Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2022 – 11:39 PM EST

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)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2
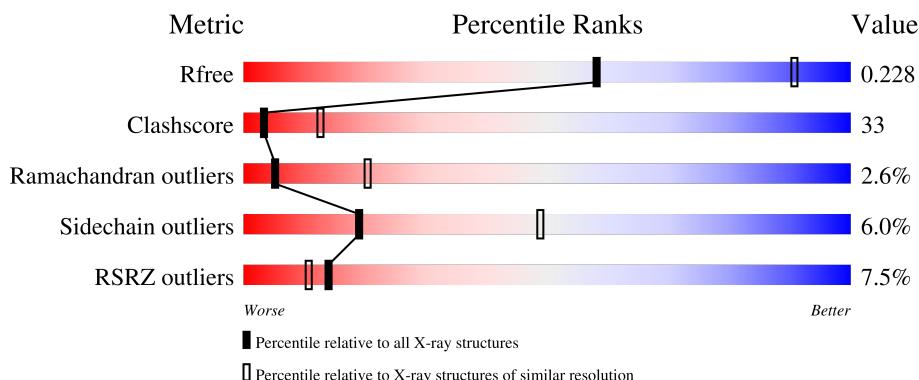
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
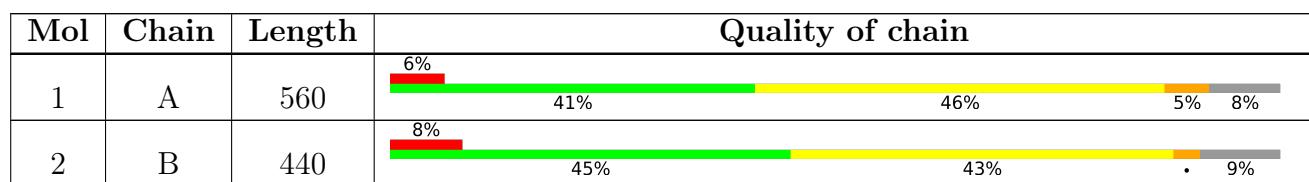
The reported resolution of this entry is 2.90 Å.

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	560	6% 41% 46% 5% 8%
2	B	440	8% 45% 43% • 9%

2 Entry composition ⓘ

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total 4247	C 2754	N 701	O 784	S 8	0	0	0
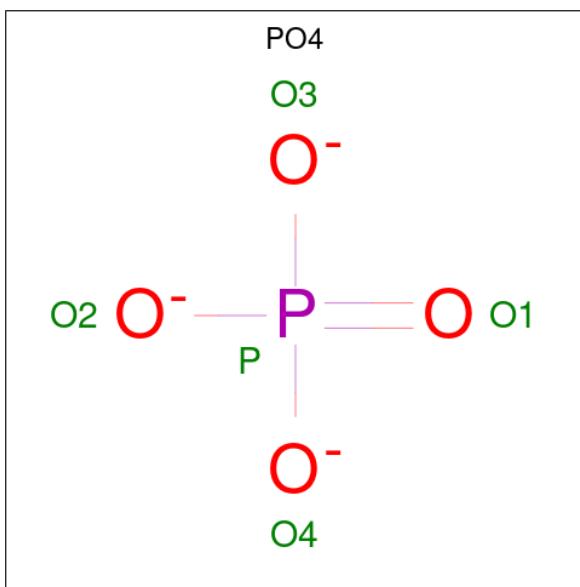
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a protein called Pol polyprotein, Reverse transcriptase, Chain B.
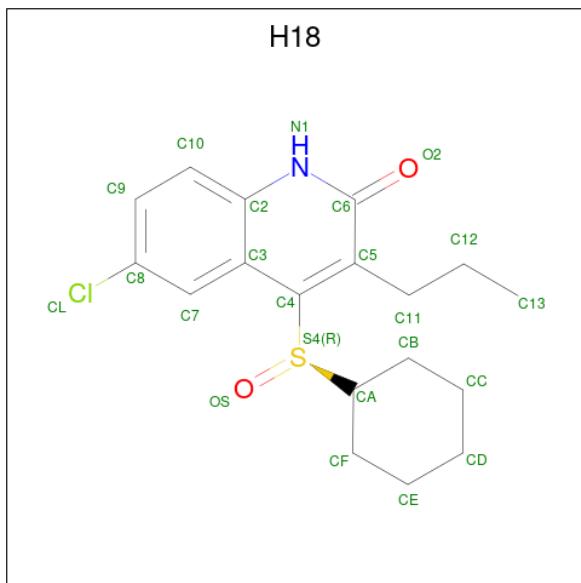
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	400	Total 3319	C 2168	N 546	O 598	S 7	0	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

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

- Molecule 4 is 6-CHLORO-4-(CYCLOHEXYLSULFINYL)-3-PROPYLQUINOLIN-2(1H)-ONE (three-letter code: H18) (formula: $C_{18}H_{22}ClNO_2S$).
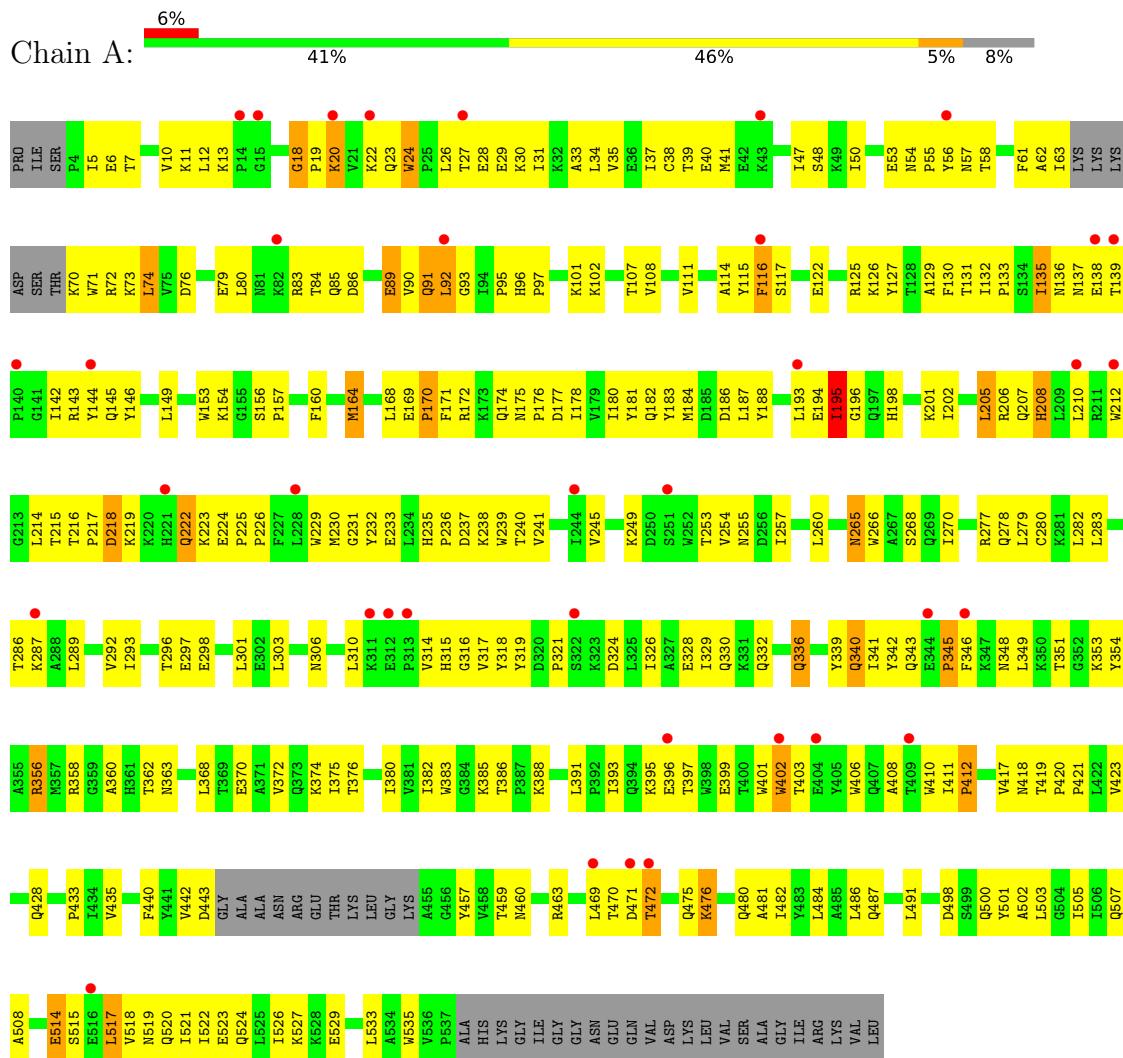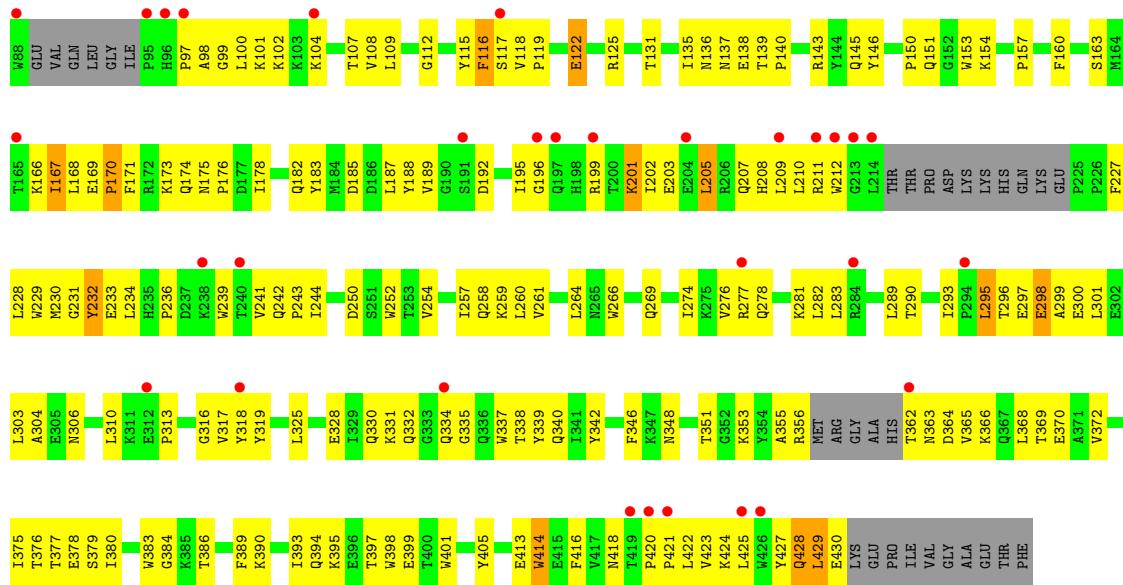
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 23	C 18	Cl 1	N 1	O 2	S 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Pol polyprotein, Reverse transcriptase, Chain A

- Molecule 2: Pol polyprotein, Reverse transcriptase, Chain B

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
$< I/\sigma(I) >$ [1]	2.25 (at 2.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221　,　0.281 0.213　,　0.228	Depositor DCC
R_{free} test set	1135 reflections (4.82%)	wwPDB-VP
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 , 88.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, H18, 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	0.51	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 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	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

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 33.

All (497) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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
1:A:70:LYS:HG3	1:A:71:TRP:H	1.38	0.85
2:B:169:GLU:O	2:B:173:LYS:HG3	1.75	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:57:ASN:HA	1:A:129:ALA:O	1.79	0.81
1:A:469:LEU:HD21	1:A:480:GLN:HG3	1.60	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:H	2:B:295:LEU:HD12	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
2:B:151:GLN:HB3	2:B:185:ASP:OD1	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE3	2:B:201:LYS:HA	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
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.74	0.69
2:B:169:GLU:HG2	2:B:170:PRO:HD3	1.74	0.69
1:A:102:LYS:HG3	1:A:237:ASP:HA	1.75	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:206:ARG:NH2	1:A:218:ASP:HA	2.08	0.68
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.26	0.68
1:A:206:ARG:CZ	1:A:217:PRO:O	2.42	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
1:A:177:ASP:OD2	1:A:193:LEU:HD21	1.94	0.67
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.75	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:HD2	1:A:208:HIS:O	1.79	0.65
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.31	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
1:A:174:GLN:HE21	1:A:174:GLN:HA	1.61	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:203:GLU:HG3	2:B:207:GLN:NE2	2.12	0.64
2:B:227:PHE:HB3	2:B:231:GLY:CA	2.26	0.64
1:A:92:LEU:HD23	1:A:92:LEU:O	1.97	0.64
2:B:104:LYS:HD2	2:B:192:ASP:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.96	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
1:A:317:VAL:HG22	1:A:318:TYR:H	1.64	0.62
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.34	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:N	1:A:195:ILE:CD1	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:HA	1:A:174:GLN:NE2	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:115:TYR:C	2:B:117:SER:H	2.05	0.60
2:B:241:VAL:O	2:B:243:PRO:HD3	2.02	0.60
1:A:507:GLN:HE22	2:B:421:PRO:HB3	1.67	0.60
2:B:85:GLN:O	2:B:85:GLN:HG3	2.01	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:101:LYS:HD2	1:A:101:LYS:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:VAL:C	1:A:293:ILE:HD12	2.21	0.59
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
1:A:89:GLU:OE1	1:A:89:GLU:HA	2.03	0.58
2:B:365:VAL:O	2:B:369:THR:HG23	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:OE1	2:B:298:GLU:N	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
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.34	0.57
1:A:491:LEU:HD23	1:A:529:GLU:CG	2.34	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: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:HD13	1:A:195:ILE:H	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:62:ALA:C	1:A:63:ILE:HD12	2.26	0.56
1:A:125:ARG:HG2	1:A:146:TYR:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ILE:O	2:B:208:HIS:CE1	2.58	0.56
1:A:491:LEU:HD23	1:A:529:GLU:HG2	1.86	0.56
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
1:A:116:PHE:N	1:A:116:PHE:CD2	2.74	0.55
1:A:440:PHE:HZ	1:A:463:ARG:HH21	1.53	0.55
2:B:31:ILE:O	2:B:35:VAL:HG23	2.06	0.55
2:B:332:GLN:CG	2:B:338:THR:HG23	2.37	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
1:A:27:THR:HG23	1:A:30:LYS:HB2	1.88	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
2:B:414:TRP:HD1	2:B:414:TRP:O	1.90	0.55
2:B:254:VAL:O	2:B:258:GLN:HG3	2.07	0.55
2:B:380:ILE:O	2:B:384:GLY:N	2.34	0.55
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.42	0.55
2:B:116:PHE:CE1	2:B:151:GLN:HG3	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
1:A:208:HIS:CD2	1:A:208:HIS:C	2.80	0.54
2:B:175:ASN:ND2	2:B:201:LYS:NZ	2.54	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:61:PHE:CE1	1:A:63:ILE:HD11	2.43	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLU:OE2	1:A:40:GLU:HA	2.08	0.53
1:A:376:THR:HG23	1:A:386:THR:CG2	2.39	0.53
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:175:ASN:N	2:B:176:PRO:HD3	2.22	0.53
1:A:358:ARG:NH2	2:B:394:GLN:HG2	2.24	0.53
2:B:203:GLU:OE2	2:B:207:GLN:NE2	2.40	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:56:TYR:O	1:A:143:ARG:NH2	2.35	0.52
1:A:70:LYS:HG3	1:A:71:TRP:N	2.16	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
1:A:469:LEU:HD21	1:A:480:GLN:CG	2.35	0.52
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.09	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
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
2:B:175:ASN:O	2:B:178:ILE:HB	2.10	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:146:TYR:CD2	2:B:150:PRO:HB3	2.45	0.51
2:B:297:GLU:HA	2:B:300:GLU:HB2	1.91	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:164:MET:HE1	1:A:168:LEU:HD21	1.92	0.51
1:A:225:PRO:HB3	1:A:236:PRO:HD3	1.92	0.51
2:B:306:ASN:O	2:B:310:LEU:HG	2.11	0.51
2:B:366:LYS:O	2:B:370:GLU:HG3	2.11	0.51
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.43	0.50
2:B:282:LEU:HB3	2:B:293:ILE:HG21	1.93	0.50
1:A:19:PRO:HD3	1:A:80:LEU:HD13	1.93	0.50
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.94	0.50
1:A:328:GLU:O	1:A:339:TYR:HA	2.10	0.50
1:A:406:TRP:HH2	2:B:418:ASN:OD1	1.94	0.50
1:A:70:LYS:CG	1:A:71:TRP:H	2.17	0.50
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
1:A:393:ILE:HD12	1:A:423:VAL:HG21	1.93	0.50
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.76	0.50
2:B:107:THR:HB	2:B:202:ILE:HD11	1.94	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: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
1:A:476:LYS:CD	1:A:517:LEU:HD12	2.41	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:207:GLN:NE2	1:A:210:LEU:HD12	2.27	0.49
1:A:278:GLN:NE2	1:A:278:GLN:HA	2.27	0.49
1:A:54:ASN:O	1:A:143:ARG:NH2	2.43	0.49
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.47	0.49
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.47	0.49
1:A:210:LEU:C	1:A:212:TRP:H	2.15	0.49
2:B:125:ARG:HB3	2:B:145:GLN:NE2	2.28	0.49
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.48	0.49
2:B:178:ILE:HD11	2:B:201:LYS:CG	2.40	0.49
1:A:10:VAL:O	1:A:11:LYS:HG3	2.13	0.49
2:B:328:GLU:CG	2:B:390:LYS:HD2	2.36	0.49
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.48	0.49
1:A:229:TRP:O	1:A:232:TYR:HB2	2.13	0.49
1:A:277:ARG:HG3	1:A:277:ARG:HH11	1.78	0.49
2:B:278:GLN:NE2	2:B:298:GLU:HB2	2.28	0.49
2:B:423:VAL:O	2:B:427:TYR:HD2	1.96	0.49
2:B:295:LEU:N	2:B:295:LEU:CD1	2.75	0.48
1:A:63:ILE:HD12	1:A:63:ILE:N	2.28	0.48
1:A:108:VAL:HG12	1:A:223:LYS:O	2.13	0.48
2:B:170:PRO:HA	2:B:173:LYS:HZ3	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:131:THR:OG1	1:A:143:ARG:CD	2.62	0.48
1:A:399:GLU:HG3	1:A:402:TRP:HE3	1.75	0.48
2:B:319:TYR:HE2	2:B:325:LEU:HD13	1.78	0.48
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:HG3	1:A:145:GLN:O	2.14	0.48
1:A:86:ASP:CA	1:A:154:LYS:HZ1	2.25	0.48
1:A:231:GLY:O	1:A:266:TRP:CZ2	2.67	0.47
1:A:293:ILE:HD12	1:A:293:ILE:N	2.29	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:130:PHE:CE2	1:A:144:TYR:HB2	2.50	0.47
1:A:225:PRO:CB	1:A:236:PRO:HD3	2.44	0.47
1:A:254:VAL:CG2	1:A:293:ILE:HD11	2.45	0.47
1:A:469:LEU:CD2	1:A:480:GLN:HG3	2.40	0.47
1:A:518:VAL:O	1:A:522:ILE:HG13	2.15	0.47
2:B:99:GLY:HA2	2:B:102:LYS:HE2	1.96	0.47
1:A:136:ASN:OD1	1:A:139:THR:HG23	2.14	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
2:B:108:VAL:HG12	2:B:228:LEU:HD12	1.96	0.47
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.49	0.47
2:B:379:SER:HA	2:B:383:TRP:CE3	2.50	0.47
1:A:346:PHE:N	1:A:346:PHE:CD1	2.82	0.46
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.97	0.46
1:A:340:GLN:HA	1:A:351:THR:HA	1.96	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:238:LYS:NZ	1:A:315:HIS:CD2	2.83	0.46
1:A:24:TRP:CZ3	1:A:61:PHE:HB3	2.51	0.46
1:A:164:MET:CE	1:A:168:LEU:HD11	2.45	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
2:B:169:GLU:N	2:B:170:PRO:CD	2.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:HG23	2:B:196:GLY:N	2.31	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:117:SER:OG	1:A:214:LEU:HD23	2.16	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:408:ALA:HB2	2:B:337:TRP:HH2	1.80	0.46
2:B:393:ILE:HD11	2:B:397:THR:CG2	2.46	0.46
1:A:417:VAL:O	1:A:417:VAL:CG1	2.61	0.46
1:A:486:LEU:HD13	1:A:524:GLN:HB2	1.98	0.46
2:B:174:GLN:C	2:B:176:PRO:HD3	2.36	0.46
2:B:195:ILE:CG2	2:B:196:GLY:N	2.79	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:238:LYS:HD2	1:A:315:HIS:CD2	2.51	0.45
1:A:317:VAL:CG2	1:A:318:TYR:N	2.76	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:18:GLY:HA3	1:A:56:TYR:CE1	2.52	0.45
1:A:28:GLU:OE1	1:A:135:ILE:CG2	2.61	0.45
1:A:306:ASN:O	1:A:310:LEU:HG	2.15	0.45
1:A:363:ASN:ND2	1:A:401:TRP:CH2	2.84	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:108:VAL:HG22	2:B:188:TYR:CD2	2.52	0.44
2:B:264:LEU:HD13	2:B:306:ASN:ND2	2.32	0.44
2:B:208:HIS:O	2:B:208:HIS:ND1	2.50	0.44
1:A:40:GLU:OE2	1:A:40:GLU:CA	2.65	0.44
1:A:240:THR:OG1	1:A:241:VAL:N	2.50	0.44
1:A:395:LYS:O	1:A:399:GLU:HB2	2.17	0.44
1:A:222:GLN:HB3	1:A:223:LYS:H	1.69	0.44
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.47	0.44
1:A:142:ILE:HD12	1:A:144:TYR:OH	2.17	0.44
1:A:324:ASP:O	1:A:343:GLN:HG2	2.17	0.44
2:B:234:LEU:N	2:B:234:LEU:HD12	2.32	0.44
2:B:278:GLN:HB3	2:B:299:ALA:HA	2.00	0.44
1:A:34:LEU:HD13	1:A:132:ILE:CD1	2.47	0.44
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.52	0.44
1:A:48:SER:O	1:A:50:ILE:HG23	2.16	0.44
1:A:332:GLN:HB3	1:A:336:GLN:HB3	2.00	0.44
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.48	0.44
2:B:339:TYR:CD1	2:B:375:ILE:HD11	2.53	0.44
2:B:414:TRP:O	2:B:414:TRP:CD1	2.71	0.44
2:B:429:LEU:CD1	2:B:430:GLU:N	2.81	0.44
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
2:B:154:LYS:O	2:B:157:PRO:HD2	2.18	0.43
1:A:95:PRO:HG2	1:A:181:TYR:CE2	2.53	0.43
1:A:237:ASP:OD2	1:A:237:ASP:N	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:296:THR:CG2	1:A:297:GLU:N	2.81	0.43
1:A:317:VAL:CG2	1:A:318:TYR:H	2.28	0.43
1:A:326:ILE:O	1:A:341:ILE:HA	2.19	0.43
1:A:360:ALA:HB1	1:A:514:GLU:OE1	2.18	0.43
1:A:401:TRP:CH2	1:A:508:ALA:O	2.71	0.43
2:B:228:LEU:HD23	2:B:228:LEU:HA	1.91	0.43
2:B:264:LEU:CD1	2:B:306:ASN:HD22	2.32	0.43
1:A:218:ASP:O	1:A:222:GLN:HG3	2.18	0.43
1:A:253:THR:CG2	1:A:255:ASN:H	2.07	0.43
2:B:100:LEU:O	2:B:100:LEU:HD12	2.19	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:472:THR:CB	1:A:476:LYS:HE3	2.48	0.43
2:B:201:LYS:HD3	2:B:201:LYS:C	2.38	0.43
1:A:131:THR:OG1	1:A:143:ARG:HD3	2.18	0.43
2:B:229:TRP:HA	2:B:229:TRP:CE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:C	1:A:212:TRP:N	2.71	0.43
1:A:253:THR:CG2	1:A:289:LEU:O	2.67	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
1:A:277:ARG:HG3	1:A:277:ARG:NH1	2.33	0.43
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.49	0.43
1:A:177:ASP:OD1	1:A:177:ASP:N	2.48	0.42
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:23:GLN:NE2	1:A:24:TRP:O	2.41	0.42
1:A:206:ARG:HH12	1:A:219:LYS:N	2.17	0.42
1:A:265:ASN:N	1:A:265:ASN:HD22	2.17	0.42
1:A:296:THR:HG22	1:A:298:GLU:H	1.85	0.42
2:B:112:GLY:HA3	2:B:151:GLN:OE1	2.18	0.42
1:A:224:GLU:HB3	1:A:225:PRO:CD	2.49	0.42
1:A:433:PRO:HB3	2:B:289:LEU:HD23	2.01	0.42
2:B:376:THR:O	2:B:377:THR:C	2.57	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
1:A:283:LEU:C	1:A:286:THR:HG23	2.40	0.42
2:B:104:LYS:CB	2:B:192:ASP:HA	2.46	0.42
2:B:182:GLN:HA	2:B:187:LEU:HD12	2.01	0.42
2:B:208:HIS:O	2:B:208:HIS:CG	2.72	0.42
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.54	0.42
2:B:355:ALA:O	2:B:356:ARG:C	2.57	0.42
2:B:378:GLU:O	2:B:379:SER:C	2.58	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:O	2:B:160:PHE:CD1	2.73	0.42
1:A:207:GLN:CD	1:A:210:LEU:HD12	2.40	0.42
1:A:63:ILE:HD13	1:A:74:LEU:HB3	2.00	0.41
1:A:233:GLU:HB3	1:A:240:THR:CG2	2.48	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:156:SER:N	1:A:157:PRO:CD	2.83	0.41
1:A:174:GLN:O	1:A:176:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:173:LYS:O	2:B:176:PRO:CD	2.66	0.41
1:A:116:PHE:H	1:A:116:PHE:HD2	1.68	0.41
2:B:136:ASN:O	2:B:137:ASN:C	2.58	0.41
1:A:160:PHE:CE2	1:A:164:MET:HG2	2.55	0.41
1:A:282:LEU:HB3	1:A:293:ILE:HG21	2.02	0.41
1:A:457:TYR:CD1	1:A:457:TYR:C	2.94	0.41
1:A:23:GLN:HE21	1:A:26:LEU:HG	1.86	0.41
1:A:324:ASP:O	1:A:343:GLN:HA	2.20	0.41
2:B:393:ILE:HG12	2:B:394:GLN: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
1:A:253:THR:HG22	1:A:254:VAL:N	2.36	0.41
2:B:259:LYS:HE2	2:B:259:LYS:HB3	1.82	0.41
1:A:116:PHE:N	1:A:116:PHE:HD2	2.19	0.41
1:A:175:ASN:OD1	1:A:201:LYS:HE2	2.20	0.41
1:A:226:PRO:HB3	1:A:235:HIS:ND1	2.36	0.41
1:A:396:GLU:HG3	1:A:397:THR:N	2.36	0.41
1:A:440:PHE:CD2	1:A:459:THR:HG22	2.56	0.41
2:B:429:LEU:HD13	2:B:430:GLU:N	2.36	0.41
1:A:33:ALA:O	1:A:37:ILE:HG13	2.21	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:338:THR:HG21	2:B:427:TYR:O	2.20	0.41
2:B:340:GLN:CG	2:B:351:THR:HG22	2.51	0.41
1:A:22:LYS:HG2	1:A:23:GLN:N	2.36	0.40
1:A:84:THR:O	1:A:154:LYS:NZ	2.53	0.40
1:A:164:MET:HE3	1:A:168:LEU:HD11	2.02	0.40
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.56	0.40
2:B:21:VAL:CG1	2:B:59:PRO:CG	2.99	0.40
2:B:395:LYS:HZ3	2:B:399:GLU:CG	2.34	0.40
1:A:171:PHE:CE1	1:A:205:LEU:CA	3.01	0.40
1:A:195:ILE:HG12	1:A:196:GLY:H	1.85	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
2:B:269:GLN:OE1	2:B:346:PHE:CZ	2.75	0.40
1:A:393:ILE:HD12	1:A:423:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:VAL:O	2:B:317:VAL:HG12	2.21	0.40
1:A:27:THR:CG2	1:A:30:LYS:HG3	2.51	0.40
1:A:216:THR:HB	1:A:217:PRO:HD2	2.03	0.40
2:B:298:GLU:CD	2:B:298:GLU:N	2.73	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%)	4	16
2	B	390/440 (89%)	349 (90%)	34 (9%)	7 (2%)	8	29
All	All	900/1000 (90%)	798 (89%)	79 (9%)	23 (3%)	5	20

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

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Mol	Chain	Res	Type
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%)	14	40
2	B	365/400 (91%)	348 (95%)	17 (5%)	26	59
All	All	831/899 (92%)	781 (94%)	50 (6%)	19	49

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

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Mol	Chain	Res	Type
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
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

Sometimes 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
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 molecules 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	3,7,8	0.76	0	1,8,10	7.42	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	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	CSD	OD1-SG-CB	7.42	119.66	105.54

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.

No monomer is involved in short contacts.

5.5　Carbohydrates ⓘ

There are no monosaccharides 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	#$|Z| > 2$
4	H18	A	999	-	23,25,25	3.03	13 (56%)	27,35,35	2.31	8 (29%)
3	PO4	A	1302	-	4,4,4	1.57	0	6,6,6	0.44	0
3	PO4	A	1300	-	4,4,4	1.61	0	6,6,6	0.42	0
3	PO4	A	1301	-	4,4,4	1.75	0	6,6,6	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	H18	A	999	-	-	4/11/19/19	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	H18	C6-N1	7.10	1.45	1.33
4	A	999	H18	C5-C6	5.75	1.53	1.41
4	A	999	H18	CF-CA	5.75	1.61	1.52
4	A	999	H18	C2-N1	4.28	1.42	1.35
4	A	999	H18	C3-C2	3.56	1.48	1.42
4	A	999	H18	C7-C8	3.21	1.42	1.36
4	A	999	H18	C10-C9	2.96	1.42	1.36
4	A	999	H18	C8-CL	-2.67	1.68	1.74
4	A	999	H18	C9-C8	2.62	1.43	1.38
4	A	999	H18	C5-C4	2.57	1.44	1.41
4	A	999	H18	CE-CF	2.27	1.59	1.53
4	A	999	H18	O2-C6	2.19	1.30	1.24
4	A	999	H18	CB-CA	2.10	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	999	H18	C4-S4-CA	7.75	106.82	97.74
4	A	999	H18	C2-N1-C6	4.34	122.78	116.83
4	A	999	H18	C3-C2-N1	-3.52	120.06	123.35
4	A	999	H18	CE-CF-CA	3.36	117.26	110.49
4	A	999	H18	OS-S4-C4	2.79	110.34	106.90
4	A	999	H18	CD-CE-CF	2.69	116.90	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	999	H18	C12-C11-C5	-2.29	107.85	113.26
4	A	999	H18	CF-CA-CB	2.28	113.76	111.59

There are no chirality outliers.

All (4) torsion outliers are listed below:
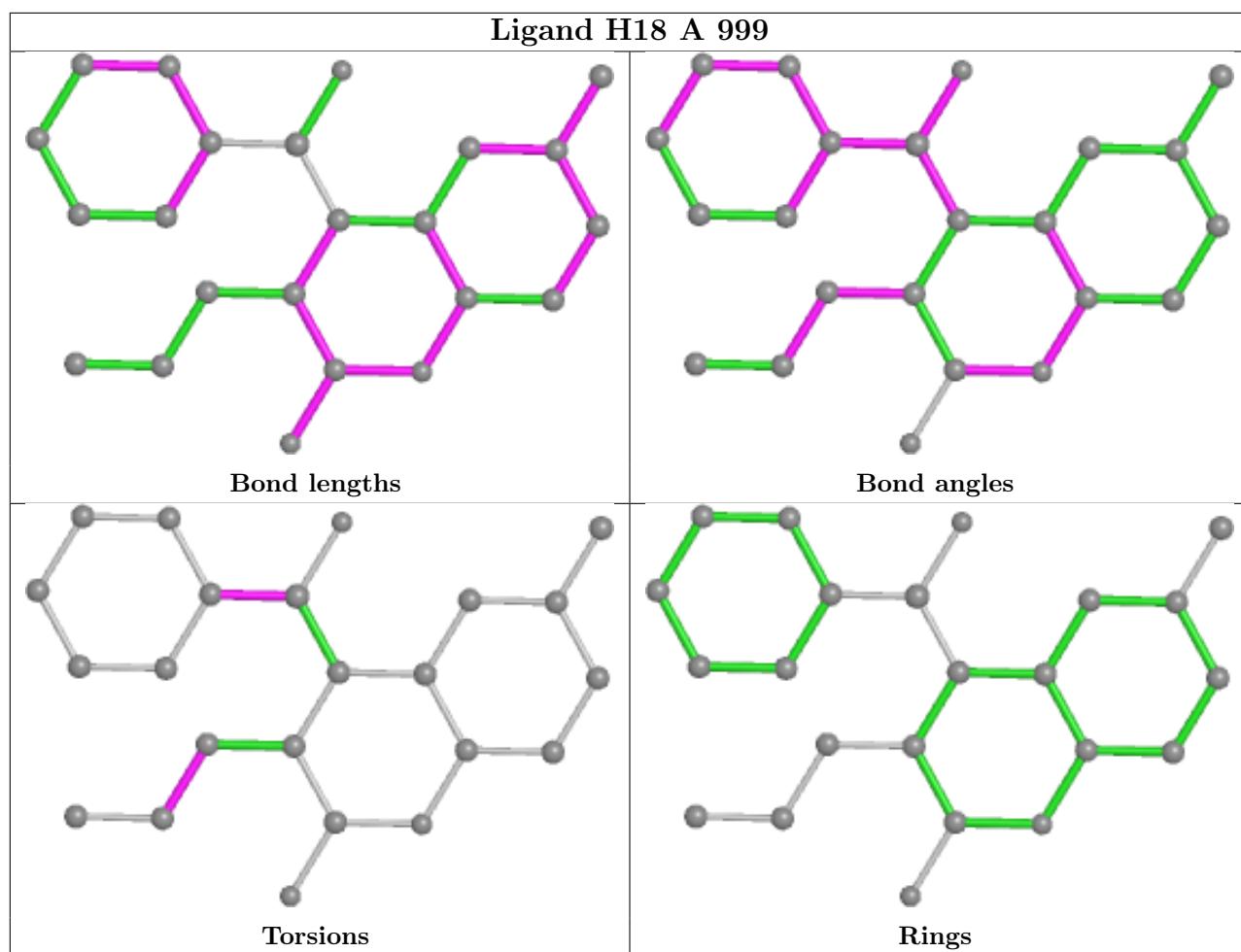
Mol	Chain	Res	Type	Atoms
4	A	999	H18	CB-CA-S4-C4
4	A	999	H18	CF-CA-S4-C4
4	A	999	H18	C5-C11-C12-C13
4	A	999	H18	CF-CA-S4-OS

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	H18	5	0
3	A	1301	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand H18 A 999

Bond lengths

Bond angles

Torsions

Rings

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	516/560 (92%)	0.24	36 (6%)	16	12	28, 65, 110, 139	0
2	B	400/440 (90%)	0.15	33 (8%)	11	8	28, 60, 117, 148	0
All	All	916/1000 (91%)	0.20	69 (7%)	14	11	28, 64, 113, 148	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	334	GLN	7.9
2	B	214	LEU	6.1
1	A	138	GLU	5.1
2	B	421	PRO	5.0
1	A	116	PHE	4.9
1	A	469	LEU	4.8
1	A	139	THR	4.7
2	B	312	GLU	4.4
1	A	251	SER	4.3
2	B	213	GLY	4.2
2	B	88	TRP	3.9
2	B	197	GLN	3.7
1	A	396	GLU	3.7
1	A	140	PRO	3.7
1	A	472	THR	3.6
2	B	419	THR	3.6
1	A	402	TRP	3.4
1	A	404	GLU	3.4
2	B	96	HIS	3.4
1	A	228	LEU	3.3
2	B	64	LYS	3.3
2	B	284	ARG	3.2
2	B	212	TRP	3.2
2	B	318	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	313	PRO	3.2
2	B	426	TRP	3.1
2	B	204	GLU	3.1
2	B	240	THR	3.1
1	A	15	GLY	3.1
2	B	117	SER	3.1
1	A	20	LYS	3.0
2	B	362	THR	3.0
2	B	165	THR	3.0
2	B	294	PRO	3.0
1	A	82	LYS	3.0
2	B	95	PRO	2.9
1	A	144	TYR	2.9
1	A	193	LEU	2.9
1	A	27	THR	2.8
1	A	22	LYS	2.8
1	A	14	PRO	2.8
2	B	15	GLY	2.8
2	B	420	PRO	2.8
2	B	191	SER	2.7
2	B	425	LEU	2.6
2	B	211	ARG	2.6
1	A	43	LYS	2.6
1	A	221	HIS	2.6
2	B	277	ARG	2.5
1	A	244	ILE	2.4
1	A	287	LYS	2.3
1	A	322	SER	2.3
2	B	97	PRO	2.3
2	B	104	LYS	2.3
1	A	92	LEU	2.3
1	A	56	TYR	2.3
1	A	346	PHE	2.3
1	A	311	LYS	2.3
1	A	409	THR	2.2
1	A	312	GLU	2.1
2	B	196	GLY	2.1
1	A	471	ASP	2.1
1	A	344	GLU	2.1
2	B	199	ARG	2.1
1	A	212	TRP	2.1
1	A	210	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	238	LYS	2.1
2	B	209	LEU	2.1
1	A	516	GLU	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSD	A	280	8/9	0.94	0.17	51,55,65,74	0

6.3 Carbohydrates ⓘ
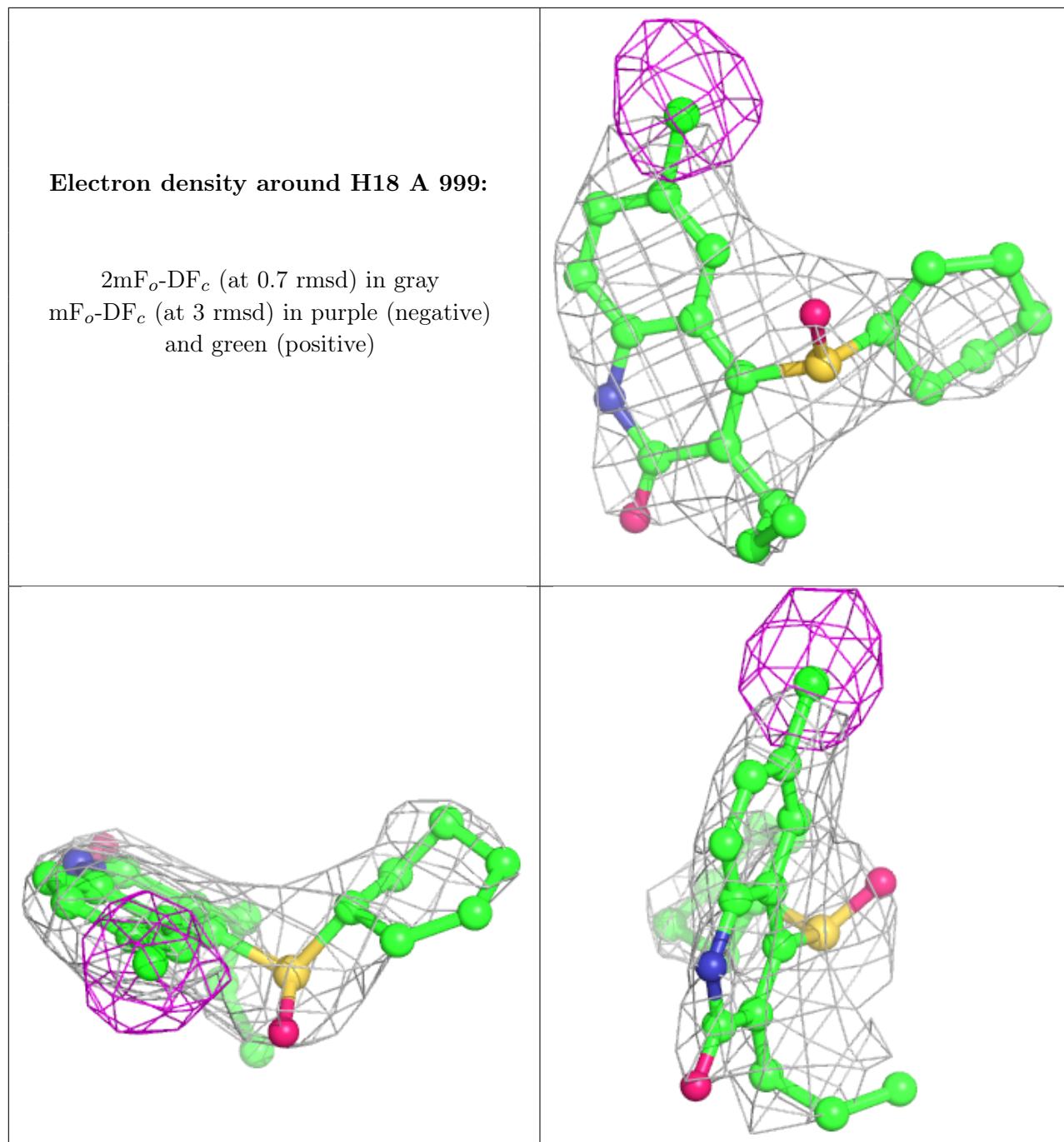
There are no monosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	A	1300	5/5	0.61	0.20	137,140,144,146	0
4	H18	A	999	23/23	0.86	0.26	45,66,78,88	0
3	PO4	A	1301	5/5	0.87	0.23	123,124,129,131	0
3	PO4	A	1302	5/5	0.88	0.26	150,150,150,150	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around H18 A 999:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.