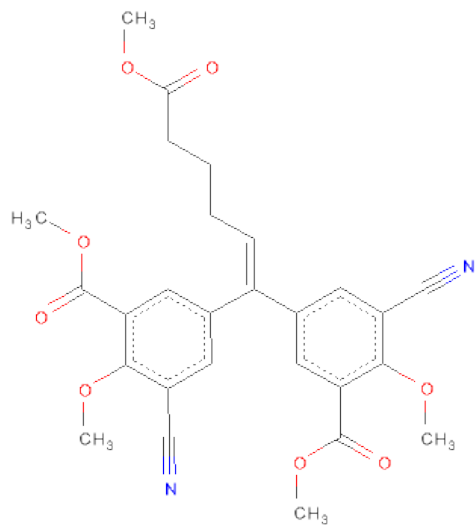
- Molecule 2 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	416	Total	C	N	O	S	0	0	0
			3441	2244	568	622	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered	UNP P03366

- Molecule 3 is DIMETHYL 3,3'-(6-METHOXY-6-OXOHEX-1-ENE-1,1-DIYL)BIS(5-CYAN O-6-METHOXYBENZOATE) (three-letter code: AC7) (formula: C₂₇H₂₆N₂O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			37	27	2	8		

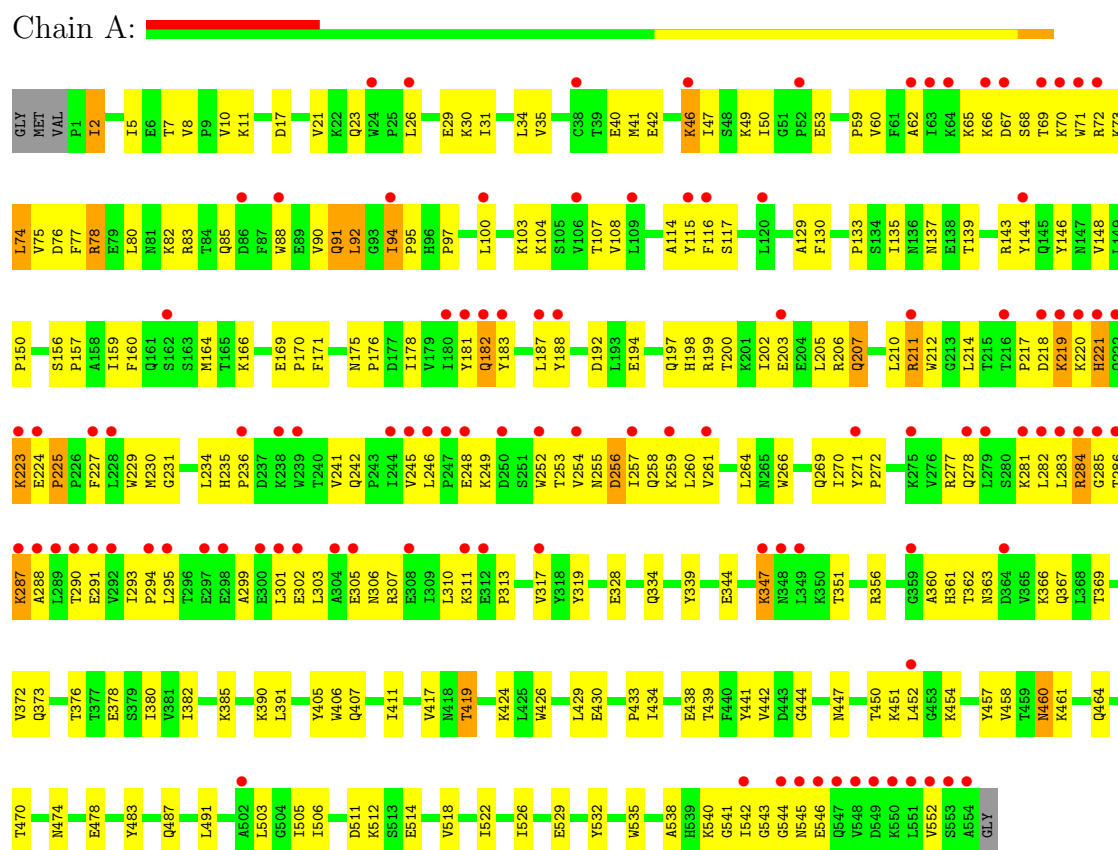
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	65	Total	O	0	0
			65	65		
4	B	59	Total	O	0	0
			59	59		

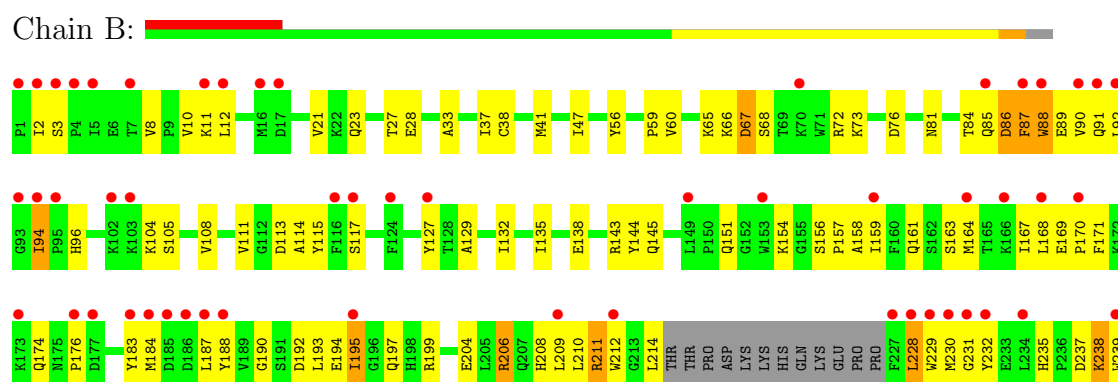
3 Residue-property plots

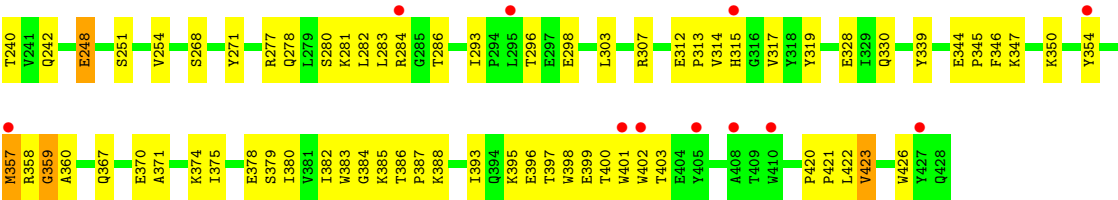
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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/ribonucleaseH



• Molecule 2: Reverse transcriptase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.82Å 73.73Å 108.69Å 90.00° 99.55° 90.00°	Depositor
Resolution (Å)	40.00 – 2.55 35.04 – 2.74	Depositor EDS
% Data completeness (in resolution range)	98.6 (40.00-2.55) 85.9 (35.04-2.74)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.72Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.250 , 0.282 0.267 , 0.279	Depositor DCC
R_{free} test set	1414 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 28872 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8103	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AC7

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	0.41	0/4619	0.63	0/6278
2	B	0.42	0/3541	0.63	0/4810
All	All	0.41	0/8160	0.63	0/11088

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4501	0	4554	244	0
2	B	3441	0	3476	198	0
3	A	37	0	26	3	0
4	A	65	0	0	3	0
4	B	59	0	0	2	0
All	All	8103	0	8056	421	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (421) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:220:LYS:O	1:A:221:HIS:CG	2.04	1.11
1:A:430:GLU:HG3	1:A:434:ILE:HD11	1.33	1.10
1:A:542:ILE:HD12	2:B:283:LEU:HD12	1.35	1.09
1:A:223:LYS:HD3	3:A:556:AC7:H25	1.37	1.04
2:B:238:LYS:HD3	2:B:239:TRP:CD1	1.92	1.04
2:B:400:THR:CG2	2:B:401:TRP:NE1	2.22	1.02
1:A:542:ILE:HD12	2:B:283:LEU:CD1	1.91	1.00
1:A:541:GLY:HA2	1:A:546:GLU:HG3	1.47	0.95
1:A:542:ILE:CD1	2:B:283:LEU:HD12	1.96	0.94
2:B:357:MET:HG3	2:B:358:ARG:N	1.80	0.93
2:B:357:MET:SD	2:B:370:GLU:OE1	2.30	0.90
2:B:11:LYS:H	2:B:85:GLN:HE21	1.18	0.90
1:A:441:TYR:HB3	1:A:544:GLY:O	1.72	0.89
1:A:544:GLY:CA	2:B:286:THR:HG22	2.03	0.88
1:A:544:GLY:HA2	2:B:286:THR:CG2	2.05	0.87
2:B:400:THR:HG21	2:B:401:TRP:NE1	1.90	0.86
1:A:544:GLY:HA3	2:B:286:THR:HG22	1.54	0.86
2:B:238:LYS:HG2	2:B:239:TRP:N	1.91	0.85
1:A:223:LYS:HD3	3:A:556:AC7:C25	2.06	0.85
2:B:2:ILE:O	2:B:117:SER:HB2	1.77	0.85
1:A:220:LYS:O	1:A:221:HIS:CD2	2.29	0.84
2:B:400:THR:HG22	2:B:401:TRP:NE1	1.94	0.83
1:A:254:VAL:HB	1:A:290:THR:HA	1.61	0.83
1:A:503:LEU:HD11	1:A:535:TRP:HB2	1.60	0.82
2:B:354:TYR:OH	2:B:357:MET:SD	2.36	0.82
1:A:70:LYS:HG2	1:A:71:TRP:H	1.44	0.82
1:A:458:VAL:HG12	1:A:464:GLN:HG2	1.60	0.81
2:B:238:LYS:CD	2:B:239:TRP:CD1	2.64	0.81
2:B:400:THR:HB	2:B:401:TRP:CD1	2.15	0.81
1:A:2:ILE:HD13	1:A:2:ILE:H	1.46	0.81
1:A:23:GLN:HA	1:A:23:GLN:HE21	1.45	0.80
1:A:253:THR:H	1:A:256:ASP:HB2	1.44	0.79
1:A:94:ILE:H	1:A:94:ILE:HD13	1.45	0.79
1:A:220:LYS:O	1:A:221:HIS:ND1	2.16	0.79
1:A:426:TRP:HB3	1:A:526:ILE:CD1	2.13	0.78
1:A:541:GLY:CA	1:A:546:GLU:HG3	2.14	0.78
2:B:206:ARG:HH11	2:B:206:ARG:HB2	1.48	0.78
1:A:220:LYS:C	1:A:221:HIS:ND1	2.38	0.77
1:A:543:GLY:HA2	1:A:546:GLU:HB2	1.64	0.77
2:B:8:VAL:HB	2:B:159:ILE:HD12	1.67	0.77
1:A:544:GLY:CA	2:B:286:THR:CG2	2.63	0.77
1:A:543:GLY:C	1:A:545:ASN:H	1.86	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:96:HIS:CE1	2:B:384:GLY:N	2.52	0.77
1:A:194:GLU:HG3	1:A:197:GLN:HE21	1.50	0.76
2:B:354:TYR:OH	2:B:357:MET:HG2	1.86	0.76
2:B:170:PRO:HB2	2:B:208:HIS:CE1	2.20	0.76
1:A:206:ARG:NH2	1:A:218:ASP:HA	2.01	0.75
1:A:439:THR:H	1:A:460:ASN:ND2	1.85	0.75
2:B:163:SER:O	2:B:167:ILE:HG13	1.87	0.75
2:B:359:GLY:HA3	2:B:367:GLN:HG3	1.66	0.75
2:B:402:TRP:CE2	2:B:403:THR:HG23	2.20	0.75
2:B:400:THR:HG22	2:B:401:TRP:CE2	2.20	0.75
1:A:376:THR:HG21	2:B:401:TRP:CZ2	2.22	0.74
1:A:543:GLY:H	1:A:546:GLU:HG2	1.50	0.74
2:B:238:LYS:HD3	2:B:239:TRP:NE1	2.02	0.74
2:B:354:TYR:OH	2:B:357:MET:CG	2.36	0.74
1:A:503:LEU:CD1	1:A:535:TRP:HB2	2.18	0.73
1:A:317:VAL:HG11	1:A:347:LYS:HG3	1.68	0.73
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.03	0.73
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.70	0.73
1:A:266:TRP:O	1:A:269:GLN:HG2	1.89	0.73
1:A:543:GLY:H	1:A:546:GLU:CG	2.02	0.73
2:B:33:ALA:O	2:B:37:ILE:HG12	1.87	0.72
1:A:66:LYS:O	1:A:67:ASP:HB2	1.89	0.72
2:B:400:THR:CG2	2:B:401:TRP:CD1	2.72	0.72
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.72	0.72
1:A:220:LYS:C	1:A:221:HIS:CG	2.62	0.72
2:B:400:THR:HG22	2:B:401:TRP:CD1	2.25	0.71
2:B:11:LYS:H	2:B:85:GLN:NE2	1.87	0.71
1:A:458:VAL:HG23	2:B:286:THR:HG21	1.70	0.71
1:A:277:ARG:NH1	1:A:334:GLN:HB3	2.05	0.70
2:B:89:GLU:HB2	2:B:91:GLN:HE21	1.55	0.70
1:A:220:LYS:O	1:A:221:HIS:CE1	2.45	0.69
1:A:285:GLY:O	1:A:286:THR:HG23	1.93	0.69
1:A:26:LEU:HB2	1:A:31:ILE:HD11	1.75	0.69
1:A:424:LYS:HB2	4:A:580:HOH:O	1.92	0.69
2:B:240:THR:O	2:B:350:LYS:HD2	1.92	0.69
2:B:254:VAL:HG22	2:B:293:ILE:HD11	1.75	0.69
1:A:69:THR:CG2	1:A:70:LYS:N	2.56	0.69
1:A:219:LYS:HD2	1:A:219:LYS:H	1.57	0.69
2:B:400:THR:HG21	2:B:401:TRP:HE1	1.58	0.68
2:B:357:MET:HG3	2:B:358:ARG:H	1.56	0.68
1:A:444:GLY:HA2	1:A:552:VAL:HG11	1.75	0.68
1:A:441:TYR:CB	1:A:544:GLY:O	2.42	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:69:THR:HG22	1:A:70:LYS:N	2.09	0.67
1:A:426:TRP:HB3	1:A:526:ILE:HD11	1.77	0.67
2:B:359:GLY:HA3	2:B:367:GLN:CG	2.24	0.67
2:B:358:ARG:O	2:B:360:ALA:N	2.27	0.67
1:A:285:GLY:O	1:A:286:THR:CG2	2.42	0.67
2:B:65:LYS:HD3	2:B:230:MET:SD	2.35	0.67
2:B:423:VAL:HG12	2:B:426:TRP:CZ3	2.29	0.67
1:A:31:ILE:O	1:A:35:VAL:HG23	1.95	0.67
2:B:400:THR:CB	2:B:401:TRP:CD1	2.77	0.67
1:A:257:ILE:O	1:A:261:VAL:HG23	1.95	0.67
2:B:371:ALA:O	2:B:375:ILE:HG12	1.96	0.66
1:A:307:ARG:O	1:A:311:LYS:HB2	1.96	0.66
1:A:444:GLY:CA	1:A:552:VAL:HG11	2.25	0.66
1:A:373:GLN:HE22	2:B:397:THR:HG23	1.61	0.66
2:B:94:ILE:HG12	2:B:94:ILE:O	1.96	0.65
2:B:206:ARG:HB2	2:B:206:ARG:NH1	2.11	0.65
1:A:277:ARG:HH11	1:A:334:GLN:HB3	1.61	0.65
1:A:426:TRP:HB3	1:A:526:ILE:HD12	1.77	0.65
2:B:358:ARG:C	2:B:360:ALA:N	2.50	0.64
1:A:219:LYS:N	1:A:219:LYS:HD2	2.13	0.64
2:B:402:TRP:CE2	2:B:403:THR:CG2	2.81	0.64
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.79	0.64
1:A:356:ARG:HD3	1:A:367:GLN:NE2	2.12	0.64
1:A:129:ALA:HA	1:A:144:TYR:O	1.98	0.64
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.28	0.63
2:B:400:THR:CG2	2:B:401:TRP:CE2	2.80	0.63
1:A:65:LYS:HE3	1:A:68:SER:HB3	1.80	0.63
1:A:73:LYS:HE3	1:A:75:VAL:HG23	1.81	0.63
2:B:210:LEU:O	2:B:210:LEU:HD23	1.99	0.62
1:A:23:GLN:HA	1:A:23:GLN:NE2	2.13	0.62
2:B:87:PHE:CD2	2:B:158:ALA:CB	2.82	0.62
2:B:67:ASP:OD1	2:B:67:ASP:C	2.37	0.62
1:A:42:GLU:OE1	1:A:49:LYS:HG3	2.00	0.62
2:B:358:ARG:C	2:B:360:ALA:H	2.02	0.62
2:B:193:LEU:HB3	2:B:197:GLN:HG3	1.82	0.62
1:A:454:LYS:O	1:A:552:VAL:HG13	2.00	0.61
2:B:72:ARG:NH2	2:B:151:GLN:NE2	2.48	0.61
1:A:369:THR:O	1:A:373:GLN:HG2	2.00	0.61
2:B:357:MET:SD	2:B:370:GLU:CD	2.79	0.61
1:A:199:ARG:O	1:A:203:GLU:HG2	2.00	0.61
1:A:474:ASN:O	1:A:478:GLU:HG3	2.01	0.61
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.64	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.81	0.61
2:B:380:ILE:HD11	2:B:386:THR:HG22	1.83	0.60
2:B:238:LYS:CG	2:B:239:TRP:N	2.60	0.60
1:A:373:GLN:NE2	2:B:397:THR:HA	2.15	0.60
1:A:272:PRO:HG3	1:A:351:THR:HG21	1.84	0.60
2:B:229:TRP:CE3	2:B:229:TRP:O	2.54	0.60
1:A:2:ILE:CD1	1:A:2:ILE:H	2.13	0.60
1:A:260:LEU:O	1:A:264:LEU:HB2	2.01	0.60
2:B:281:LYS:HD2	2:B:284:ARG:NH1	2.17	0.60
1:A:107:THR:HG22	1:A:108:VAL:N	2.17	0.60
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.84	0.59
1:A:253:THR:H	1:A:256:ASP:CB	2.14	0.59
2:B:194:GLU:HG2	2:B:197:GLN:HG2	1.84	0.59
1:A:543:GLY:C	1:A:545:ASN:N	2.54	0.59
2:B:229:TRP:O	2:B:229:TRP:CD2	2.56	0.59
1:A:287:LYS:NZ	1:A:287:LYS:HB3	2.17	0.58
2:B:209:LEU:O	2:B:214:LEU:HB2	2.03	0.58
1:A:182:GLN:HB3	1:A:187:LEU:CD2	2.33	0.58
2:B:238:LYS:CG	2:B:239:TRP:CD1	2.86	0.58
1:A:107:THR:OG1	1:A:202:ILE:HD11	2.04	0.58
1:A:285:GLY:C	1:A:286:THR:HG23	2.24	0.58
1:A:258:GLN:HB2	1:A:283:LEU:HD22	1.85	0.58
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.85	0.58
1:A:65:LYS:HE3	1:A:68:SER:CB	2.34	0.57
1:A:17:ASP:O	1:A:83:ARG:HD3	2.05	0.57
2:B:87:PHE:CD2	2:B:158:ALA:HB1	2.40	0.57
1:A:92:LEU:HD12	1:A:92:LEU:O	2.03	0.57
1:A:224:GLU:HA	1:A:227:PHE:HE2	1.69	0.57
1:A:31:ILE:CD1	1:A:133:PRO:HG2	2.33	0.57
1:A:73:LYS:NZ	1:A:130:PHE:CZ	2.72	0.57
1:A:417:VAL:HG22	1:A:419:THR:HG22	1.86	0.57
2:B:238:LYS:HG2	2:B:239:TRP:CD1	2.40	0.57
2:B:357:MET:CG	2:B:358:ARG:H	2.18	0.56
1:A:303:LEU:O	1:A:306:ASN:HB2	2.04	0.56
1:A:277:ARG:HH11	1:A:277:ARG:HG2	1.71	0.56
2:B:183:TYR:CE2	2:B:184:MET:HG2	2.41	0.56
2:B:10:VAL:HA	2:B:85:GLN:NE2	2.21	0.56
2:B:208:HIS:O	2:B:211:ARG:HG2	2.06	0.56
2:B:277:ARG:NH1	2:B:281:LYS:HZ2	2.03	0.56
1:A:175:ASN:O	1:A:178:ILE:HG13	2.06	0.55
1:A:278:GLN:HB2	1:A:302:GLU:OE2	2.05	0.55
1:A:458:VAL:CG2	2:B:286:THR:HG21	2.35	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:167:ILE:HG22	2:B:167:ILE:O	2.06	0.55
2:B:402:TRP:CZ2	2:B:403:THR:CG2	2.89	0.55
1:A:293:ILE:CG2	1:A:294:PRO:HD2	2.36	0.55
2:B:135:ILE:O	2:B:138:GLU:HG3	2.07	0.55
2:B:68:SER:H	2:B:230:MET:CE	2.20	0.55
1:A:31:ILE:HD11	1:A:133:PRO:HG2	1.88	0.54
2:B:240:THR:O	2:B:350:LYS:HA	2.06	0.54
1:A:361:HIS:NE2	1:A:505:ILE:HD12	2.22	0.54
2:B:402:TRP:CZ2	2:B:403:THR:HG22	2.43	0.54
1:A:107:THR:HG22	1:A:108:VAL:H	1.72	0.54
1:A:366:LYS:HE2	1:A:405:TYR:OH	2.08	0.54
1:A:94:ILE:HD13	1:A:94:ILE:N	2.20	0.54
2:B:206:ARG:HH21	2:B:229:TRP:HA	1.73	0.54
2:B:96:HIS:CD2	2:B:383:TRP:HA	2.43	0.53
1:A:429:LEU:HD11	1:A:506:ILE:CG2	2.37	0.53
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.89	0.53
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.24	0.53
1:A:53:GLU:CD	1:A:53:GLU:H	2.11	0.53
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.90	0.53
1:A:97:PRO:HA	1:A:100:LEU:HG	1.91	0.53
1:A:74:LEU:HD13	1:A:74:LEU:O	2.09	0.53
1:A:246:LEU:HB3	1:A:307:ARG:HH12	1.74	0.53
1:A:46:LYS:HD3	1:A:116:PHE:CD1	2.44	0.53
2:B:396:GLU:H	2:B:396:GLU:CD	2.13	0.53
2:B:72:ARG:HH11	2:B:72:ARG:HG2	1.73	0.53
2:B:239:TRP:O	2:B:242:GLN:NE2	2.42	0.53
1:A:2:ILE:HD13	1:A:2:ILE:N	2.20	0.53
1:A:483:TYR:O	1:A:487:GLN:HG3	2.09	0.53
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.08	0.52
1:A:10:VAL:HG12	1:A:11:LYS:N	2.24	0.52
2:B:113:ASP:HB2	2:B:228:LEU:HD21	1.91	0.52
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.10	0.52
1:A:114:ALA:CB	1:A:214:LEU:HD22	2.40	0.52
2:B:96:HIS:CE1	2:B:384:GLY:CA	2.93	0.52
1:A:73:LYS:HE3	1:A:75:VAL:CG2	2.39	0.52
2:B:11:LYS:N	2:B:85:GLN:HE21	1.99	0.52
1:A:225:PRO:HB3	1:A:235:HIS:ND1	2.25	0.52
1:A:70:LYS:CG	1:A:71:TRP:H	2.19	0.52
2:B:3:SER:HA	2:B:117:SER:O	2.10	0.51
2:B:47:ILE:HD12	2:B:144:TYR:CD2	2.45	0.51
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.45	0.51
1:A:211:ARG:HG2	1:A:211:ARG:NH1	2.24	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.50	0.51
2:B:56:TYR:O	2:B:129:ALA:HB3	2.09	0.51
2:B:88:TRP:O	2:B:89:GLU:C	2.48	0.51
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.40	0.51
2:B:174:GLN:O	2:B:176:PRO:HD3	2.10	0.51
2:B:169:GLU:OE2	2:B:169:GLU:HA	2.10	0.51
1:A:257:ILE:HA	1:A:260:LEU:HB3	1.93	0.51
2:B:68:SER:H	2:B:230:MET:HE3	1.76	0.50
1:A:378:GLU:O	1:A:382:ILE:HG12	2.10	0.50
1:A:542:ILE:O	1:A:542:ILE:HG22	2.10	0.50
1:A:245:VAL:HG13	1:A:245:VAL:O	2.12	0.50
1:A:229:TRP:CE2	1:A:230:MET:HG2	2.47	0.50
1:A:91:GLN:NE2	1:A:183:TYR:HE1	2.09	0.50
1:A:207:GLN:O	1:A:210:LEU:HB3	2.11	0.50
1:A:206:ARG:HH22	1:A:218:ASP:HA	1.74	0.50
2:B:423:VAL:HG12	2:B:426:TRP:HZ3	1.73	0.50
2:B:156:SER:N	2:B:157:PRO:HD2	2.26	0.50
1:A:328:GLU:O	1:A:339:TYR:HA	2.12	0.49
2:B:254:VAL:HG22	2:B:293:ILE:CD1	2.41	0.49
1:A:117:SER:HB2	1:A:214:LEU:CD2	2.42	0.49
1:A:225:PRO:HG3	1:A:236:PRO:HD3	1.94	0.49
2:B:167:ILE:HG12	2:B:212:TRP:CE3	2.47	0.49
2:B:89:GLU:C	2:B:91:GLN:H	2.15	0.49
2:B:239:TRP:O	2:B:240:THR:C	2.51	0.49
1:A:544:GLY:HA2	2:B:286:THR:HG23	1.89	0.49
1:A:356:ARG:HH11	1:A:362:THR:HG21	1.78	0.49
1:A:295:LEU:HD12	1:A:295:LEU:N	2.27	0.49
2:B:317:VAL:HG22	2:B:347:LYS:HD2	1.94	0.49
2:B:400:THR:HB	2:B:401:TRP:HD1	1.74	0.49
2:B:84:THR:O	2:B:85:GLN:C	2.51	0.49
1:A:90:VAL:O	1:A:90:VAL:HG22	2.13	0.49
1:A:178:ILE:HD12	1:A:178:ILE:C	2.33	0.49
2:B:395:LYS:HE2	2:B:399:GLU:OE1	2.13	0.49
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.77	0.48
2:B:251:SER:HB3	4:B:456:HOH:O	2.13	0.48
2:B:357:MET:CG	2:B:358:ARG:N	2.57	0.48
1:A:255:ASN:HB3	1:A:259:LYS:HD3	1.95	0.48
1:A:249:LYS:HD3	1:A:256:ASP:OD1	2.13	0.48
2:B:67:ASP:O	2:B:68:SER:C	2.52	0.48
2:B:87:PHE:CD2	2:B:158:ALA:HB3	2.47	0.48
1:A:78:ARG:O	1:A:82:LYS:HG3	2.13	0.48
1:A:135:ILE:HD12	1:A:135:ILE:H	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:447:ASN:OD1	1:A:450:THR:HG23	2.13	0.48
2:B:72:ARG:NH2	2:B:151:GLN:HE22	2.11	0.48
1:A:450:THR:O	1:A:451:LYS:HB2	2.13	0.48
2:B:81:ASN:OD1	2:B:154:LYS:N	2.38	0.48
1:A:284:ARG:HG2	1:A:284:ARG:HH11	1.79	0.48
2:B:164:MET:O	2:B:168:LEU:HG	2.14	0.48
1:A:76:ASP:OD1	1:A:78:ARG:HD3	2.13	0.48
1:A:29:GLU:HG3	1:A:30:LYS:N	2.28	0.48
2:B:328:GLU:O	2:B:339:TYR:HA	2.14	0.48
1:A:360:ALA:O	1:A:514:GLU:HG2	2.14	0.48
1:A:224:GLU:HB2	1:A:225:PRO:HD2	1.95	0.48
2:B:280:SER:O	2:B:283:LEU:HB2	2.14	0.47
2:B:248:GLU:HG2	2:B:248:GLU:O	2.13	0.47
1:A:503:LEU:HD13	2:B:422:LEU:CD1	2.44	0.47
2:B:379:SER:OG	2:B:387:PRO:HD3	2.15	0.47
2:B:206:ARG:CB	2:B:206:ARG:HH11	2.25	0.47
2:B:170:PRO:HB2	2:B:208:HIS:HE1	1.74	0.47
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.97	0.47
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.77	0.47
1:A:311:LYS:O	1:A:313:PRO:HD3	2.14	0.47
1:A:417:VAL:O	1:A:417:VAL:HG13	2.14	0.47
2:B:238:LYS:HG2	2:B:239:TRP:CG	2.50	0.47
1:A:116:PHE:O	1:A:148:VAL:HG11	2.15	0.47
2:B:11:LYS:O	2:B:85:GLN:HG2	2.15	0.47
1:A:287:LYS:O	1:A:288:ALA:HB3	2.15	0.47
2:B:312:GLU:HB3	2:B:313:PRO:HD2	1.96	0.47
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.97	0.47
2:B:277:ARG:O	2:B:281:LYS:HG2	2.15	0.46
1:A:391:LEU:C	1:A:417:VAL:HG12	2.35	0.46
2:B:278:GLN:NE2	2:B:298:GLU:HB3	2.30	0.46
2:B:96:HIS:NE2	2:B:383:TRP:CA	2.79	0.46
1:A:454:LYS:HB2	1:A:552:VAL:O	2.15	0.46
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.97	0.46
1:A:66:LYS:O	1:A:67:ASP:CB	2.61	0.46
2:B:67:ASP:OD1	2:B:68:SER:N	2.49	0.46
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.97	0.46
2:B:65:LYS:HB2	2:B:230:MET:SD	2.56	0.46
1:A:77:PHE:O	1:A:80:LEU:N	2.48	0.46
1:A:7:THR:HG23	4:A:610:HOH:O	2.14	0.46
2:B:194:GLU:OE1	2:B:194:GLU:N	2.49	0.46
1:A:278:GLN:O	1:A:282:LEU:HG	2.15	0.46
2:B:10:VAL:HA	2:B:85:GLN:HE22	1.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:85:GLN:O	2:B:85:GLN:HG3	2.16	0.46
1:A:269:GLN:HA	1:A:351:THR:O	2.15	0.46
1:A:255:ASN:O	1:A:259:LYS:HB2	2.16	0.46
1:A:40:GLU:HG3	1:A:41:MET:N	2.31	0.46
2:B:277:ARG:NH1	2:B:281:LYS:NZ	2.64	0.45
1:A:361:HIS:HE2	1:A:505:ILE:HD12	1.80	0.45
2:B:12:LEU:HG	2:B:127:TYR:CE1	2.52	0.45
1:A:257:ILE:O	1:A:260:LEU:HB3	2.16	0.45
1:A:282:LEU:HD13	1:A:295:LEU:HA	1.98	0.45
1:A:181:TYR:HD2	1:A:188:TYR:CD1	2.34	0.45
1:A:199:ARG:HA	1:A:202:ILE:HD12	1.98	0.45
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.98	0.45
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.52	0.45
1:A:546:GLU:OE1	1:A:546:GLU:HA	2.16	0.45
2:B:91:GLN:O	2:B:92:LEU:HB2	2.16	0.45
1:A:278:GLN:O	1:A:299:ALA:HB2	2.17	0.45
2:B:65:LYS:CB	2:B:230:MET:SD	3.04	0.45
2:B:90:VAL:O	2:B:90:VAL:HG12	2.16	0.45
1:A:457:TYR:C	1:A:457:TYR:CD1	2.90	0.45
1:A:217:PRO:O	1:A:219:LYS:NZ	2.42	0.45
1:A:252:TRP:HB3	1:A:257:ILE:HG13	1.97	0.45
1:A:306:ASN:O	1:A:310:LEU:N	2.44	0.45
1:A:160:PHE:CZ	1:A:164:MET:HE2	2.52	0.45
1:A:270:ILE:O	1:A:272:PRO:HD3	2.17	0.45
1:A:277:ARG:NH1	1:A:334:GLN:O	2.50	0.45
1:A:293:ILE:HG23	1:A:294:PRO:HD2	1.97	0.45
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.51	0.45
2:B:169:GLU:C	2:B:171:PHE:H	2.19	0.45
1:A:73:LYS:HE2	1:A:146:TYR:OH	2.16	0.45
2:B:303:LEU:O	2:B:307:ARG:HB2	2.17	0.45
1:A:542:ILE:HD13	2:B:283:LEU:HD12	1.92	0.45
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.98	0.45
1:A:543:GLY:O	1:A:545:ASN:N	2.44	0.45
1:A:23:GLN:HE22	1:A:60:VAL:H	1.66	0.44
1:A:223:LYS:HB2	3:A:556:AC7:H25	1.98	0.44
2:B:8:VAL:O	2:B:10:VAL:HG23	2.17	0.44
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.32	0.44
1:A:8:VAL:HG21	1:A:159:ILE:HG23	1.99	0.44
1:A:543:GLY:CA	1:A:546:GLU:HB2	2.43	0.44
2:B:91:GLN:CD	2:B:161:GLN:HE22	2.19	0.44
2:B:350:LYS:NZ	2:B:378:GLU:OE1	2.50	0.44
1:A:281:LYS:O	1:A:284:ARG:HD2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:277:ARG:NH2	2:B:281:LYS:HZ1	2.15	0.44
2:B:229:TRP:CG	2:B:229:TRP:O	2.71	0.44
2:B:423:VAL:HG12	2:B:426:TRP:CE3	2.52	0.44
1:A:94:ILE:HB	1:A:95:PRO:CD	2.46	0.44
1:A:115:TYR:HA	1:A:160:PHE:CD2	2.53	0.44
1:A:94:ILE:HB	1:A:95:PRO:HD2	2.00	0.44
2:B:76:ASP:OD1	2:B:76:ASP:C	2.55	0.44
2:B:113:ASP:O	2:B:114:ALA:C	2.56	0.44
2:B:108:VAL:O	2:B:231:GLY:HA2	2.18	0.43
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.18	0.43
1:A:542:ILE:HD12	2:B:283:LEU:HD13	1.89	0.43
1:A:246:LEU:CB	1:A:307:ARG:HH12	2.30	0.43
1:A:406:TRP:CE2	1:A:407:GLN:HG3	2.52	0.43
2:B:345:PRO:O	2:B:346:PHE:HB2	2.17	0.43
1:A:231:GLY:O	1:A:242:GLN:HG3	2.18	0.43
1:A:373:GLN:NE2	2:B:397:THR:OG1	2.52	0.43
1:A:287:LYS:HG2	1:A:287:LYS:H	1.58	0.43
2:B:115:TYR:OH	2:B:157:PRO:HA	2.18	0.43
1:A:7:THR:HG21	4:A:612:HOH:O	2.17	0.43
1:A:175:ASN:N	1:A:176:PRO:HD3	2.34	0.43
1:A:253:THR:HA	1:A:291:GLU:O	2.19	0.43
2:B:89:GLU:C	2:B:91:GLN:N	2.72	0.43
2:B:89:GLU:HB3	2:B:91:GLN:HG3	2.01	0.43
2:B:66:LYS:HG3	2:B:67:ASP:H	1.82	0.43
1:A:148:VAL:O	1:A:150:PRO:HD3	2.19	0.43
1:A:390:LYS:HB3	1:A:390:LYS:HE3	1.71	0.43
1:A:50:ILE:HG13	1:A:143:ARG:HB3	2.01	0.43
1:A:26:LEU:HB2	1:A:31:ILE:CD1	2.45	0.43
1:A:442:VAL:HG12	1:A:457:TYR:HB3	2.00	0.43
1:A:541:GLY:C	1:A:546:GLU:HG3	2.39	0.43
1:A:69:THR:CG2	1:A:70:LYS:H	2.30	0.43
2:B:41:MET:CE	2:B:73:LYS:HE2	2.48	0.43
1:A:156:SER:N	1:A:157:PRO:CD	2.82	0.43
1:A:254:VAL:H	1:A:291:GLU:H	1.67	0.42
2:B:251:SER:HA	4:B:484:HOH:O	2.19	0.42
1:A:439:THR:H	1:A:460:ASN:HD21	1.63	0.42
1:A:285:GLY:C	1:A:286:THR:CG2	2.87	0.42
1:A:540:LYS:O	2:B:280:SER:HB3	2.19	0.42
2:B:171:PHE:HE1	2:B:204:GLU:HG2	1.83	0.42
1:A:444:GLY:HA2	1:A:552:VAL:CG1	2.47	0.42
1:A:460:ASN:H	1:A:460:ASN:HD22	1.66	0.42
1:A:246:LEU:HD21	1:A:310:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:PHE:O	1:A:78:ARG:C	2.58	0.42
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.50	0.42
2:B:379:SER:CB	2:B:387:PRO:HD3	2.49	0.42
1:A:518:VAL:O	1:A:522:ILE:HG12	2.20	0.42
1:A:253:THR:N	1:A:256:ASP:HB2	2.22	0.42
2:B:339:TYR:CD1	2:B:375:ILE:HD12	2.55	0.42
1:A:198:HIS:C	1:A:200:THR:N	2.72	0.42
2:B:401:TRP:N	2:B:401:TRP:CD1	2.87	0.42
1:A:103:LYS:HA	1:A:192:ASP:OD1	2.19	0.42
2:B:268:SER:HA	2:B:271:TYR:O	2.20	0.42
2:B:28:GLU:HB2	2:B:135:ILE:HD11	2.02	0.42
1:A:50:ILE:CG1	1:A:143:ARG:HB3	2.49	0.42
2:B:283:LEU:O	2:B:284:ARG:C	2.57	0.42
1:A:171:PHE:CD2	1:A:205:LEU:HD13	2.55	0.42
1:A:223:LYS:O	1:A:224:GLU:HB3	2.20	0.41
1:A:301:LEU:O	1:A:305:GLU:HG3	2.20	0.41
2:B:111:VAL:HG11	2:B:187:LEU:HD22	2.02	0.41
2:B:357:MET:HE2	2:B:357:MET:HB2	1.88	0.41
2:B:357:MET:CG	2:B:370:GLU:OE1	2.68	0.41
1:A:5:ILE:N	1:A:5:ILE:HD12	2.35	0.41
1:A:241:VAL:CG2	1:A:271:TYR:HE1	2.32	0.41
1:A:380:ILE:HD12	2:B:27:THR:HG22	2.03	0.41
1:A:538:ALA:O	1:A:540:LYS:HG2	2.21	0.41
2:B:72:ARG:HH22	2:B:151:GLN:NE2	2.18	0.41
2:B:23:GLN:OE1	2:B:60:VAL:HG12	2.20	0.41
1:A:182:GLN:H	1:A:182:GLN:HG3	1.72	0.41
1:A:210:LEU:C	1:A:212:TRP:H	2.23	0.41
2:B:41:MET:HE3	2:B:73:LYS:HE2	2.03	0.41
2:B:315:HIS:O	2:B:315:HIS:ND1	2.53	0.41
2:B:237:ASP:HB2	2:B:238:LYS:H	1.65	0.41
2:B:232:TYR:OH	2:B:374:LYS:HE2	2.20	0.41
2:B:187:LEU:HA	2:B:187:LEU:HD12	1.87	0.40
2:B:96:HIS:NE2	2:B:382:ILE:C	2.75	0.40
2:B:105:SER:O	2:B:190:GLY:HA2	2.22	0.40
2:B:104:LYS:NZ	2:B:192:ASP:HB3	2.36	0.40
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.56	0.40
1:A:503:LEU:HD12	1:A:535:TRP:CD1	2.56	0.40
1:A:23:GLN:CA	1:A:23:GLN:NE2	2.74	0.40
2:B:211:ARG:HH11	2:B:211:ARG:CB	2.35	0.40
1:A:491:LEU:HB3	1:A:529:GLU:HG3	2.03	0.40
1:A:438:GLU:HG3	1:A:461:LYS:HD3	2.03	0.40
1:A:281:LYS:HD3	1:A:281:LYS:O	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	552/558 (99%)	487 (88%)	62 (11%)	3 (0%)	38 60
2	B	412/428 (96%)	354 (86%)	53 (13%)	5 (1%)	19 31
All	All	964/986 (98%)	841 (87%)	115 (12%)	8 (1%)	27 45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	359	GLY
1	A	92	LEU
2	B	86	ASP
2	B	87	PHE
1	A	85	GLN
1	A	225	PRO
2	B	195	ILE
2	B	423	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	493/495 (100%)	468 (95%)	25 (5%)	33 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	378/390 (97%)	362 (96%)	16 (4%)	40	65
All	All	871/885 (98%)	830 (95%)	41 (5%)	36	59

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	46	LYS
1	A	72	ARG
1	A	74	LEU
1	A	78	ARG
1	A	91	GLN
1	A	94	ILE
1	A	137	ASN
1	A	139	THR
1	A	166	LYS
1	A	182	GLN
1	A	207	GLN
1	A	211	ARG
1	A	219	LYS
1	A	221	HIS
1	A	223	LYS
1	A	248	GLU
1	A	256	ASP
1	A	284	ARG
1	A	287	LYS
1	A	344	GLU
1	A	347	LYS
1	A	419	THR
1	A	460	ASN
1	A	512	LYS
2	B	67	ASP
2	B	86	ASP
2	B	88	TRP
2	B	94	ILE
2	B	145	GLN
2	B	206	ARG
2	B	211	ARG
2	B	228	LEU
2	B	235	HIS
2	B	238	LYS
2	B	248	GLU

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Mol	Chain	Res	Type
2	B	314	VAL
2	B	330	GLN
2	B	344	GLU
2	B	357	MET
2	B	388	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	151	GLN
1	A	197	GLN
1	A	242	GLN
1	A	255	ASN
1	A	332	GLN
1	A	373	GLN
1	A	460	ASN
1	A	475	GLN
1	A	545	ASN
2	B	85	GLN
2	B	91	GLN
2	B	151	GLN
2	B	161	GLN
2	B	174	GLN
2	B	197	GLN
2	B	208	HIS
2	B	242	GLN
2	B	278	GLN
2	B	330	GLN
2	B	340	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand 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	$\# Z > 2$
3	AC7	A	556	-	38,38,38	2.99	15 (39%)	51,51,51	1.71	8 (15%)

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	AC7	A	556	-	-	0/37/37/37	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	556	AC7	C4-C77	-9.93	1.28	1.44
3	A	556	AC7	C11-C82	-8.23	1.31	1.44
3	A	556	AC7	C6-C8	5.33	1.56	1.49
3	A	556	AC7	O5-C7	5.20	1.46	1.33
3	A	556	AC7	O7-C16	4.58	1.44	1.33
3	A	556	AC7	C13-C8	4.00	1.54	1.49
3	A	556	AC7	O3-C20	3.67	1.46	1.32
3	A	556	AC7	C1-C6	3.30	1.44	1.39
3	A	556	AC7	C9-C8	2.86	1.37	1.34
3	A	556	AC7	C12-C13	2.62	1.43	1.39
3	A	556	AC7	C12-C11	2.56	1.43	1.39
3	A	556	AC7	C1-C2	2.24	1.43	1.39
3	A	556	AC7	C5-C6	2.13	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	556	AC7	C2-C3	2.11	1.45	1.40
3	A	556	AC7	C15-C10	2.06	1.44	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	556	AC7	O7-C16-C15	6.95	124.10	112.29
3	A	556	AC7	O5-C7-C2	4.44	119.83	112.29
3	A	556	AC7	C22-O1-C3	3.31	123.96	114.90
3	A	556	AC7	O7-C16-O36	-3.10	116.48	123.39
3	A	556	AC7	O5-C7-O35	-2.25	118.38	123.39
3	A	556	AC7	C19-C18-C17	-2.17	109.17	113.25
3	A	556	AC7	C13-C8-C9	-2.12	118.81	121.88
3	A	556	AC7	C24-O5-C7	2.10	120.46	115.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	554/558 (99%)	1.22	105 (18%) 2 2	29, 78, 144, 186	0
2	B	416/428 (97%)	1.12	64 (15%) 3 2	36, 69, 145, 173	0
All	All	970/986 (98%)	1.18	169 (17%) 2 2	29, 73, 145, 186	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	ILE	16.7
2	B	1	PRO	13.3
2	B	230	MET	12.3
2	B	227	PHE	12.1
2	B	90	VAL	11.3
1	A	554	ALA	10.9
1	A	553	SER	10.7
1	A	552	VAL	9.2
1	A	287	LYS	8.7
2	B	92	LEU	8.4
1	A	286	THR	8.3
1	A	547	GLN	7.9
1	A	548	VAL	7.8
2	B	93	GLY	7.8
1	A	551	LEU	7.6
2	B	3	SER	7.4
1	A	549	ASP	6.5
2	B	229	TRP	6.5
1	A	67	ASP	6.4
1	A	301	LEU	6.3
1	A	292	VAL	5.8
2	B	173	LYS	5.6
1	A	220	LYS	5.6
1	A	219	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	218	ASP	5.4
2	B	357	MET	5.3
1	A	24	TRP	5.3
1	A	71	TRP	5.3
1	A	298	GLU	5.3
2	B	16	MET	5.2
1	A	304	ALA	5.2
1	A	257	ILE	5.1
1	A	109	LEU	5.1
2	B	94	ILE	5.1
1	A	282	LEU	5.0
2	B	228	LEU	5.0
1	A	283	LEU	4.9
2	B	85	GLN	4.8
1	A	550	LYS	4.7
1	A	305	GLU	4.7
2	B	166	LYS	4.7
1	A	100	LEU	4.6
1	A	284	ARG	4.5
1	A	221	HIS	4.5
1	A	69	THR	4.5
1	A	63	ILE	4.5
2	B	4	PRO	4.5
1	A	544	GLY	4.4
1	A	278	GLN	4.4
1	A	26	LEU	4.3
1	A	545	ASN	4.3
2	B	87	PHE	4.3
1	A	70	LYS	4.2
1	A	244	ILE	4.2
1	A	216	THR	4.2
2	B	232	TYR	4.1
1	A	182	GLN	4.1
1	A	288	ALA	4.0
2	B	164	MET	4.0
1	A	290	THR	3.9
2	B	212	TRP	3.9
2	B	70	LYS	3.8
2	B	231	GLY	3.7
1	A	183	TYR	3.7
2	B	95	PRO	3.6
2	B	401	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	88	TRP	3.4
2	B	209	LEU	3.4
1	A	546	GLU	3.4
1	A	308	GLU	3.4
1	A	247	PRO	3.4
1	A	291	GLU	3.3
1	A	66	LYS	3.3
1	A	289	LEU	3.3
1	A	252	TRP	3.3
1	A	275	LYS	3.3
1	A	38	CYS	3.2
2	B	5	ILE	3.2
2	B	183	TYR	3.2
1	A	285	GLY	3.2
1	A	261	VAL	3.1
1	A	279	LEU	3.1
2	B	284	ARG	3.1
1	A	228	LEU	3.1
1	A	238	LYS	3.0
2	B	186	ASP	2.9
1	A	223	LYS	2.9
1	A	248	GLU	2.9
2	B	405	TYR	2.9
1	A	281	LYS	2.9
1	A	311	LYS	2.9
2	B	124	PHE	2.9
1	A	115	TYR	2.9
1	A	245	VAL	2.8
1	A	86	ASP	2.8
1	A	542	ILE	2.8
1	A	120	LEU	2.8
1	A	300	GLU	2.8
2	B	239	TRP	2.8
2	B	295	LEU	2.8
2	B	354	TYR	2.7
2	B	427	TYR	2.7
2	B	91	GLN	2.7
1	A	302	GLU	2.7
1	A	52	PRO	2.7
1	A	188	TYR	2.7
1	A	106	VAL	2.6
1	A	46	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	254	VAL	2.6
2	B	185	ASP	2.6
1	A	349	LEU	2.6
2	B	177	ASP	2.6
1	A	317	VAL	2.6
1	A	187	LEU	2.5
1	A	295	LEU	2.5
1	A	180	ILE	2.5
1	A	203	GLU	2.5
1	A	347	LYS	2.5
1	A	181	TYR	2.5
1	A	259	LYS	2.5
2	B	187	LEU	2.5
2	B	168	LEU	2.5
1	A	359	GLY	2.4
1	A	452	LEU	2.4
1	A	297	GLU	2.4
2	B	170	PRO	2.4
1	A	62	ALA	2.4
2	B	17	ASP	2.4
2	B	184	MET	2.4
2	B	410	TRP	2.3
1	A	72	ARG	2.3
1	A	348	ASN	2.3
1	A	162	SER	2.3
2	B	11	LYS	2.3
2	B	176	PRO	2.3
2	B	195	ILE	2.3
1	A	250	ASP	2.3
2	B	12	LEU	2.3
2	B	127	TYR	2.3
1	A	211	ARG	2.3
2	B	159	ILE	2.3
1	A	239	TRP	2.2
1	A	116	PHE	2.2
1	A	364	ASP	2.2
1	A	88	TRP	2.2
2	B	117	SER	2.2
2	B	153	TRP	2.2
1	A	294	PRO	2.1
1	A	312	GLU	2.1
2	B	103	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	188	TYR	2.1
2	B	116	PHE	2.1
2	B	234	LEU	2.1
1	A	227	PHE	2.1
1	A	246	LEU	2.1
2	B	149	LEU	2.1
1	A	64	LYS	2.1
2	B	7	THR	2.1
1	A	236	PRO	2.1
1	A	222	GLN	2.1
1	A	502	ALA	2.1
1	A	94	ILE	2.1
2	B	408	ALA	2.0
2	B	315	HIS	2.0
1	A	144	TYR	2.0
1	A	271	TYR	2.0
2	B	402	TRP	2.0
1	A	224	GLU	2.0
2	B	102	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	AC7	A	556	37/37	0.45	2.35	80,88,100,100	0

6.5 Other polymers ⓘ

There are no such residues in this entry.