



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:03 PM GMT

PDB ID : 1TL1
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN
COMPLEX WITH GW451211
Authors : Hopkins, A.L.; Ren, J.; Stuart, D.I.; Stammers, D.K.
Deposited on : 2004-06-09
Resolution : 2.90 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>

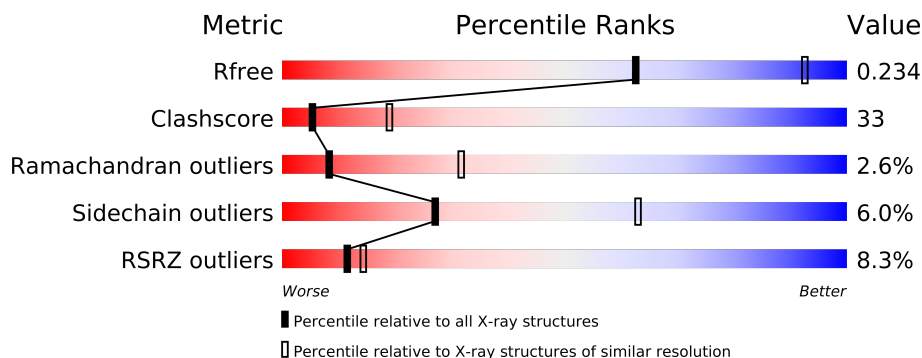
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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	560	
2	B	440	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	H18	A	999	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7604 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 Pol polyprotein, Reverse transcriptase, Chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			4247	2754	701	784	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	OXIDIZED CYS	UNP P04585

- Molecule 2 is a protein called Pol polyprotein, Reverse transcriptase, Chain B.

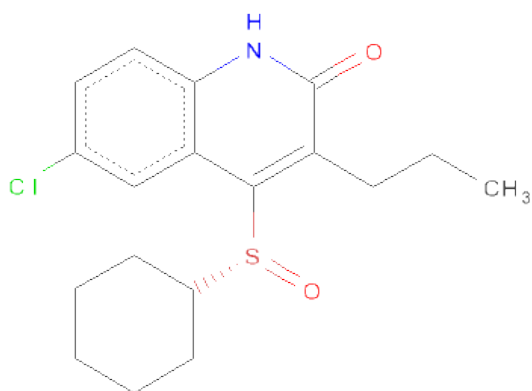
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	400	Total	C	N	O	S	0	0	0
			3319	2168	546	598	7			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

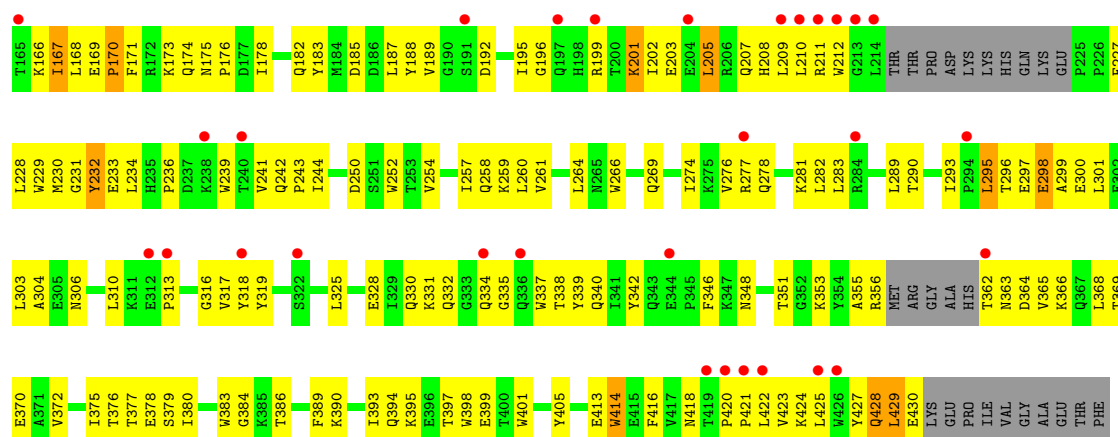


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 6-CHLORO-4-(CYCLOHEXYLSULFINYL)-3-PROPYLQUINOLIN-2(1H)-ONE (three-letter code: H18) (formula: C₁₈H₂₂ClNO₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			23	18	1	1	2	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.50Å 115.30Å 65.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.91 – 2.90 24.91 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (24.91-2.90) 99.3 (24.91-2.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.281 0.218 , 0.234	Depositor DCC
R_{free} test set	1135 reflections (4.82%)	DCC
Wilson B-factor (Å ²)	71.7	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 23552 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7604	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: H18, CSD, PO4

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	0.51	0/4352	0.72	0/5918
2	B	0.50	1/3415 (0.0%)	0.72	0/4639
All	All	0.51	1/7767 (0.0%)	0.72	0/10557

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	24	TRP	CB-CG	5.12	1.59	1.50

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	4247	0	4274	309	0
2	B	3319	0	3341	210	0
3	A	15	0	0	1	0
4	A	23	0	22	5	0
All	All	7604	0	7637	497	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 33.

All (497) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:178:ILE:HD11	1:A:201:LYS:HG2	1.31	1.13
1:A:91:GLN:NE2	2:B:137:ASN:HB3	1.72	1.05
1:A:253:THR:HG22	1:A:255:ASN:H	1.17	1.02
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.43	1.00
2:B:63:ILE:HD11	2:B:72:ARG:HD3	1.44	0.99
2:B:227:PHE:HB3	2:B:231:GLY:HA2	1.46	0.95
2:B:332:GLN:HB3	2:B:428:GLN:NE2	1.80	0.95
2:B:266:TRP:O	2:B:269:GLN:HG2	1.69	0.92
1:A:91:GLN:HE21	2:B:137:ASN:HB3	1.34	0.88
2:B:169:GLU:O	2:B:173:LYS:HG3	1.75	0.85
1:A:70:LYS:HG3	1:A:71:TRP:H	1.38	0.85
1:A:253:THR:HG22	1:A:255:ASN:N	1.93	0.84
1:A:195:ILE:HD13	1:A:195:ILE:N	1.93	0.84
1:A:522:ILE:O	1:A:526:ILE:HG13	1.79	0.82
2:B:328:GLU:HG2	2:B:390:LYS:HD2	1.61	0.82
2:B:429:LEU:HD13	2:B:430:GLU:O	1.80	0.81
1:A:469:LEU:HD21	1:A:480:GLN:HG3	1.60	0.81
1:A:57:ASN:HA	1:A:129:ALA:O	1.79	0.81
1:A:225:PRO:HG2	1:A:236:PRO:HG3	1.60	0.81
2:B:332:GLN:HA	2:B:424:LYS:HE3	1.62	0.80
1:A:41:MET:HB2	1:A:47:ILE:HD11	1.64	0.80
1:A:206:ARG:HH22	1:A:218:ASP:HA	1.48	0.79
2:B:178:ILE:HD11	2:B:201:LYS:HG3	1.64	0.79
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.63	0.79
1:A:319:TYR:OH	1:A:385:LYS:HE2	1.83	0.78
1:A:399:GLU:HG3	1:A:402:TRP:CE3	2.18	0.78
2:B:362:THR:HG22	2:B:366:LYS:HD3	1.65	0.78
2:B:295:LEU:HD12	2:B:295:LEU:H	1.49	0.77
1:A:122:GLU:HG3	1:A:125:ARG:NH1	1.99	0.77
2:B:420:PRO:O	2:B:423:VAL:HG12	1.86	0.76
1:A:28:GLU:OE1	1:A:135:ILE:HG22	1.86	0.75
1:A:178:ILE:CD1	1:A:201:LYS:HG2	2.12	0.74
1:A:107:THR:HG21	1:A:202:ILE:HG21	1.68	0.74
1:A:354:TYR:HD2	1:A:374:LYS:HD3	1.52	0.74
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.70	0.73
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.53	0.73
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.24	0.73
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.54	0.73
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.25	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:151:GLN:HB3	2:B:185:ASP:OD1	1.89	0.72
1:A:198:HIS:O	1:A:202:ILE:HG12	1.89	0.72
2:B:241:VAL:HG11	2:B:313:PRO:HG3	1.70	0.72
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.71	0.72
2:B:201:LYS:HA	2:B:201:LYS:HE3	1.70	0.72
2:B:295:LEU:HD12	2:B:295:LEU:N	2.05	0.71
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.72	0.70
1:A:500:GLN:HE21	2:B:422:LEU:HD12	1.56	0.70
2:B:169:GLU:N	2:B:170:PRO:HD2	2.06	0.70
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.72	0.70
1:A:500:GLN:NE2	2:B:422:LEU:HD12	2.08	0.69
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.72	0.69
2:B:169:GLU:HG2	2:B:170:PRO:HD3	1.74	0.69
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.74	0.69
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.74	0.69
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.27	0.69
1:A:102:LYS:HG3	1:A:237:ASP:HA	1.75	0.69
1:A:206:ARG:NH2	1:A:218:ASP:HA	2.08	0.68
1:A:206:ARG:CZ	1:A:217:PRO:O	2.42	0.68
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.26	0.68
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.29	0.68
2:B:203:GLU:HG3	2:B:207:GLN:HE22	1.58	0.67
1:A:317:VAL:HG22	1:A:318:TYR:N	2.09	0.67
1:A:480:GLN:HG2	1:A:517:LEU:HD11	1.76	0.67
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.75	0.67
1:A:177:ASP:OD2	1:A:193:LEU:HD21	1.94	0.67
1:A:417:VAL:O	1:A:417:VAL:HG13	1.95	0.66
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.30	0.66
1:A:503:LEU:HD12	1:A:533:LEU:HD23	1.78	0.66
1:A:174:GLN:C	1:A:176:PRO:HD3	2.15	0.66
1:A:164:MET:O	1:A:168:LEU:HG	1.96	0.65
1:A:208:HIS:O	1:A:208:HIS:HD2	1.79	0.65
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.31	0.65
1:A:174:GLN:HE21	1:A:174:GLN:HA	1.61	0.65
1:A:54:ASN:ND2	1:A:126:LYS:HB2	2.12	0.65
1:A:72:ARG:HG2	1:A:73:LYS:N	2.11	0.65
2:B:242:GLN:HG2	2:B:353:LYS:HE3	1.78	0.65
2:B:202:ILE:HG21	2:B:227:PHE:HE1	1.61	0.64
2:B:227:PHE:HB3	2:B:231:GLY:CA	2.26	0.64
2:B:203:GLU:HG3	2:B:207:GLN:NE2	2.12	0.64
1:A:92:LEU:O	1:A:92:LEU:HD23	1.97	0.64
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.96	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:104:LYS:HD2	2:B:192:ASP:O	1.97	0.64
1:A:20:LYS:HD2	1:A:55:PRO:HB2	1.78	0.64
2:B:298:GLU:CD	2:B:298:GLU:H	2.01	0.64
1:A:107:THR:HB	1:A:202:ILE:HD12	1.79	0.64
1:A:108:VAL:HG13	1:A:223:LYS:HB2	1.80	0.64
2:B:27:THR:OG1	2:B:30:LYS:HG2	1.98	0.64
1:A:500:GLN:HE21	2:B:422:LEU:CD1	2.10	0.64
1:A:31:ILE:O	1:A:35:VAL:HG23	1.98	0.63
1:A:472:THR:OG1	1:A:476:LYS:HE3	1.98	0.63
2:B:173:LYS:O	2:B:176:PRO:HD3	1.99	0.63
1:A:363:ASN:ND2	1:A:401:TRP:CZ3	2.67	0.63
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.34	0.62
1:A:317:VAL:HG22	1:A:318:TYR:H	1.64	0.62
1:A:96:HIS:H	2:B:136:ASN:HD21	1.47	0.62
1:A:41:MET:HB2	1:A:47:ILE:CD1	2.28	0.62
1:A:86:ASP:HA	1:A:154:LYS:HZ1	1.65	0.62
1:A:238:LYS:HD2	1:A:315:HIS:CG	2.33	0.62
1:A:13:LYS:HE3	1:A:84:THR:O	1.99	0.62
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.80	0.62
1:A:195:ILE:CD1	1:A:195:ILE:N	2.63	0.62
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.34	0.62
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.34	0.62
1:A:279:LEU:HD23	1:A:282:LEU:HD11	1.82	0.62
1:A:523:GLU:O	1:A:527:LYS:HG2	1.99	0.61
1:A:174:GLN:NE2	1:A:174:GLN:HA	2.15	0.61
2:B:234:LEU:HD21	2:B:377:THR:CG2	2.30	0.61
1:A:417:VAL:O	1:A:419:THR:N	2.33	0.61
1:A:460:ASN:ND2	3:A:1301:PO4:O4	2.33	0.61
1:A:368:LEU:O	1:A:372:VAL:HG23	2.01	0.61
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.36	0.61
2:B:167:ILE:O	2:B:208:HIS:HE1	1.82	0.61
2:B:395:LYS:HG3	2:B:416:PHE:CE1	2.36	0.61
1:A:91:GLN:C	1:A:93:GLY:H	2.05	0.60
2:B:203:GLU:CG	2:B:207:GLN:HE22	2.14	0.60
2:B:241:VAL:O	2:B:243:PRO:HD3	2.02	0.60
2:B:115:TYR:C	2:B:117:SER:H	2.05	0.60
2:B:85:GLN:O	2:B:85:GLN:HG3	2.01	0.60
1:A:507:GLN:HE22	2:B:421:PRO:HB3	1.67	0.60
1:A:476:LYS:HD2	1:A:476:LYS:O	2.02	0.60
1:A:171:PHE:HB2	1:A:208:HIS:CE1	2.37	0.60
1:A:292:VAL:C	1:A:293:ILE:HD12	2.21	0.59
1:A:101:LYS:N	1:A:101:LYS:HD2	2.16	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:403:THR:CG2	2:B:334:GLN:H	2.14	0.59
1:A:354:TYR:CD2	1:A:374:LYS:HD3	2.37	0.59
1:A:229:TRP:CE2	4:A:999:H18:HD1	2.37	0.59
1:A:399:GLU:HG3	1:A:402:TRP:CZ3	2.37	0.59
1:A:85:GLN:C	1:A:154:LYS:HZ3	2.06	0.59
1:A:411:ILE:O	1:A:412:PRO:O	2.20	0.59
2:B:395:LYS:NZ	2:B:399:GLU:HG3	2.17	0.59
2:B:139:THR:HB	2:B:140:PRO:HD2	1.84	0.59
2:B:365:VAL:O	2:B:369:THR:HG23	2.03	0.58
1:A:89:GLU:OE1	1:A:89:GLU:HA	2.03	0.58
1:A:10:VAL:HG12	1:A:11:LYS:N	2.18	0.58
1:A:172:ARG:NH1	1:A:180:ILE:HB	2.18	0.58
2:B:298:GLU:N	2:B:298:GLU:OE1	2.35	0.58
2:B:261:VAL:HG13	2:B:276:VAL:CG1	2.24	0.58
2:B:295:LEU:H	2:B:295:LEU:CD1	2.15	0.58
2:B:170:PRO:HA	2:B:173:LYS:NZ	2.19	0.58
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.34	0.57
2:B:205:LEU:O	2:B:209:LEU:HG	2.03	0.57
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.85	0.57
1:A:233:GLU:HB3	1:A:240:THR:HG23	1.86	0.57
2:B:168:LEU:C	2:B:170:PRO:HD2	2.24	0.57
2:B:234:LEU:HD21	2:B:377:THR:HG21	1.87	0.57
1:A:491:LEU:HD23	1:A:529:GLU:CG	2.34	0.57
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.34	0.57
1:A:58:THR:HG23	1:A:76:ASP:O	2.04	0.57
2:B:195:ILE:HG13	2:B:199:ARG:HE	1.69	0.57
1:A:34:LEU:HD13	1:A:132:ILE:HD12	1.86	0.57
1:A:181:TYR:HH	1:A:183:TYR:HD2	1.53	0.57
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.87	0.57
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.86	0.57
1:A:195:ILE:H	1:A:195:ILE:HD13	1.70	0.57
1:A:208:HIS:O	1:A:208:HIS:CD2	2.57	0.56
2:B:115:TYR:O	2:B:117:SER:N	2.37	0.56
1:A:107:THR:HG23	1:A:222:GLN:NE2	2.19	0.56
1:A:131:THR:HG23	1:A:143:ARG:HG2	1.86	0.56
1:A:231:GLY:O	1:A:266:TRP:HZ2	1.88	0.56
2:B:38:CYS:SG	2:B:73:LYS:HE2	2.46	0.56
2:B:58:THR:HG21	2:B:77:PHE:CD2	2.39	0.56
1:A:125:ARG:HG2	1:A:146:TYR:O	2.06	0.56
2:B:167:ILE:O	2:B:208:HIS:CE1	2.58	0.56
1:A:62:ALA:C	1:A:63:ILE:HD12	2.26	0.56
1:A:491:LEU:HD23	1:A:529:GLU:HG2	1.86	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:91:GLN:O	1:A:93:GLY:N	2.39	0.56
2:B:257:ILE:HG21	2:B:283:LEU:HD13	1.89	0.55
2:B:332:GLN:CG	2:B:338:THR:HG23	2.37	0.55
2:B:31:ILE:O	2:B:35:VAL:HG23	2.06	0.55
1:A:116:PHE:CD2	1:A:116:PHE:N	2.74	0.55
1:A:440:PHE:HZ	1:A:463:ARG:HH21	1.53	0.55
1:A:206:ARG:HH12	1:A:218:ASP:HA	1.71	0.55
1:A:376:THR:HG23	1:A:386:THR:HG22	1.89	0.55
2:B:175:ASN:HD21	2:B:201:LYS:HZ2	1.54	0.55
2:B:170:PRO:HG2	2:B:171:PHE:H	1.71	0.55
2:B:183:TYR:OH	2:B:386:THR:HG23	2.07	0.55
1:A:27:THR:HG23	1:A:30:LYS:HB2	1.88	0.55
2:B:414:TRP:O	2:B:414:TRP:HD1	1.90	0.55
2:B:380:ILE:O	2:B:384:GLY:N	2.34	0.55
2:B:254:VAL:O	2:B:258:GLN:HG3	2.07	0.55
2:B:116:PHE:CE1	2:B:151:GLN:HG3	2.42	0.55
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.42	0.55
1:A:219:LYS:HD2	1:A:222:GLN:NE2	2.23	0.54
1:A:348:ASN:ND2	1:A:351:THR:CG2	2.71	0.54
2:B:169:GLU:HG2	2:B:170:PRO:CD	2.38	0.54
2:B:178:ILE:CD1	2:B:201:LYS:HD2	2.37	0.54
2:B:175:ASN:ND2	2:B:201:LYS:NZ	2.54	0.54
1:A:208:HIS:C	1:A:208:HIS:CD2	2.80	0.54
1:A:296:THR:HG22	1:A:297:GLU:N	2.21	0.54
1:A:58:THR:CG2	1:A:76:ASP:O	2.56	0.54
1:A:96:HIS:H	2:B:136:ASN:ND2	2.05	0.54
1:A:380:ILE:HD13	2:B:27:THR:HG22	1.90	0.54
1:A:61:PHE:CE1	1:A:63:ILE:HD11	2.43	0.54
1:A:171:PHE:HB2	1:A:208:HIS:ND1	2.23	0.54
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.89	0.54
1:A:470:THR:O	1:A:471:ASP:HB2	2.08	0.54
2:B:227:PHE:CB	2:B:231:GLY:HA2	2.30	0.54
2:B:335:GLY:O	2:B:355:ALA:HA	2.08	0.54
1:A:340:GLN:CB	1:A:351:THR:HG22	2.37	0.53
1:A:358:ARG:HD3	1:A:370:GLU:CD	2.29	0.53
1:A:253:THR:CG2	1:A:254:VAL:N	2.70	0.53
2:B:277:ARG:O	2:B:281:LYS:HG3	2.08	0.53
2:B:201:LYS:HD3	2:B:201:LYS:O	2.08	0.53
1:A:26:LEU:HD12	1:A:133:PRO:CD	2.39	0.53
1:A:376:THR:HG23	1:A:386:THR:CG2	2.39	0.53
1:A:40:GLU:HA	1:A:40:GLU:OE2	2.08	0.53
2:B:175:ASN:N	2:B:176:PRO:HD3	2.22	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:29:GLU:HG2	1:A:29:GLU:O	2.09	0.53
1:A:115:TYR:O	1:A:149:LEU:HB2	2.09	0.53
2:B:203:GLU:OE2	2:B:207:GLN:NE2	2.40	0.53
1:A:358:ARG:NH2	2:B:394:GLN:HG2	2.24	0.53
1:A:476:LYS:HD3	1:A:517:LEU:HD12	1.90	0.52
2:B:425:LEU:HD23	2:B:425:LEU:O	2.09	0.52
1:A:70:LYS:HG3	1:A:71:TRP:N	2.16	0.52
1:A:56:TYR:O	1:A:143:ARG:NH2	2.35	0.52
1:A:194:GLU:O	1:A:196:GLY:N	2.42	0.52
2:B:203:GLU:CD	2:B:207:GLN:HE22	2.11	0.52
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.90	0.52
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.09	0.52
1:A:469:LEU:HD21	1:A:480:GLN:CG	2.35	0.52
2:B:79:GLU:O	2:B:83:ARG:HG3	2.09	0.52
1:A:236:PRO:HA	4:A:999:H18:H9	1.92	0.52
2:B:175:ASN:O	2:B:178:ILE:HB	2.10	0.52
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.25	0.52
1:A:268:SER:OG	1:A:353:LYS:HE2	2.09	0.52
1:A:498:ASP:O	1:A:535:TRP:NE1	2.41	0.51
1:A:507:GLN:NE2	2:B:421:PRO:HB3	2.25	0.51
1:A:86:ASP:HA	1:A:154:LYS:NZ	2.24	0.51
1:A:108:VAL:CG1	1:A:223:LYS:HB2	2.40	0.51
2:B:297:GLU:HA	2:B:300:GLU:HB2	1.91	0.51
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.45	0.51
2:B:125:ARG:HB3	2:B:145:GLN:HE21	1.75	0.51
1:A:382:ILE:O	2:B:136:ASN:HB2	2.11	0.51
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.92	0.51
2:B:264:LEU:HD13	2:B:306:ASN:HD22	1.75	0.51
1:A:515:SER:O	1:A:519:ASN:ND2	2.42	0.51
2:B:115:TYR:OH	2:B:157:PRO:HG3	2.11	0.51
1:A:225:PRO:HB3	1:A:236:PRO:HD3	1.92	0.51
2:B:366:LYS:O	2:B:370:GLU:HG3	2.11	0.51
1:A:164:MET:HE1	1:A:168:LEU:HD21	1.92	0.51
2:B:306:ASN:O	2:B:310:LEU:HG	2.11	0.51
2:B:282:LEU:HB3	2:B:293:ILE:HG21	1.93	0.50
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.43	0.50
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.93	0.50
1:A:19:PRO:HD3	1:A:80:LEU:HD13	1.93	0.50
1:A:406:TRP:HH2	2:B:418:ASN:OD1	1.94	0.50
1:A:328:GLU:O	1:A:339:TYR:HA	2.10	0.50
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.94	0.50
1:A:70:LYS:CG	1:A:71:TRP:H	2.17	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.47	0.50
2:B:372:VAL:HG13	2:B:389:PHE:CZ	2.47	0.50
2:B:107:THR:HB	2:B:202:ILE:HD11	1.94	0.50
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.76	0.50
1:A:393:ILE:HD12	1:A:423:VAL:HG21	1.93	0.50
1:A:260:LEU:HD23	1:A:279:LEU:HD13	1.94	0.50
2:B:393:ILE:HD11	2:B:397:THR:HG22	1.94	0.50
1:A:111:VAL:CG1	1:A:114:ALA:HB2	2.41	0.49
1:A:476:LYS:CD	1:A:517:LEU:HD12	2.41	0.49
1:A:188:TYR:CD2	4:A:999:H18:HF1	2.47	0.49
1:A:319:TYR:O	1:A:321:PRO:HD3	2.12	0.49
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.42	0.49
2:B:175:ASN:ND2	2:B:201:LYS:HZ2	2.10	0.49
1:A:175:ASN:N	1:A:176:PRO:HD3	2.26	0.49
1:A:278:GLN:HA	1:A:278:GLN:NE2	2.27	0.49
1:A:207:GLN:NE2	1:A:210:LEU:HD12	2.27	0.49
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.47	0.49
1:A:54:ASN:O	1:A:143:ARG:NH2	2.43	0.49
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.47	0.49
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.48	0.49
2:B:125:ARG:HB3	2:B:145:GLN:NE2	2.28	0.49
1:A:210:LEU:C	1:A:212:TRP:H	2.15	0.49
2:B:178:ILE:HD11	2:B:201:LYS:CG	2.40	0.49
2:B:328:GLU:CG	2:B:390:LYS:HD2	2.36	0.49
1:A:10:VAL:O	1:A:11:LYS:HG3	2.13	0.49
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.48	0.49
2:B:423:VAL:O	2:B:427:TYR:HD2	1.96	0.49
1:A:229:TRP:O	1:A:232:TYR:HB2	2.13	0.49
2:B:278:GLN:NE2	2:B:298:GLU:HB2	2.28	0.49
1:A:277:ARG:HH11	1:A:277:ARG:HG3	1.78	0.49
2:B:295:LEU:CD1	2:B:295:LEU:N	2.75	0.48
2:B:170:PRO:HA	2:B:173:LYS:HZ3	1.77	0.48
1:A:108:VAL:HG12	1:A:223:LYS:O	2.13	0.48
1:A:63:ILE:N	1:A:63:ILE:HD12	2.28	0.48
1:A:181:TYR:OH	1:A:183:TYR:HD2	1.95	0.48
2:B:136:ASN:O	2:B:138:GLU:HG3	2.14	0.48
2:B:178:ILE:HD12	2:B:201:LYS:HD2	1.95	0.48
1:A:10:VAL:HG21	1:A:153:TRP:CH2	2.43	0.48
1:A:500:GLN:O	1:A:503:LEU:HB3	2.12	0.48
1:A:399:GLU:HG3	1:A:402:TRP:HE3	1.75	0.48
1:A:131:THR:OG1	1:A:143:ARG:CD	2.62	0.48
2:B:319:TYR:HE2	2:B:325:LEU:HD13	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:208:HIS:HA	2:B:211:ARG:HD3	1.95	0.48
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.96	0.48
1:A:145:GLN:O	1:A:145:GLN:HG3	2.14	0.48
1:A:86:ASP:CA	1:A:154:LYS:HZ1	2.25	0.48
1:A:293:ILE:HD12	1:A:293:ILE:N	2.29	0.47
1:A:231:GLY:O	1:A:266:TRP:CZ2	2.67	0.47
2:B:368:LEU:O	2:B:372:VAL:HG23	2.14	0.47
1:A:23:GLN:NE2	1:A:26:LEU:HG	2.28	0.47
1:A:38:CYS:SG	1:A:73:LYS:HE3	2.54	0.47
1:A:107:THR:HG21	1:A:202:ILE:CG2	2.41	0.47
1:A:255:ASN:HB2	1:A:289:LEU:O	2.15	0.47
1:A:241:VAL:HG22	1:A:270:ILE:HG21	1.95	0.47
2:B:10:VAL:HG21	2:B:153:TRP:HH2	1.79	0.47
1:A:254:VAL:CG2	1:A:293:ILE:HD11	2.45	0.47
1:A:518:VAL:O	1:A:522:ILE:HG13	2.15	0.47
1:A:469:LEU:CD2	1:A:480:GLN:HG3	2.40	0.47
1:A:225:PRO:CB	1:A:236:PRO:HD3	2.44	0.47
1:A:130:PHE:CE2	1:A:144:TYR:HB2	2.50	0.47
2:B:99:GLY:HA2	2:B:102:LYS:HE2	1.96	0.47
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.49	0.47
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.12	0.47
2:B:97:PRO:C	2:B:99:GLY:N	2.66	0.47
1:A:136:ASN:OD1	1:A:139:THR:HG23	2.14	0.47
2:B:108:VAL:HG12	2:B:228:LEU:HD12	1.96	0.47
2:B:379:SER:HA	2:B:383:TRP:CE3	2.50	0.47
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.97	0.46
1:A:346:PHE:CD1	1:A:346:PHE:N	2.82	0.46
2:B:189:VAL:HG11	2:B:202:ILE:HD13	1.97	0.46
2:B:332:GLN:OE1	2:B:428:GLN:CD	2.53	0.46
1:A:340:GLN:HA	1:A:351:THR:HA	1.96	0.46
1:A:238:LYS:NZ	1:A:315:HIS:CD2	2.83	0.46
2:B:169:GLU:N	2:B:170:PRO:CD	2.76	0.46
1:A:164:MET:CE	1:A:168:LEU:HD11	2.45	0.46
2:B:195:ILE:HG23	2:B:196:GLY:N	2.31	0.46
1:A:24:TRP:CZ3	1:A:61:PHE:HB3	2.51	0.46
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.97	0.46
2:B:97:PRO:C	2:B:99:GLY:H	2.18	0.46
1:A:348:ASN:ND2	1:A:351:THR:HG21	2.31	0.46
2:B:348:ASN:HD22	2:B:351:THR:CG2	2.29	0.46
1:A:224:GLU:HB3	1:A:225:PRO:HD2	1.96	0.46
2:B:24:TRP:CD1	2:B:25:PRO:HD2	2.51	0.46
1:A:117:SER:OG	1:A:214:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:393:ILE:HD11	2:B:397:THR:CG2	2.46	0.46
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.80	0.46
2:B:174:GLN:C	2:B:176:PRO:HD3	2.36	0.46
1:A:417:VAL:O	1:A:417:VAL:CG1	2.61	0.46
2:B:195:ILE:CG2	2:B:196:GLY:N	2.79	0.46
1:A:486:LEU:HD13	1:A:524:GLN:HB2	1.98	0.46
1:A:270:ILE:HG13	1:A:314:VAL:HG23	1.98	0.45
1:A:183:TYR:O	1:A:184:MET:HB2	2.17	0.45
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.45	0.45
1:A:317:VAL:CG2	1:A:318:TYR:N	2.76	0.45
1:A:238:LYS:HD2	1:A:315:HIS:CD2	2.51	0.45
2:B:40:GLU:HG3	2:B:44:GLU:OE2	2.16	0.45
1:A:283:LEU:O	1:A:286:THR:HG23	2.15	0.45
1:A:235:HIS:O	4:A:999:H18:H9	2.16	0.45
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.51	0.45
1:A:28:GLU:OE1	1:A:135:ILE:CG2	2.61	0.45
1:A:18:GLY:HA3	1:A:56:TYR:CE1	2.52	0.45
1:A:363:ASN:ND2	1:A:401:TRP:CH2	2.84	0.45
1:A:306:ASN:O	1:A:310:LEU:HG	2.15	0.45
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.52	0.45
1:A:27:THR:O	1:A:30:LYS:N	2.48	0.45
1:A:53:GLU:O	1:A:55:PRO:HD3	2.16	0.45
1:A:401:TRP:HH2	1:A:508:ALA:O	2.00	0.45
1:A:482:ILE:HD12	1:A:502:ALA:HB1	1.99	0.45
1:A:27:THR:HG23	1:A:30:LYS:CB	2.46	0.45
1:A:95:PRO:HG3	2:B:137:ASN:O	2.17	0.44
4:A:999:H18:H7	4:A:999:H18:OS	2.17	0.44
2:B:264:LEU:HD13	2:B:306:ASN:ND2	2.32	0.44
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.52	0.44
2:B:208:HIS:ND1	2:B:208:HIS:O	2.50	0.44
1:A:395:LYS:O	1:A:399:GLU:HB2	2.17	0.44
1:A:240:THR:OG1	1:A:241:VAL:N	2.50	0.44
1:A:40:GLU:CA	1:A:40:GLU:OE2	2.65	0.44
1:A:222:GLN:HB3	1:A:223:LYS:H	1.69	0.44
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.47	0.44
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.53	0.44
1:A:324:ASP:O	1:A:343:GLN:HG2	2.17	0.44
2:B:234:LEU:HD12	2:B:234:LEU:N	2.32	0.44
1:A:142:ILE:HD12	1:A:144:TYR:OH	2.17	0.44
2:B:278:GLN:HB3	2:B:299:ALA:HA	2.00	0.44
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.52	0.44
1:A:34:LEU:HD13	1:A:132:ILE:CD1	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:429:LEU:CD1	2:B:430:GLU:N	2.81	0.44
1:A:48:SER:O	1:A:50:ILE:HG23	2.16	0.44
2:B:414:TRP:O	2:B:414:TRP:CD1	2.71	0.44
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.48	0.44
1:A:332:GLN:HB3	1:A:336:GLN:HB3	2.00	0.44
2:B:339:TYR:CD1	2:B:375:ILE:HD11	2.53	0.44
2:B:154:LYS:O	2:B:157:PRO:HD2	2.18	0.43
1:A:74:LEU:C	1:A:74:LEU:HD12	2.38	0.43
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.53	0.43
2:B:118:VAL:HG21	2:B:160:PHE:HD2	1.83	0.43
1:A:95:PRO:HG2	1:A:181:TYR:CE2	2.53	0.43
1:A:237:ASP:N	1:A:237:ASP:OD2	2.44	0.43
2:B:163:SER:O	2:B:167:ILE:HG13	2.18	0.43
1:A:164:MET:HE1	1:A:187:LEU:HD21	2.00	0.43
1:A:194:GLU:O	1:A:195:ILE:C	2.57	0.43
1:A:317:VAL:CG2	1:A:318:TYR:H	2.28	0.43
1:A:401:TRP:CH2	1:A:508:ALA:O	2.71	0.43
2:B:264:LEU:CD1	2:B:306:ASN:HD22	2.32	0.43
1:A:296:THR:CG2	1:A:297:GLU:N	2.81	0.43
2:B:228:LEU:HD23	2:B:228:LEU:HA	1.91	0.43
1:A:360:ALA:HB1	1:A:514:GLU:OE1	2.18	0.43
1:A:326:ILE:O	1:A:341:ILE:HA	2.19	0.43
1:A:253:THR:CG2	1:A:255:ASN:H	2.07	0.43
1:A:218:ASP:O	1:A:222:GLN:HG3	2.18	0.43
2:B:100:LEU:HD12	2:B:100:LEU:O	2.19	0.43
2:B:201:LYS:HD3	2:B:201:LYS:C	2.38	0.43
1:A:472:THR:CB	1:A:476:LYS:HE3	2.48	0.43
1:A:79:GLU:O	1:A:83:ARG:HG3	2.17	0.43
1:A:245:VAL:HG23	1:A:245:VAL:O	2.18	0.43
1:A:420:PRO:HA	1:A:421:PRO:C	2.39	0.43
1:A:131:THR:OG1	1:A:143:ARG:HD3	2.18	0.43
2:B:229:TRP:CE3	2:B:229:TRP:HA	2.53	0.43
1:A:111:VAL:HG12	1:A:114:ALA:HB2	1.99	0.43
2:B:150:PRO:HG2	2:B:153:TRP:HB2	2.01	0.43
1:A:253:THR:CG2	1:A:289:LEU:O	2.67	0.43
1:A:210:LEU:C	1:A:212:TRP:N	2.71	0.43
2:B:230:MET:C	2:B:232:TYR:N	2.72	0.43
1:A:174:GLN:HE21	1:A:174:GLN:CA	2.27	0.43
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.54	0.43
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.49	0.43
1:A:277:ARG:NH1	1:A:277:ARG:HG3	2.33	0.43
1:A:177:ASP:OD1	1:A:177:ASP:N	2.48	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:520:GLN:HE21	1:A:520:GLN:HB2	1.57	0.42
2:B:98:ALA:O	2:B:101:LYS:HE3	2.19	0.42
1:A:206:ARG:HH12	1:A:219:LYS:N	2.17	0.42
2:B:112:GLY:HA3	2:B:151:GLN:OE1	2.18	0.42
1:A:23:GLN:NE2	1:A:24:TRP:O	2.41	0.42
1:A:296:THR:HG22	1:A:298:GLU:H	1.85	0.42
1:A:265:ASN:N	1:A:265:ASN:HD22	2.17	0.42
1:A:224:GLU:HB3	1:A:225:PRO:CD	2.49	0.42
2:B:376:THR:O	2:B:377:THR:C	2.57	0.42
1:A:433:PRO:HB3	2:B:289:LEU:HD23	2.01	0.42
1:A:239:TRP:NE1	1:A:316:GLY:HA3	2.35	0.42
2:B:316:GLY:HA2	2:B:318:TYR:CE2	2.54	0.42
1:A:91:GLN:C	1:A:93:GLY:N	2.71	0.42
2:B:104:LYS:CB	2:B:192:ASP:HA	2.46	0.42
2:B:378:GLU:O	2:B:379:SER:C	2.58	0.42
2:B:208:HIS:CG	2:B:208:HIS:O	2.72	0.42
2:B:355:ALA:O	2:B:356:ARG:C	2.57	0.42
1:A:283:LEU:C	1:A:286:THR:HG23	2.40	0.42
2:B:182:GLN:HA	2:B:187:LEU:HD12	2.01	0.42
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.54	0.42
1:A:503:LEU:HD22	1:A:535:TRP:HB2	2.01	0.42
1:A:131:THR:OG1	1:A:143:ARG:HD2	2.19	0.42
2:B:98:ALA:O	2:B:101:LYS:HG2	2.19	0.42
2:B:301:LEU:O	2:B:304:ALA:HB3	2.19	0.42
2:B:160:PHE:CD1	2:B:160:PHE:O	2.73	0.42
1:A:207:GLN:CD	1:A:210:LEU:HD12	2.40	0.42
1:A:233:GLU:HB3	1:A:240:THR:CG2	2.48	0.41
1:A:63:ILE:HD13	1:A:74:LEU:HB3	2.00	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD2	1.83	0.41
1:A:257:ILE:HD13	1:A:282:LEU:HD13	2.02	0.41
2:B:429:LEU:HB2	2:B:430:GLU:H	1.38	0.41
1:A:174:GLN:O	1:A:176:PRO:HD3	2.20	0.41
1:A:324:ASP:CG	1:A:388:LYS:HE3	2.40	0.41
1:A:391:LEU:HB2	1:A:393:ILE:HG22	2.02	0.41
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.50	0.41
1:A:156:SER:N	1:A:157:PRO:CD	2.83	0.41
2:B:173:LYS:O	2:B:176:PRO:CD	2.66	0.41
1:A:10:VAL:CG1	1:A:11:LYS:N	2.82	0.41
1:A:115:TYR:N	1:A:115:TYR:CD2	2.89	0.41
2:B:136:ASN:O	2:B:137:ASN:C	2.58	0.41
1:A:116:PHE:H	1:A:116:PHE:HD2	1.68	0.41
1:A:282:LEU:HB3	1:A:293:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:160:PHE:CE2	1:A:164:MET:HG2	2.55	0.41
1:A:457:TYR:C	1:A:457:TYR:CD1	2.94	0.41
1:A:324:ASP:O	1:A:343:GLN:HA	2.20	0.41
1:A:23:GLN:HE21	1:A:26:LEU:HG	1.86	0.41
2:B:393:ILE:HG12	2:B:394:GLN:N	2.36	0.41
1:A:253:THR:HG22	1:A:254:VAL:N	2.36	0.41
1:A:54:ASN:HD21	1:A:126:LYS:HB2	1.84	0.41
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.56	0.41
2:B:259:LYS:HE2	2:B:259:LYS:HB3	1.82	0.41
1:A:175:ASN:OD1	1:A:201:LYS:HE2	2.20	0.41
2:B:429:LEU:HD13	2:B:430:GLU:N	2.36	0.41
1:A:226:PRO:HB3	1:A:235:HIS:ND1	2.36	0.41
1:A:116:PHE:HD2	1:A:116:PHE:N	2.19	0.41
1:A:440:PHE:CD2	1:A:459:THR:HG22	2.56	0.41
1:A:396:GLU:HG3	1:A:397:THR:N	2.36	0.41
2:B:338:THR:HG21	2:B:427:TYR:O	2.20	0.41
1:A:354:TYR:HD2	1:A:374:LYS:CD	2.26	0.41
1:A:362:THR:OG1	1:A:363:ASN:N	2.54	0.41
2:B:340:GLN:CG	2:B:351:THR:HG22	2.51	0.41
1:A:33:ALA:O	1:A:37:ILE:HG13	2.21	0.41
1:A:164:MET:HE3	1:A:168:LEU:HD11	2.02	0.40
1:A:84:THR:O	1:A:154:LYS:NZ	2.53	0.40
2:B:395:LYS:HZ3	2:B:399:GLU:CG	2.34	0.40
1:A:22:LYS:HG2	1:A:23:GLN:N	2.36	0.40
2:B:21:VAL:CG1	2:B:59:PRO:CG	2.99	0.40
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.56	0.40
2:B:269:GLN:OE1	2:B:346:PHE:CZ	2.75	0.40
1:A:195:ILE:HG12	1:A:196:GLY:H	1.85	0.40
1:A:171:PHE:CE1	1:A:205:LEU:CA	3.01	0.40
1:A:207:GLN:NE2	1:A:207:GLN:HA	2.36	0.40
2:B:40:GLU:OE2	2:B:40:GLU:HA	2.21	0.40
1:A:393:ILE:HD12	1:A:423:VAL:CG2	2.51	0.40
2:B:317:VAL:O	2:B:317:VAL:HG12	2.21	0.40
1:A:216:THR:HB	1:A:217:PRO:HD2	2.03	0.40
2:B:298:GLU:N	2:B:298:GLU:CD	2.73	0.40
1:A:27:THR:CG2	1:A:30:LYS:HG3	2.51	0.40
1:A:26:LEU:HD12	1:A:133:PRO:CG	2.52	0.40
2:B:230:MET:C	2:B:232:TYR:H	2.24	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	510/560 (91%)	449 (88%)	45 (9%)	16 (3%)	7	26
2	B	390/440 (89%)	349 (90%)	34 (9%)	7 (2%)	13	44
All	All	900/1000 (90%)	798 (89%)	79 (9%)	23 (3%)	8	32

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	195	ILE
1	A	222	GLN
1	A	412	PRO
2	B	116	PHE
2	B	428	GLN
1	A	18	GLY
1	A	402	TRP
1	A	418	ASN
2	B	122	GLU
2	B	167	ILE
1	A	137	ASN
1	A	230	MET
1	A	249	LYS
1	A	345	PRO
1	A	356	ARG
1	A	472	THR
2	B	85	GLN
2	B	170	PRO
1	A	91	GLN
1	A	92	LEU
2	B	166	LYS
1	A	170	PRO

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	466/499 (93%)	433 (93%)	33 (7%)	21	52
2	B	365/400 (91%)	348 (95%)	17 (5%)	36	75
All	All	831/899 (92%)	781 (94%)	50 (6%)	27	63

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	GLU
1	A	7	THR
1	A	20	LYS
1	A	24	TRP
1	A	39	THR
1	A	74	LEU
1	A	89	GLU
1	A	116	PHE
1	A	135	ILE
1	A	138	GLU
1	A	164	MET
1	A	182	GLN
1	A	195	ILE
1	A	205	LEU
1	A	208	HIS
1	A	215	THR
1	A	218	ASP
1	A	265	ASN
1	A	287	LYS
1	A	301	LEU
1	A	303	LEU
1	A	336	GLN
1	A	340	GLN
1	A	345	PRO
1	A	356	ARG
1	A	428	GLN
1	A	443	ASP
1	A	476	LYS

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Mol	Chain	Res	Type
1	A	484	LEU
1	A	487	GLN
1	A	514	GLU
1	A	517	LEU
2	B	10	VAL
2	B	55	PRO
2	B	109	LEU
2	B	122	GLU
2	B	201	LYS
2	B	205	LEU
2	B	210	LEU
2	B	212	TRP
2	B	232	TYR
2	B	233	GLU
2	B	250	ASP
2	B	295	LEU
2	B	298	GLU
2	B	303	LEU
2	B	413	GLU
2	B	414	TRP
2	B	429	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	174	GLN
1	A	207	GLN
1	A	208	HIS
1	A	222	GLN
1	A	242	GLN
1	A	265	ASN
1	A	278	GLN
1	A	315	HIS
1	A	336	GLN
1	A	348	ASN
1	A	475	GLN
1	A	480	GLN
1	A	487	GLN
1	A	500	GLN
1	A	507	GLN
1	A	520	GLN

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Mol	Chain	Res	Type
2	B	57	ASN
2	B	137	ASN
2	B	175	ASN
2	B	207	GLN
2	B	235	HIS
2	B	278	GLN
2	B	336	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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	7,7,8	6.74	2 (28%)	6,8,10	3.71	4 (66%)

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	-	1/3/6/8	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	O-C	17.45	1.23	1.11
1	A	280	CSD	CA-C	3.18	1.54	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	5.43	119.66	105.25
1	A	280	CSD	OD2-SG-OD1	5.07	117.81	109.39
1	A	280	CSD	CA-CB-SG	4.50	117.24	110.82
1	A	280	CSD	C-CA-N	-2.60	111.23	113.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	A	1300	-	4,4,4	0.84	0	6,6,6	0.31	0
3	PO4	A	1301	-	4,4,4	0.94	0	6,6,6	0.31	0
3	PO4	A	1302	-	4,4,4	0.81	0	6,6,6	0.31	0
4	H18	A	999	-	25,25,25	2.57	14 (56%)	33,35,35	2.00	7 (21%)

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	PO4	A	1300	-	-	0/0/0/0	0/0/0/0
3	PO4	A	1301	-	-	0/0/0/0	0/0/0/0
3	PO4	A	1302	-	-	0/0/0/0	0/0/0/0
4	H18	A	999	-	-	0/11/19/19	0/1/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	H18	CF-CA	5.55	1.61	1.52
4	A	999	H18	C6-C5	4.94	1.53	1.42
4	A	999	H18	C6-N1	4.89	1.45	1.37
4	A	999	H18	C3-C2	3.51	1.48	1.41
4	A	999	H18	C10-C9	2.96	1.42	1.36
4	A	999	H18	O2-C6	2.83	1.30	1.24
4	A	999	H18	C7-C8	2.77	1.42	1.36
4	A	999	H18	C5-C4	2.75	1.44	1.41
4	A	999	H18	C9-C8	2.54	1.43	1.38
4	A	999	H18	C8-CL	-2.47	1.68	1.74
4	A	999	H18	C2-N1	2.37	1.42	1.38
4	A	999	H18	C4-S4	-2.30	1.77	1.81
4	A	999	H18	CE-CF	2.08	1.59	1.53
4	A	999	H18	CB-CA	2.02	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	H18	C4-S4-CA	7.34	106.82	97.86
4	A	999	H18	OS-S4-CA	4.91	110.42	107.16
4	A	999	H18	CE-CF-CA	3.22	117.26	110.50
4	A	999	H18	C12-C11-C5	-3.05	107.85	113.42
4	A	999	H18	OS-S4-C4	2.69	110.34	106.81
4	A	999	H18	CD-CE-CF	2.46	116.90	111.45
4	A	999	H18	CF-CA-CB	2.20	113.76	111.57

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	517/560 (92%)	0.26	37 (7%)	15 18	28, 65, 110, 139	0
2	B	400/440 (90%)	0.17	39 (9%)	8 10	28, 60, 117, 148	0
All	All	917/1000 (91%)	0.22	76 (8%)	11 14	28, 63, 113, 148	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	421	PRO	7.6
2	B	334	GLN	7.2
2	B	214	LEU	6.3
1	A	138	GLU	5.7
2	B	312	GLU	4.8
2	B	213	GLY	4.6
1	A	469	LEU	4.3
1	A	139	THR	4.2
2	B	88	TRP	4.1
1	A	140	PRO	4.0
1	A	15	GLY	4.0
2	B	165	THR	3.9
1	A	144	TYR	3.9
1	A	251	SER	3.9
1	A	402	TRP	3.6
2	B	197	GLN	3.6
1	A	472	THR	3.5
1	A	396	GLU	3.5
2	B	362	THR	3.4
1	A	220	LYS	3.4
2	B	240	THR	3.4
1	A	14	PRO	3.4
1	A	82	LYS	3.4
2	B	420	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	294	PRO	3.3
2	B	64	LYS	3.3
1	A	43	LYS	3.2
1	A	228	LEU	3.2
1	A	116	PHE	3.2
2	B	425	LEU	3.1
2	B	212	TRP	3.1
2	B	426	TRP	3.1
2	B	95	PRO	3.1
2	B	211	ARG	3.1
2	B	284	ARG	3.0
2	B	419	THR	3.0
2	B	238	LYS	2.9
2	B	204	GLU	2.9
2	B	117	SER	2.9
2	B	96	HIS	2.9
1	A	287	LYS	2.9
1	A	193	LEU	2.9
2	B	97	PRO	2.8
1	A	404	GLU	2.8
2	B	318	TYR	2.7
1	A	27	THR	2.6
2	B	277	ARG	2.6
1	A	20	LYS	2.6
1	A	322	SER	2.6
2	B	104	LYS	2.6
2	B	210	LEU	2.5
1	A	221	HIS	2.5
1	A	409	THR	2.5
1	A	36	GLU	2.5
2	B	322	SER	2.5
2	B	191	SER	2.5
1	A	313	PRO	2.4
1	A	29	GLU	2.4
1	A	311	LYS	2.3
1	A	192	ASP	2.3
2	B	344	GLU	2.3
1	A	56	TYR	2.3
1	A	346	PHE	2.3
2	B	313	PRO	2.2
1	A	71	TRP	2.2
1	A	336	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	15	GLY	2.2
2	B	164	MET	2.2
1	A	210	LEU	2.2
2	B	422	LEU	2.2
1	A	113	ASP	2.1
2	B	209	LEU	2.1
2	B	199	ARG	2.0
1	A	112	GLY	2.0
1	A	90	VAL	2.0
2	B	336	GLN	2.0

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

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
1	CSD	A	280	8/9	0.17	0.09	51,55,65,74	0

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
4	H18	A	999	23/23	0.24	2.16	45,66,78,88	0
3	PO4	A	1301	5/5	0.22	1.02	123,124,129,131	0
3	PO4	A	1302	5/5	0.24	-0.37	150,150,150,150	0
3	PO4	A	1300	5/5	0.18	-0.42	137,140,144,146	0

6.5 Other polymers ⓘ

There are no such residues in this entry.