Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 02:09 PM EDT

PDB ID	:	1EP4
Title	:	Crystal structure of HIV-1 reverse transcriptase in complex with S-1153
Authors	:	Ren, J.; Nichols, C.; Bird, L.E.; Fujiwara, T.; Suginoto, H.; Stuart, D.I.; Stammers, D.K.
Deposited on	:	2000-03-27
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

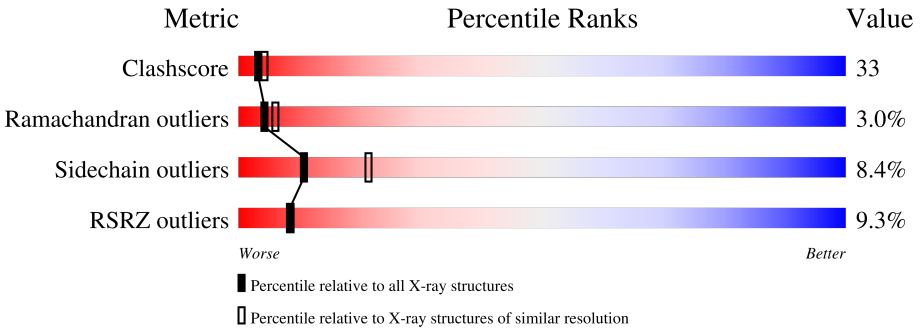
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	9%; 44%, 42%, 7%, •, 7%
2	B	440	8%; 42%, 42%, 5%, 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7791 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

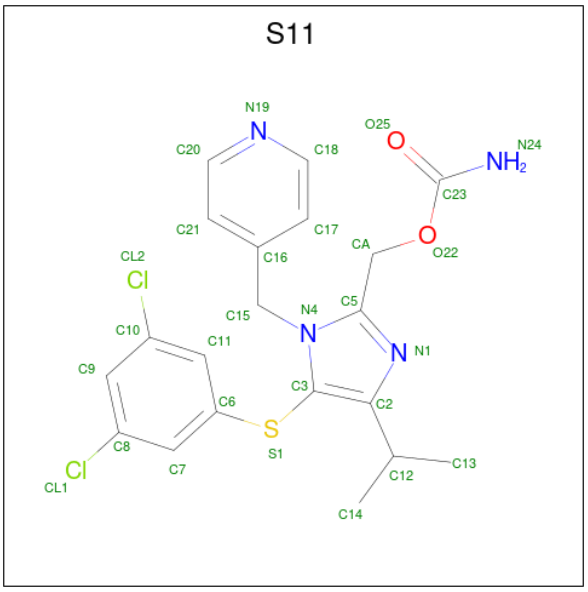
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	523	4288	2778	712	790	8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	395	3277	2135	541	595	6	0	0	0

- Molecule 3 is 5-(3,5-DICHLOROPHENYL)THIO-4-ISOPROPYL-1-(PYRIDIN-4-YL-METHYL)-1H-IMIDAZOL-2-YL-METHYL CARBAMATE (three-letter code: S11) (formula: $C_{20}H_{20}Cl_2N_4O_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
3	A	1	29	20	2	4	2	1	0	0

- Molecule 4 is water.

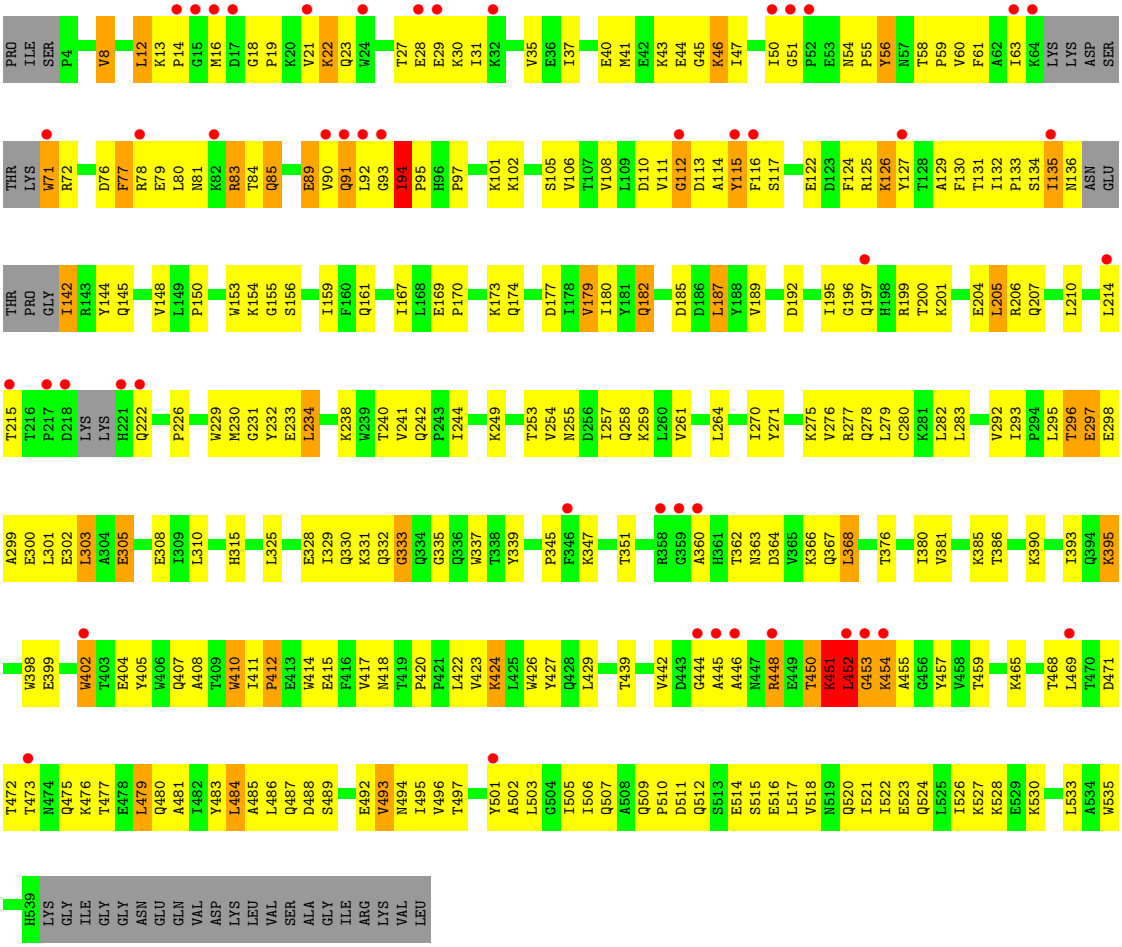
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	121	121	121	0	0
			Total	O		
4	B	76	76	76	0	0

3 Residue-property plots (i)

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.

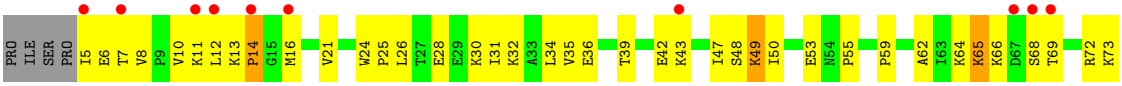
• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE

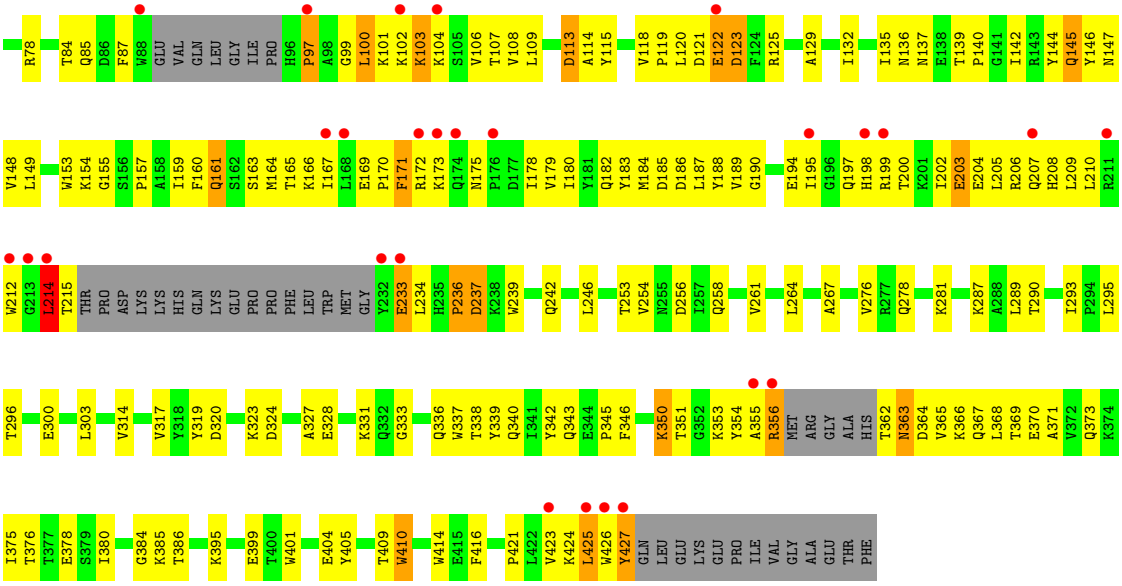
Chain A: 9% 44% 42% 7% • 7%



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE

Chain B: 8% 42% 42% 5% 10%




R78
T84
Q85
D86
F87
W88
GLU
VAL
GLN
LEU
GLY
ILE
PRO
H96
P97
A98
G99
L100
K101
K102
K103
K104
S105
V106
T107
V108
L109
D113
A114
Y115
V118
P119
L120
D121
E122
D123
F124
R125
A129
I132
I135
N136
N137
E138
T139
P140
G141
I142
R143
Y144
Q145
Y146
N147
V148
L149
W153
K154
G155
S156
P157
A158
I159
F160
Q161
S162
S163
M164
T165
K166
I167
L168
E169
P170
F171
R172
K173
Q174
N175
P176
D177
I178
V179
I180
Y181
Q182
Y183
M184
D185
D186
L187
Y188
V189
G190
E194
I195
G196
Q197
H198
R199
T200
K201
I202
E203
E204
L205
R206
Q207
H208
L209
L210
R211
W212
G213
L214
T215
THR
PRO
ASP
LYS
LYS
HIS
GLN
LYS
GLU
PRO
PRO
PHE
LEU
TRP
MET
GLY
Y232
E233
L234
H235
P236
D237
K238
W239
Q242
L246
T253
V254
M255
D256
I257
Q258
V261
L264
A267
V276
R277
Q278
K281
K287
A288
L289
T290
I293
P294
L295
T296
E300
L303
V314
V317
Y318
Y319
D320
K323
D324
A327
E328
K331
Q332
G333
Q336
W337
T338
Y339
Q340
I341
Y342
Q343
E344
P345
F346
K350
T351
G352
K353
Y354
A355
R356
MET
ARG
GLY
ALA
HIS
T362
N363
D364
V365
K366
Q367
L368
T369
E370
A371
V372
Q373
K374
I375
T376
T377
E378
S379
I380
G384
K385
T386
K395
E399
T400
W401
E404
Y405
T409
W410
W414
E415
F416
P421
L422
V423
K424
L425
W426
Y427
GLN
LEU
GLU
LYS
GLU
PRO
ILE
VAL
GLY
ALA
GLU
THR
PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	135.70Å 118.00Å 67.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 27.02 – 2.48	Depositor EDS
% Data completeness (in resolution range)	91.0 (30.00-2.50) 90.0 (27.02-2.48)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.98 (at 2.47Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.254 , 0.330 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	56.2	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 80.3	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	0.94	EDS
Total number of atoms	7791	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: S11, 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	0.47	0/4392	0.70	3/5969 (0.1%)
2	B	0.46	0/3368	0.70	0/4574
All	All	0.47	0/7760	0.70	3/10543 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	94	ILE	C-N-CD	-6.23	106.89	120.60
1	A	451	LYS	N-CA-C	5.64	126.24	111.00
1	A	452	LEU	N-CA-C	-5.43	96.33	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4288	0	4315	307	0
2	B	3277	0	3306	214	0
3	A	29	0	20	2	0
4	A	121	0	0	9	0
4	B	76	0	0	10	0
All	All	7791	0	7641	505	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 (505) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:GLU:HB3	2:B:197:GLN:HB2	1.33	1.11
1:A:451:LYS:H	1:A:451:LYS:HE2	0.95	1.06
2:B:50:ILE:HG21	2:B:145:GLN:HB3	1.37	1.03
2:B:84:THR:HG21	2:B:153:TRP:HE1	1.21	1.01
1:A:451:LYS:CD	1:A:472:THR:H	1.73	1.01
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.46	0.98
2:B:100:LEU:HD23	2:B:100:LEU:H	1.28	0.96
1:A:451:LYS:HE2	1:A:451:LYS:N	1.79	0.96
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.47	0.94
1:A:19:PRO:O	1:A:56:TYR:HB3	1.67	0.93
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.52	0.91
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.51	0.91
1:A:451:LYS:HD3	1:A:472:THR:H	1.32	0.91
1:A:451:LYS:H	1:A:451:LYS:CE	1.84	0.90
1:A:465:LYS:HE3	1:A:484:LEU:HD11	1.54	0.89
2:B:423:VAL:HG23	2:B:426:TRP:HB2	1.54	0.89
1:A:31:ILE:O	1:A:35:VAL:HG23	1.72	0.88
1:A:452:LEU:O	1:A:452:LEU:HG	1.74	0.88
2:B:170:PRO:HB2	2:B:208:HIS:CE1	2.09	0.87
1:A:516:GLU:O	1:A:520:GLN:HG3	1.73	0.87
1:A:195:ILE:HD12	1:A:199:ARG:HH12	1.38	0.86
1:A:444:GLY:HA3	1:A:477:THR:HG22	1.57	0.85
2:B:164:MET:O	2:B:167:ILE:HG13	1.76	0.85
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.56	0.84
1:A:46:LYS:HD2	1:A:116:PHE:HB3	1.59	0.84
1:A:332:GLN:HG2	1:A:333:GLY:H	1.43	0.83
1:A:363:ASN:HB2	1:A:511:ASP:OD2	1.78	0.83
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.10	0.82
1:A:29:GLU:HG2	1:A:71:TRP:HZ2	1.46	0.81
1:A:457:TYR:HE2	1:A:484:LEU:HD12	1.46	0.81
1:A:296:THR:HG22	1:A:299:ALA:H	1.44	0.80
1:A:301:LEU:HD11	1:A:305:GLU:OE1	1.82	0.80
2:B:363:ASN:ND2	2:B:366:LYS:H	1.79	0.80
2:B:107:THR:HG21	2:B:202:ILE:HG12	1.62	0.80
2:B:50:ILE:CG2	2:B:145:GLN:HB3	2.10	0.80
1:A:150:PRO:HG2	1:A:153:TRP:HB2	1.64	0.79
1:A:94:ILE:HG22	1:A:95:PRO:C	2.02	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:ILE:HG22	2:B:189:VAL:HG22	1.62	0.79
1:A:177:ASP:HA	4:A:1010:HOH:O	1.80	0.79
2:B:287:LYS:HD2	2:B:293:ILE:HD11	1.65	0.79
2:B:200:THR:O	2:B:204:GLU:HG3	1.82	0.79
2:B:10:VAL:HG13	2:B:87:PHE:HZ	1.49	0.78
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.67	0.77
2:B:69:THR:HG22	2:B:69:THR:O	1.85	0.76
1:A:523:GLU:O	1:A:527:LYS:HG3	1.85	0.76
1:A:451:LYS:HD2	1:A:471:ASP:N	2.01	0.75
2:B:104:LYS:HA	2:B:237:ASP:OD1	1.87	0.75
2:B:163:SER:O	2:B:167:ILE:HG23	1.87	0.75
2:B:210:LEU:HG	2:B:215:THR:HA	1.68	0.74
2:B:210:LEU:O	2:B:210:LEU:HD23	1.87	0.74
1:A:132:ILE:O	1:A:142:ILE:HD12	1.88	0.74
2:B:171:PHE:O	2:B:175:ASN:HB2	1.88	0.73
1:A:452:LEU:HD11	1:A:454:LYS:HD3	1.71	0.73
1:A:95:PRO:HB3	2:B:136:ASN:O	1.90	0.72
2:B:170:PRO:HB2	2:B:208:HIS:NE2	2.05	0.72
2:B:369:THR:O	2:B:373:GLN:HG3	1.91	0.71
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.72	0.71
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.73	0.71
2:B:8:VAL:HG21	2:B:159:ILE:HG23	1.73	0.70
2:B:424:LYS:HE2	4:B:1051:HOH:O	1.91	0.70
2:B:189:VAL:HG11	2:B:202:ILE:HG13	1.74	0.69
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.23	0.69
1:A:210:LEU:HD12	1:A:215:THR:HA	1.74	0.69
1:A:398:TRP:CZ2	1:A:411:ILE:HB	2.28	0.69
2:B:338:THR:HG22	2:B:353:LYS:HG2	1.74	0.69
2:B:28:GLU:HG2	2:B:32:LYS:HE3	1.74	0.68
1:A:411:ILE:HD12	1:A:412:PRO:HD2	1.75	0.68
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.75	0.68
1:A:200:THR:O	1:A:204:GLU:HG3	1.94	0.68
2:B:24:TRP:HB2	4:B:1065:HOH:O	1.93	0.67
1:A:507:GLN:HE21	1:A:507:GLN:HA	1.59	0.67
1:A:442:VAL:HG11	1:A:485:ALA:HB2	1.77	0.67
2:B:194:GLU:CB	2:B:197:GLN:HB2	2.20	0.67
1:A:278:GLN:NE2	1:A:278:GLN:HA	2.10	0.67
1:A:451:LYS:HD2	1:A:471:ASP:CA	2.25	0.66
1:A:453:GLY:O	1:A:469:LEU:N	2.29	0.66
1:A:507:GLN:HA	1:A:507:GLN:NE2	2.10	0.66
2:B:425:LEU:HD23	2:B:425:LEU:H	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLU:CD	1:A:92:LEU:HD23	2.16	0.66
1:A:451:LYS:HD2	1:A:472:THR:H	1.58	0.66
1:A:114:ALA:HA	1:A:117:SER:CB	2.26	0.66
2:B:42:GLU:HA	2:B:47:ILE:O	1.95	0.66
1:A:180:ILE:HG12	1:A:189:VAL:HG22	1.78	0.66
1:A:94:ILE:HG22	1:A:95:PRO:CA	2.25	0.66
2:B:10:VAL:HG13	2:B:87:PHE:CZ	2.31	0.66
1:A:27:THR:O	1:A:31:ILE:HG13	1.97	0.65
2:B:107:THR:CG2	2:B:189:VAL:HB	2.27	0.65
2:B:100:LEU:HD23	2:B:100:LEU:N	2.08	0.65
2:B:157:PRO:HG2	2:B:184:MET:HA	1.78	0.65
1:A:170:PRO:O	1:A:173:LYS:HB2	1.96	0.65
1:A:448:ARG:H	1:A:448:ARG:NE	1.94	0.65
1:A:451:LYS:CD	1:A:472:THR:N	2.55	0.65
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.78	0.65
1:A:21:VAL:HG13	1:A:59:PRO:CD	2.27	0.64
1:A:114:ALA:HB1	1:A:214:LEU:HD13	1.77	0.64
2:B:194:GLU:HB3	2:B:197:GLN:CB	2.19	0.64
1:A:132:ILE:O	1:A:142:ILE:N	2.30	0.64
2:B:99:GLY:HA2	2:B:102:LYS:HD2	1.79	0.64
1:A:71:TRP:HA	1:A:71:TRP:CE3	2.33	0.64
2:B:363:ASN:HD21	2:B:366:LYS:H	1.45	0.64
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.80	0.63
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.79	0.63
2:B:366:LYS:O	2:B:370:GLU:HG3	1.98	0.63
1:A:167:ILE:O	1:A:170:PRO:HD2	1.97	0.63
1:A:278:GLN:HA	1:A:278:GLN:HE21	1.62	0.63
2:B:180:ILE:HA	2:B:188:TYR:O	1.99	0.63
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.34	0.63
1:A:63:ILE:HG13	1:A:72:ARG:HB3	1.81	0.63
1:A:135:ILE:HG22	1:A:136:ASN:ND2	2.14	0.63
1:A:19:PRO:HG2	1:A:80:LEU:HB2	1.80	0.62
1:A:113:ASP:C	1:A:115:TYR:H	2.03	0.62
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.81	0.62
1:A:29:GLU:HG2	1:A:71:TRP:CZ2	2.31	0.62
1:A:296:THR:HG22	1:A:299:ALA:N	2.14	0.62
1:A:418:ASN:O	1:A:420:PRO:HD3	1.98	0.62
1:A:94:ILE:HG22	1:A:95:PRO:O	1.99	0.62
2:B:101:LYS:HA	2:B:236:PRO:HB3	1.82	0.62
1:A:31:ILE:HG12	1:A:133:PRO:HG2	1.82	0.62
2:B:13:LYS:HG2	2:B:85:GLN:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:GLU:HA	2:B:206:ARG:HD2	1.80	0.62
2:B:31:ILE:O	2:B:35:VAL:HG12	1.99	0.62
2:B:278:GLN:O	2:B:281:LYS:HB2	2.00	0.62
1:A:114:ALA:HA	1:A:117:SER:HB2	1.81	0.61
2:B:132:ILE:HB	2:B:142:ILE:HB	1.81	0.61
1:A:142:ILE:HD12	1:A:142:ILE:N	2.16	0.61
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.82	0.61
1:A:410:TRP:HA	1:A:410:TRP:CE3	2.35	0.61
2:B:115:TYR:OH	2:B:157:PRO:HG3	2.00	0.61
1:A:518:VAL:O	1:A:522:ILE:HG13	2.01	0.61
1:A:411:ILE:CD1	1:A:412:PRO:HD2	2.31	0.60
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.36	0.60
2:B:84:THR:HG21	2:B:153:TRP:NE1	2.05	0.60
1:A:79:GLU:O	1:A:83:ARG:HD3	2.02	0.60
1:A:325:LEU:HD12	1:A:385:LYS:HD2	1.84	0.60
1:A:451:LYS:HD3	1:A:472:THR:N	2.10	0.60
1:A:40:GLU:O	1:A:44:GLU:HG3	2.02	0.60
1:A:111:VAL:HG22	1:A:185:ASP:O	2.02	0.60
2:B:363:ASN:HB2	4:B:1054:HOH:O	2.02	0.60
2:B:8:VAL:O	2:B:121:ASP:HB2	2.02	0.59
1:A:507:GLN:HE21	1:A:507:GLN:CA	2.14	0.59
1:A:410:TRP:HA	1:A:410:TRP:HE3	1.67	0.59
2:B:99:GLY:O	2:B:103:LYS:HG2	2.02	0.59
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.37	0.59
1:A:23:GLN:HB2	1:A:131:THR:CG2	2.32	0.59
2:B:165:THR:HG22	2:B:172:ARG:NH2	2.18	0.59
1:A:111:VAL:HG23	1:A:112:GLY:N	2.17	0.59
1:A:296:THR:HG23	1:A:298:GLU:OE1	2.03	0.59
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.85	0.59
1:A:19:PRO:O	1:A:56:TYR:CB	2.46	0.59
1:A:257:ILE:HD12	1:A:293:ILE:HD12	1.85	0.59
1:A:337:TRP:HE1	1:A:367:GLN:NE2	2.01	0.59
1:A:135:ILE:H	1:A:135:ILE:CD1	2.16	0.59
1:A:253:THR:O	1:A:257:ILE:HG13	2.01	0.59
1:A:446:ALA:C	1:A:452:LEU:HD23	2.23	0.59
1:A:455:ALA:HB2	1:A:477:THR:HG23	1.84	0.59
1:A:486:LEU:CB	1:A:524:GLN:HG2	2.27	0.59
1:A:452:LEU:O	1:A:454:LYS:N	2.37	0.58
1:A:524:GLN:HE21	1:A:528:LYS:HE2	1.68	0.58
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.32	0.58
1:A:424:LYS:HB2	1:A:424:LYS:NZ	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LEU:O	1:A:454:LYS:HG2	2.03	0.58
2:B:169:GLU:CG	2:B:173:LYS:HB2	2.33	0.58
2:B:320:ASP:OD2	2:B:323:LYS:HE3	2.02	0.58
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.69	0.58
1:A:395:LYS:HE2	1:A:399:GLU:OE2	2.04	0.58
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.37	0.58
1:A:23:GLN:HE22	1:A:60:VAL:H	1.50	0.58
2:B:102:LYS:O	2:B:237:ASP:HB3	2.03	0.58
2:B:108:VAL:HA	2:B:187:LEU:O	2.04	0.58
1:A:261:VAL:HG13	1:A:276:VAL:CG1	2.31	0.58
1:A:418:ASN:OD1	1:A:422:LEU:HD11	2.03	0.58
1:A:101:LYS:HE2	4:B:1003:HOH:O	2.04	0.57
1:A:503:LEU:HD13	1:A:503:LEU:C	2.24	0.57
1:A:12:LEU:N	1:A:12:LEU:HD22	2.18	0.57
1:A:468:THR:C	1:A:469:LEU:HD22	2.24	0.57
2:B:125:ARG:HB3	2:B:146:TYR:O	2.03	0.57
1:A:85:GLN:HE22	2:B:53:GLU:HB2	1.68	0.57
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.33	0.57
2:B:239:TRP:CZ2	2:B:378:GLU:HG2	2.39	0.57
1:A:270:ILE:HG13	1:A:271:TYR:CD2	2.40	0.57
2:B:185:ASP:HB2	2:B:409:THR:HG21	1.87	0.56
1:A:114:ALA:HB1	1:A:214:LEU:CD1	2.35	0.56
1:A:195:ILE:HD12	1:A:199:ARG:NH1	2.16	0.56
1:A:410:TRP:HB2	2:B:365:VAL:HG21	1.86	0.56
2:B:108:VAL:O	2:B:109:LEU:HD13	2.05	0.56
1:A:114:ALA:CB	1:A:214:LEU:HD13	2.36	0.56
2:B:107:THR:HG23	2:B:189:VAL:HB	1.86	0.56
1:A:275:LYS:HD3	4:A:1117:HOH:O	2.05	0.56
1:A:408:ALA:CB	2:B:364:ASP:HB3	2.35	0.56
2:B:10:VAL:HG22	2:B:159:ILE:HD11	1.88	0.56
2:B:69:THR:O	2:B:69:THR:CG2	2.54	0.56
1:A:480:GLN:NE2	1:A:517:LEU:HD11	2.21	0.56
2:B:30:LYS:HD2	4:B:1067:HOH:O	2.06	0.56
1:A:45:GLY:O	1:A:47:ILE:N	2.39	0.56
1:A:43:LYS:O	1:A:43:LYS:HG2	2.06	0.55
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.36	0.55
1:A:337:TRP:HE1	1:A:367:GLN:HE21	1.53	0.55
1:A:453:GLY:HA3	1:A:469:LEU:HB2	1.88	0.55
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.41	0.55
1:A:111:VAL:HG23	1:A:112:GLY:H	1.72	0.55
1:A:426:TRP:O	1:A:427:TYR:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:HD21	1:A:501:TYR:CE2	2.42	0.55
1:A:28:GLU:OE1	1:A:135:ILE:O	2.25	0.55
1:A:296:THR:HG22	1:A:298:GLU:N	2.22	0.55
2:B:97:PRO:O	2:B:100:LEU:CD2	2.54	0.55
2:B:363:ASN:HD21	2:B:366:LYS:HB2	1.72	0.55
1:A:297:GLU:HG3	1:A:298:GLU:N	2.22	0.55
1:A:19:PRO:CG	1:A:80:LEU:HB2	2.37	0.54
1:A:475:GLN:HB2	1:A:501:TYR:CD2	2.41	0.54
1:A:182:GLN:HB2	4:A:1177:HOH:O	2.07	0.54
2:B:172:ARG:HA	2:B:175:ASN:HB2	1.88	0.54
1:A:46:LYS:CD	1:A:116:PHE:HB3	2.35	0.54
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.43	0.54
1:A:332:GLN:HG2	1:A:333:GLY:N	2.17	0.54
1:A:71:TRP:HA	1:A:71:TRP:HE3	1.70	0.54
1:A:331:LYS:HE3	1:A:364:ASP:OD1	2.08	0.54
1:A:448:ARG:H	1:A:448:ARG:HE	1.55	0.54
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.90	0.54
2:B:161:GLN:C	2:B:161:GLN:HE21	2.11	0.54
2:B:395:LYS:O	2:B:399:GLU:HG3	2.08	0.54
1:A:277:ARG:HG2	1:A:277:ARG:HH11	1.72	0.54
2:B:214:LEU:H	2:B:214:LEU:HD23	1.73	0.54
1:A:452:LEU:HD11	1:A:454:LYS:CD	2.38	0.53
2:B:423:VAL:HG22	2:B:427:TYR:HB2	1.91	0.53
2:B:118:VAL:HB	2:B:149:LEU:HG	1.89	0.53
2:B:371:ALA:O	2:B:375:ILE:HG13	2.09	0.53
1:A:135:ILE:H	1:A:135:ILE:HD12	1.73	0.53
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.91	0.53
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.44	0.53
1:A:150:PRO:HG2	1:A:153:TRP:CB	2.36	0.53
2:B:199:ARG:O	2:B:203:GLU:HB2	2.09	0.53
1:A:496:VAL:CG2	2:B:289:LEU:HD11	2.38	0.53
2:B:363:ASN:HD21	2:B:366:LYS:CB	2.22	0.53
1:A:91:GLN:HE21	1:A:91:GLN:CA	2.21	0.53
2:B:24:TRP:CG	2:B:25:PRO:HD2	2.43	0.53
2:B:296:THR:O	2:B:300:GLU:HG3	2.09	0.53
2:B:363:ASN:C	2:B:363:ASN:HD22	2.12	0.53
2:B:26:LEU:HA	4:B:1067:HOH:O	2.08	0.53
2:B:345:PRO:O	2:B:346:PHE:HB2	2.08	0.52
1:A:210:LEU:CD1	1:A:215:THR:HA	2.39	0.52
1:A:453:GLY:O	1:A:468:THR:HA	2.08	0.52
1:A:472:THR:OG1	1:A:476:LYS:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:ASP:HB3	2:B:188:TYR:CE1	2.45	0.52
2:B:354:TYR:OH	2:B:370:GLU:OE1	2.28	0.52
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.91	0.52
2:B:161:GLN:HE21	2:B:161:GLN:CA	2.23	0.52
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.33	0.52
1:A:92:LEU:HD12	2:B:140:PRO:O	2.10	0.52
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.42	0.52
1:A:13:LYS:HB2	1:A:16:MET:HG3	1.92	0.52
1:A:40:GLU:HG3	1:A:44:GLU:OE2	2.09	0.52
1:A:376:THR:O	1:A:380:ILE:HG13	2.10	0.52
1:A:295:LEU:HD12	1:A:300:GLU:OE2	2.10	0.52
2:B:423:VAL:CG2	2:B:426:TRP:HB2	2.33	0.52
1:A:480:GLN:HG2	1:A:517:LEU:HD21	1.92	0.52
1:A:457:TYR:CE2	1:A:484:LEU:HD12	2.35	0.51
2:B:153:TRP:CE2	2:B:155:GLY:HA3	2.45	0.51
2:B:32:LYS:O	2:B:35:VAL:HG13	2.10	0.51
1:A:81:ASN:HB3	1:A:154:LYS:HB2	1.91	0.51
2:B:261:VAL:HG13	2:B:276:VAL:CG2	2.32	0.51
1:A:480:GLN:HE21	1:A:517:LEU:HD11	1.76	0.51
1:A:517:LEU:O	1:A:521:ILE:HG13	2.09	0.51
2:B:5:ILE:HG22	2:B:6:GLU:N	2.26	0.51
1:A:8:VAL:HG11	1:A:159:ILE:HG23	1.91	0.51
1:A:135:ILE:HD12	1:A:135:ILE:N	2.25	0.51
1:A:451:LYS:HD2	1:A:472:THR:N	2.20	0.51
2:B:167:ILE:C	2:B:167:ILE:HD12	2.30	0.51
2:B:166:LYS:O	2:B:166:LYS:HG2	2.10	0.51
2:B:423:VAL:HG13	2:B:423:VAL:O	2.10	0.51
2:B:287:LYS:CD	2:B:293:ILE:HD11	2.40	0.51
1:A:366:LYS:HE3	1:A:405:TYR:OH	2.11	0.50
1:A:446:ALA:O	1:A:452:LEU:HD23	2.11	0.50
1:A:94:ILE:HG22	1:A:95:PRO:N	2.26	0.50
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.46	0.50
1:A:19:PRO:HD3	1:A:80:LEU:HD13	1.94	0.50
1:A:395:LYS:HD3	1:A:395:LYS:C	2.32	0.50
2:B:169:GLU:HG3	2:B:173:LYS:HB2	1.92	0.50
2:B:209:LEU:HB3	2:B:214:LEU:HD21	1.92	0.50
2:B:254:VAL:O	2:B:258:GLN:HG3	2.10	0.50
2:B:376:THR:O	2:B:380:ILE:HG13	2.11	0.50
1:A:106:VAL:HG13	3:A:999:S11:H133	1.93	0.50
1:A:410:TRP:CE3	1:A:411:ILE:N	2.80	0.50
1:A:255:ASN:OD1	1:A:259:LYS:HE2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLU:O	1:A:339:TYR:HA	2.12	0.50
2:B:164:MET:HG2	2:B:182:GLN:HE22	1.77	0.50
1:A:50:ILE:HD12	1:A:54:ASN:CB	2.42	0.50
2:B:395:LYS:HG3	2:B:416:PHE:CE1	2.47	0.50
1:A:257:ILE:O	1:A:261:VAL:HG23	2.12	0.49
1:A:399:GLU:HG3	1:A:402:TRP:CE3	2.47	0.49
1:A:308:GLU:OE2	1:A:308:GLU:HA	2.11	0.49
2:B:202:ILE:N	2:B:202:ILE:HD12	2.26	0.49
1:A:362:THR:HG23	1:A:512:GLN:HE22	1.77	0.49
1:A:410:TRP:HD1	2:B:401:TRP:CD1	2.31	0.49
2:B:64:LYS:O	2:B:64:LYS:HG3	2.13	0.49
2:B:129:ALA:HA	2:B:144:TYR:O	2.12	0.49
2:B:207:GLN:O	2:B:207:GLN:HG2	2.12	0.49
1:A:102:LYS:HG3	3:A:999:S11:N24	2.27	0.49
1:A:113:ASP:C	1:A:115:TYR:N	2.64	0.49
1:A:244:ILE:HB	1:A:310:LEU:HD22	1.94	0.49
1:A:95:PRO:CB	2:B:136:ASN:O	2.57	0.49
1:A:495:ILE:HB	1:A:533:LEU:HD13	1.95	0.49
2:B:423:VAL:HG22	2:B:423:VAL:O	2.12	0.49
1:A:296:THR:CG2	1:A:298:GLU:H	2.26	0.49
1:A:332:GLN:O	1:A:333:GLY:O	2.30	0.49
1:A:276:VAL:HG12	1:A:276:VAL:O	2.12	0.49
1:A:515:SER:HB3	1:A:518:VAL:HB	1.94	0.49
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.94	0.49
2:B:214:LEU:H	2:B:214:LEU:CD2	2.25	0.49
1:A:60:VAL:HG12	1:A:61:PHE:N	2.27	0.49
1:A:125:ARG:O	1:A:127:TYR:N	2.46	0.49
1:A:514:GLU:CD	1:A:514:GLU:H	2.16	0.49
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.95	0.49
1:A:368:LEU:HD12	1:A:423:VAL:HG21	1.93	0.49
2:B:160:PHE:CD1	2:B:164:MET:HB2	2.47	0.49
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.95	0.48
2:B:202:ILE:C	2:B:204:GLU:N	2.66	0.48
2:B:12:LEU:O	2:B:13:LYS:C	2.52	0.48
2:B:314:VAL:HG13	2:B:317:VAL:HG21	1.94	0.48
1:A:444:GLY:CA	1:A:477:THR:HG22	2.35	0.48
2:B:170:PRO:O	2:B:208:HIS:CE1	2.67	0.48
2:B:180:ILE:O	2:B:180:ILE:HG13	2.13	0.48
1:A:197:GLN:O	1:A:201:LYS:HG2	2.12	0.48
2:B:85:GLN:O	2:B:85:GLN:HG3	2.12	0.48
1:A:50:ILE:HG13	1:A:51:GLY:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:HG13	1:A:161:GLN:NE2	2.29	0.48
2:B:333:GLY:O	2:B:336:GLN:HB2	2.13	0.48
1:A:114:ALA:HA	1:A:117:SER:HB3	1.94	0.48
2:B:107:THR:HG22	2:B:189:VAL:O	2.13	0.48
2:B:154:LYS:O	2:B:157:PRO:HD2	2.13	0.48
1:A:479:LEU:CD2	1:A:501:TYR:HE2	2.27	0.48
2:B:169:GLU:HG2	2:B:173:LYS:HB2	1.94	0.48
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.94	0.48
1:A:480:GLN:HE21	1:A:517:LEU:CD1	2.27	0.48
1:A:58:THR:HG23	1:A:76:ASP:O	2.14	0.47
1:A:241:VAL:HG12	1:A:242:GLN:O	2.14	0.47
1:A:111:VAL:HG22	1:A:185:ASP:C	2.34	0.47
1:A:404:GLU:HB2	4:A:1141:HOH:O	2.14	0.47
1:A:398:TRP:CH2	1:A:411:ILE:HB	2.49	0.47
1:A:417:VAL:O	1:A:417:VAL:HG13	2.14	0.47
1:A:489:SER:OG	1:A:493:VAL:HG21	2.14	0.47
2:B:10:VAL:HG12	2:B:11:LYS:N	2.30	0.47
1:A:50:ILE:HG13	1:A:51:GLY:H	1.79	0.47
1:A:126:LYS:HG3	1:A:127:TYR:N	2.29	0.47
1:A:278:GLN:HE21	1:A:278:GLN:CA	2.18	0.47
2:B:48:SER:O	2:B:49:LYS:C	2.52	0.47
2:B:214:LEU:HD23	2:B:214:LEU:N	2.30	0.47
1:A:368:LEU:O	1:A:368:LEU:HD23	2.15	0.47
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.96	0.47
1:A:427:TYR:OH	1:A:509:GLN:HA	2.14	0.47
2:B:34:LEU:HG	2:B:62:ALA:HB2	1.97	0.47
2:B:328:GLU:OE1	2:B:342:TYR:OH	2.29	0.47
2:B:421:PRO:HG2	2:B:424:LYS:HB3	1.96	0.47
1:A:360:ALA:HB1	1:A:514:GLU:OE1	2.15	0.46
1:A:195:ILE:HG13	1:A:196:GLY:N	2.30	0.46
2:B:253:THR:H	2:B:256:ASP:HB2	1.81	0.46
2:B:97:PRO:O	2:B:100:LEU:HD21	2.14	0.46
2:B:160:PHE:HD1	2:B:164:MET:HB2	1.81	0.46
2:B:205:LEU:HG	2:B:209:LEU:CD1	2.46	0.46
2:B:276:VAL:HG12	4:B:1086:HOH:O	2.15	0.46
2:B:380:ILE:O	2:B:384:GLY:HA2	2.16	0.46
1:A:23:GLN:HB2	1:A:131:THR:HG21	1.96	0.46
2:B:236:PRO:HA	2:B:239:TRP:CE3	2.50	0.46
2:B:314:VAL:HG13	2:B:317:VAL:CG2	2.45	0.46
1:A:495:ILE:HB	1:A:533:LEU:CD1	2.46	0.46
1:A:255:ASN:HB3	4:A:1023:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:LYS:HD2	1:A:347:LYS:HA	1.81	0.46
2:B:78:ARG:HA	4:B:1195:HOH:O	2.16	0.46
1:A:93:GLY:HA3	2:B:137:ASN:ND2	2.31	0.46
1:A:445:ALA:H	1:A:477:THR:HG21	1.80	0.46
2:B:276:VAL:HG22	2:B:276:VAL:O	2.16	0.46
1:A:153:TRP:HZ3	1:A:159:ILE:HD12	1.81	0.46
1:A:124:PHE:O	1:A:127:TYR:HD2	1.98	0.45
1:A:411:ILE:HD12	1:A:412:PRO:CD	2.44	0.45
2:B:203:GLU:OE2	2:B:203:GLU:O	2.34	0.45
1:A:426:TRP:HB3	1:A:526:ILE:CD1	2.46	0.45
2:B:103:LYS:NZ	2:B:179:VAL:HG12	2.31	0.45
1:A:71:TRP:CE3	1:A:71:TRP:CA	2.99	0.45
1:A:393:ILE:HD13	1:A:398:TRP:HB2	1.99	0.45
2:B:43:LYS:HE3	2:B:43:LYS:HB2	1.85	0.45
1:A:402:TRP:CD1	1:A:402:TRP:C	2.90	0.45
2:B:13:LYS:HA	2:B:14:PRO:HD2	1.80	0.45
1:A:155:GLY:O	1:A:159:ILE:HG13	2.17	0.45
1:A:390:LYS:HA	1:A:415:GLU:O	2.16	0.45
2:B:169:GLU:O	2:B:171:PHE:N	2.40	0.45
1:A:229:TRP:O	1:A:230:MET:C	2.55	0.45
2:B:423:VAL:O	2:B:427:TYR:HB2	2.17	0.45
1:A:179:VAL:O	1:A:189:VAL:HA	2.16	0.45
2:B:65:LYS:CE	2:B:72:ARG:HD2	2.47	0.45
2:B:106:VAL:HG21	2:B:236:PRO:HG2	1.98	0.45
1:A:108:VAL:HA	1:A:187:LEU:O	2.15	0.45
1:A:381:VAL:HG22	2:B:25:PRO:HB3	1.99	0.45
1:A:329:ILE:HG22	1:A:330:GLN:N	2.31	0.44
1:A:487:GLN:HG3	1:A:488:ASP:OD1	2.17	0.44
2:B:113:ASP:O	2:B:114:ALA:C	2.55	0.44
2:B:183:TYR:O	2:B:186:ASP:HB2	2.17	0.44
1:A:77:PHE:HB3	1:A:81:ASN:HD21	1.82	0.44
1:A:439:THR:HG23	2:B:289:LEU:HD13	1.97	0.44
1:A:29:GLU:CG	1:A:71:TRP:HZ2	2.23	0.44
1:A:240:THR:HG22	1:A:315:HIS:HB3	1.99	0.44
1:A:410:TRP:CE3	1:A:410:TRP:CA	3.00	0.44
2:B:120:LEU:HB2	2:B:148:VAL:O	2.18	0.44
1:A:148:VAL:O	1:A:150:PRO:N	2.51	0.44
1:A:325:LEU:HD12	1:A:385:LYS:CD	2.48	0.44
2:B:421:PRO:HG3	4:B:1051:HOH:O	2.16	0.44
1:A:296:THR:HG22	1:A:298:GLU:H	1.82	0.44
2:B:28:GLU:CG	2:B:135:ILE:HD11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:VAL:HG12	2:B:107:THR:N	2.33	0.44
2:B:319:TYR:OH	2:B:385:LYS:HD3	2.17	0.44
2:B:363:ASN:ND2	2:B:366:LYS:CB	2.81	0.44
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.99	0.44
2:B:179:VAL:O	2:B:190:GLY:N	2.44	0.44
1:A:465:LYS:NZ	1:A:488:ASP:OD2	2.48	0.44
2:B:363:ASN:ND2	2:B:363:ASN:N	2.65	0.44
1:A:395:LYS:HD3	1:A:395:LYS:O	2.18	0.44
2:B:202:ILE:C	2:B:204:GLU:H	2.22	0.44
1:A:253:THR:HG22	1:A:292:VAL:HG22	2.00	0.43
1:A:472:THR:OG1	1:A:476:LYS:CB	2.66	0.43
1:A:12:LEU:HD22	1:A:12:LEU:H	1.80	0.43
1:A:303:LEU:CD2	1:A:303:LEU:O	2.66	0.43
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.99	0.43
1:A:226:PRO:HA	1:A:234:LEU:O	2.18	0.43
1:A:279:LEU:HD12	1:A:302:GLU:OE1	2.18	0.43
1:A:376:THR:HG23	1:A:386:THR:HG22	1.99	0.43
2:B:39:THR:O	2:B:42:GLU:HB3	2.18	0.43
2:B:376:THR:CG2	2:B:386:THR:HG22	2.48	0.43
1:A:479:LEU:CD2	1:A:501:TYR:CE2	3.02	0.43
2:B:425:LEU:HD23	2:B:425:LEU:N	2.30	0.43
1:A:77:PHE:HE1	1:A:150:PRO:HB2	1.83	0.43
1:A:457:TYR:CD1	1:A:457:TYR:C	2.92	0.43
1:A:479:LEU:HD21	1:A:501:TYR:HE2	1.82	0.43
1:A:517:LEU:HD12	1:A:517:LEU:HA	1.78	0.43
2:B:103:LYS:HZ2	2:B:179:VAL:HG12	1.83	0.43
1:A:37:ILE:O	1:A:41:MET:HG3	2.18	0.43
1:A:110:ASP:OD1	1:A:111:VAL:N	2.51	0.43
2:B:107:THR:CG2	2:B:202:ILE:HG12	2.41	0.43
2:B:355:ALA:O	2:B:356:ARG:C	2.56	0.43
2:B:32:LYS:O	2:B:35:VAL:CG1	2.66	0.43
2:B:139:THR:CG2	2:B:140:PRO:HD2	2.48	0.43
2:B:165:THR:C	2:B:167:ILE:H	2.22	0.43
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.53	0.42
1:A:12:LEU:H	1:A:12:LEU:CD2	2.32	0.42
1:A:134:SER:O	1:A:136:ASN:N	2.51	0.42
1:A:231:GLY:C	1:A:242:GLN:HG3	2.40	0.42
2:B:178:ILE:HG12	2:B:179:VAL:N	2.33	0.42
1:A:153:TRP:HE3	1:A:156:SER:OG	2.01	0.42
2:B:327:ALA:HA	2:B:340:GLN:O	2.19	0.42
1:A:56:TYR:HE2	1:A:126:LYS:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ALA:HA	1:A:144:TYR:O	2.20	0.42
1:A:135:ILE:CD1	1:A:135:ILE:N	2.80	0.42
1:A:205:LEU:O	1:A:206:ARG:C	2.56	0.42
1:A:497:THR:O	1:A:535:TRP:HA	2.19	0.42
2:B:164:MET:HG2	2:B:182:GLN:NE2	2.33	0.42
2:B:404:GLU:HB3	2:B:405:TYR:CD1	2.54	0.42
2:B:157:PRO:CG	2:B:184:MET:HA	2.46	0.42
2:B:362:THR:HB	2:B:367:GLN:HE21	1.84	0.42
2:B:47:ILE:HA	2:B:145:GLN:O	2.20	0.42
2:B:65:LYS:NZ	2:B:72:ARG:HD2	2.34	0.42
2:B:324:ASP:O	2:B:343:GLN:HG2	2.20	0.42
2:B:410:TRP:HE3	2:B:410:TRP:O	2.03	0.42
1:A:112:GLY:C	1:A:114:ALA:N	2.73	0.42
1:A:125:ARG:O	1:A:126:LYS:C	2.58	0.42
1:A:522:ILE:O	1:A:526:ILE:HG13	2.20	0.42
2:B:328:GLU:O	2:B:339:TYR:HA	2.20	0.42
1:A:448:ARG:NE	1:A:448:ARG:N	2.66	0.42
1:A:195:ILE:CD1	1:A:199:ARG:HH12	2.20	0.41
1:A:506:ILE:HD12	1:A:533:LEU:HD21	2.02	0.41
1:A:12:LEU:HB3	1:A:83:ARG:O	2.20	0.41
1:A:503:LEU:HD22	1:A:507:GLN:HG2	2.02	0.41
1:A:22:LYS:HG2	1:A:23:GLN:N	2.36	0.41
2:B:100:LEU:H	2:B:100:LEU:CD2	2.11	0.41
2:B:13:LYS:CG	2:B:85:GLN:HA	2.47	0.41
2:B:103:LYS:HD3	2:B:103:LYS:HA	1.76	0.41
1:A:80:LEU:O	1:A:84:THR:OG1	2.36	0.41
1:A:254:VAL:O	1:A:258:GLN:HG3	2.21	0.41
1:A:445:ALA:N	1:A:477:THR:HG21	2.35	0.41
1:A:509:GLN:N	1:A:510:PRO:CD	2.82	0.41
2:B:53:GLU:O	2:B:55:PRO:HD3	2.21	0.41
1:A:12:LEU:N	1:A:12:LEU:CD2	2.81	0.41
1:A:58:THR:N	4:A:1001:HOH:O	2.54	0.41
1:A:249:LYS:HE2	4:A:1020:HOH:O	2.20	0.41
1:A:13:LYS:HB3	1:A:14:PRO:CD	2.38	0.41
1:A:479:LEU:HD12	1:A:479:LEU:HA	1.79	0.41
1:A:27:THR:H	1:A:30:LYS:HD2	1.86	0.41
1:A:91:GLN:CA	1:A:91:GLN:NE2	2.84	0.41
1:A:92:LEU:HG	4:A:1157:HOH:O	2.20	0.41
1:A:134:SER:O	1:A:135:ILE:C	2.58	0.41
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.85	0.41
1:A:450:THR:HA	1:A:451:LYS:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:LEU:HD13	1:A:524:GLN:HB3	2.03	0.41
2:B:32:LYS:O	2:B:36:GLU:HG3	2.21	0.41
2:B:161:GLN:CA	2:B:161:GLN:NE2	2.84	0.41
2:B:202:ILE:O	2:B:205:LEU:N	2.53	0.41
1:A:111:VAL:CG2	1:A:112:GLY:H	2.34	0.41
1:A:153:TRP:HB3	1:A:156:SER:OG	2.21	0.41
2:B:7:THR:HG22	2:B:119:PRO:HB2	2.02	0.41
2:B:350:LYS:HG3	2:B:351:THR:N	2.35	0.41
1:A:233:GLU:HB2	1:A:240:THR:OG1	2.21	0.40
2:B:198:HIS:O	2:B:199:ARG:C	2.59	0.40
1:A:479:LEU:HD11	1:A:502:ALA:HA	2.03	0.40
2:B:233:GLU:CD	2:B:233:GLU:H	2.24	0.40
1:A:19:PRO:O	1:A:56:TYR:CA	2.69	0.40
2:B:290:THR:HB	4:B:1057:HOH:O	2.21	0.40
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.56	0.40
1:A:192:ASP:HB2	4:A:1108:HOH:O	2.20	0.40
1:A:362:THR:HG23	1:A:512:GLN:NE2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	514/560 (92%)	435 (85%)	66 (13%)	13 (2%)	5 8
2	B	387/440 (88%)	331 (86%)	42 (11%)	14 (4%)	3 4
All	All	901/1000 (90%)	766 (85%)	108 (12%)	27 (3%)	4 6

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	LYS

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Mol	Chain	Res	Type
1	A	46	LYS
1	A	333	GLY
1	A	453	GLY
1	A	126	LYS
1	A	473	THR
2	B	14	PRO
2	B	103	LYS
2	B	171	PHE
2	B	214	LEU
1	A	112	GLY
2	B	49	LYS
1	A	85	GLN
1	A	94	ILE
1	A	451	LYS
2	B	237	ASP
2	B	68	SER
2	B	122	GLU
2	B	123	ASP
1	A	135	ILE
2	B	97	PRO
2	B	267	ALA
2	B	195	ILE
1	A	55	PRO
1	A	345	PRO
2	B	236	PRO
2	B	242	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	468/499 (94%)	421 (90%)	47 (10%)	7 15
2	B	361/400 (90%)	338 (94%)	23 (6%)	17 33
All	All	829/899 (92%)	759 (92%)	70 (8%)	11 21

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	12	LEU
1	A	56	TYR
1	A	71	TRP
1	A	77	PHE
1	A	78	ARG
1	A	83	ARG
1	A	89	GLU
1	A	91	GLN
1	A	94	ILE
1	A	105	SER
1	A	115	TYR
1	A	142	ILE
1	A	145	GLN
1	A	174	GLN
1	A	179	VAL
1	A	182	GLN
1	A	187	LEU
1	A	205	LEU
1	A	207	GLN
1	A	222	GLN
1	A	234	LEU
1	A	238	LYS
1	A	264	LEU
1	A	282	LEU
1	A	283	LEU
1	A	296	THR
1	A	297	GLU
1	A	303	LEU
1	A	305	GLU
1	A	351	THR
1	A	368	LEU
1	A	395	LYS
1	A	402	TRP
1	A	410	TRP
1	A	412	PRO
1	A	414	TRP
1	A	424	LYS
1	A	448	ARG
1	A	450	THR
1	A	451	LYS
1	A	452	LEU
1	A	454	LYS

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Mol	Chain	Res	Type
1	A	459	THR
1	A	479	LEU
1	A	484	LEU
1	A	493	VAL
2	B	65	LYS
2	B	66	LYS
2	B	100	LEU
2	B	113	ASP
2	B	122	GLU
2	B	123	ASP
2	B	145	GLN
2	B	161	GLN
2	B	203	GLU
2	B	212	TRP
2	B	214	LEU
2	B	233	GLU
2	B	234	LEU
2	B	295	LEU
2	B	303	LEU
2	B	350	LYS
2	B	356	ARG
2	B	363	ASN
2	B	368	LEU
2	B	410	TRP
2	B	414	TRP
2	B	425	LEU
2	B	427	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	161	GLN
1	A	222	GLN
1	A	242	GLN
1	A	265	ASN
1	A	269	GLN
1	A	278	GLN
1	A	334	GLN
1	A	367	GLN
1	A	464	GLN
1	A	480	GLN

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Mol	Chain	Res	Type
1	A	487	GLN
1	A	507	GLN
1	A	509	GLN
1	A	512	GLN
1	A	524	GLN
2	B	57	ASN
2	B	85	GLN
2	B	147	ASN
2	B	151	GLN
2	B	161	GLN
2	B	182	GLN
2	B	208	HIS
2	B	242	GLN
2	B	278	GLN
2	B	332	GLN
2	B	334	GLN
2	B	363	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	0.99	0	1,8,10	5.96	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	5.96	116.88	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	S11	A	999	-	26,31,31	1.79	6 (23%)	34,43,43	1.54	6 (17%)

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	S11	A	999	-	-	4/13/17/17	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	S11	C5-N1	-4.36	1.26	1.35
3	A	999	S11	C2-C3	-3.42	1.35	1.42
3	A	999	S11	C11-C10	3.00	1.43	1.38
3	A	999	S11	C9-C8	2.29	1.42	1.38
3	A	999	S11	C7-C8	2.06	1.41	1.38
3	A	999	S11	C17-C16	2.01	1.43	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	999	S11	C5-N1-C2	4.33	109.84	104.13
3	A	999	S11	C12-C2-N1	3.24	126.04	120.46
3	A	999	S11	C8-C7-C6	2.52	120.71	118.74
3	A	999	S11	C2-C3-N4	2.49	110.09	106.20
3	A	999	S11	C10-C9-C8	2.14	119.87	117.37
3	A	999	S11	C18-N19-C20	2.12	121.83	116.85

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	S11	N24-C23-O22-CA
3	A	999	S11	O25-C23-O22-CA
3	A	999	S11	N4-C15-C16-C21
3	A	999	S11	N4-C15-C16-C17

There are no ring outliers.

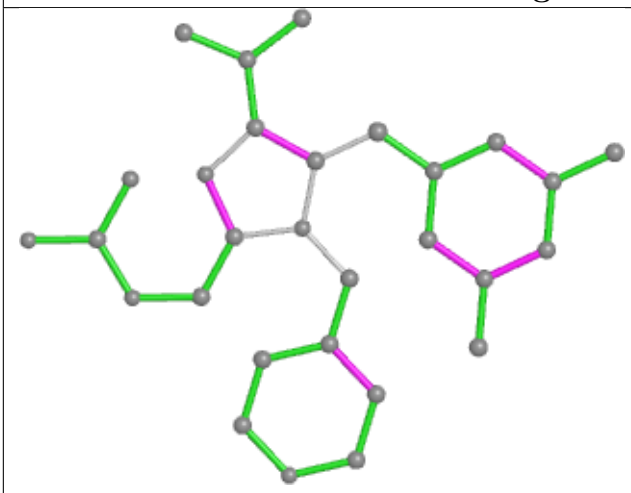
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	S11	2	0

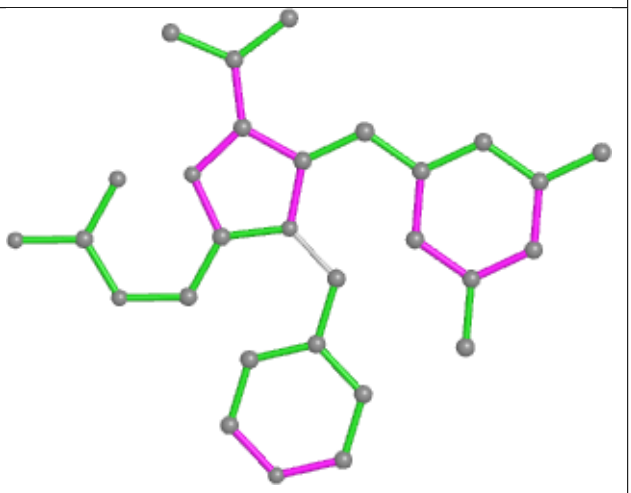
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

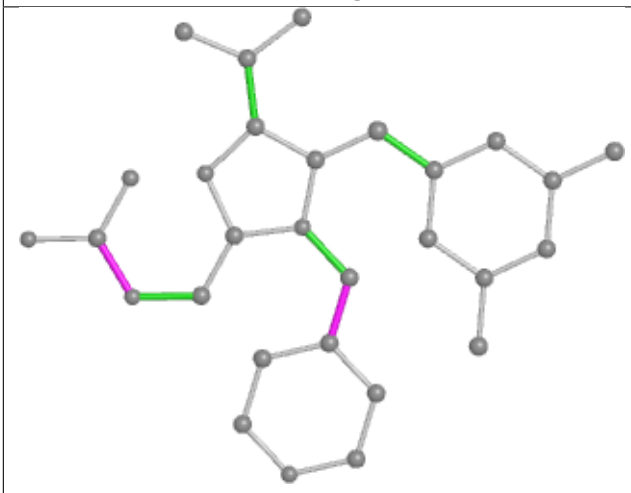
Ligand S11 A 999



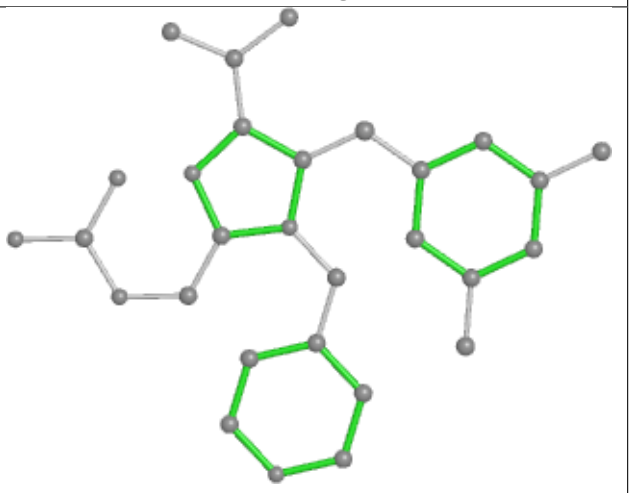
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	522/560 (93%)	0.39	48 (9%)	9	9	34, 67, 109, 132	0
2	B	395/440 (89%)	0.51	37 (9%)	8	8	31, 64, 114, 134	0
All	All	917/1000 (91%)	0.45	85 (9%)	8	8	31, 66, 112, 134	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	GLY	7.0
1	A	92	LEU	6.9
2	B	174	GLN	6.3
1	A	452	LEU	6.1
1	A	115	TYR	5.9
2	B	213	GLY	5.7
2	B	426	TRP	5.3
2	B	173	LYS	5.2
2	B	67	ASP	5.1
1	A	116	PHE	4.7
1	A	78	ARG	4.7
2	B	176	PRO	4.6
2	B	69	THR	4.5
1	A	346	PHE	4.4
1	A	453	GLY	4.2
1	A	21	VAL	4.2
1	A	71	TRP	4.1
1	A	221	HIS	4.1
1	A	51	GLY	4.1
2	B	11	LYS	4.0
1	A	91	GLN	4.0
2	B	233	GLU	4.0
2	B	12	LEU	4.0
1	A	90	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	52	PRO	3.8
1	A	24	TRP	3.7
2	B	199	ARG	3.7
1	A	358	ARG	3.6
2	B	168	LEU	3.6
1	A	135	ILE	3.4
1	A	444	GLY	3.4
1	A	127	TYR	3.4
2	B	195	ILE	3.3
2	B	14	PRO	3.2
1	A	214	LEU	3.2
2	B	88	TRP	3.2
2	B	232	TYR	3.2
2	B	167	ILE	3.2
1	A	469	LEU	3.2
2	B	16	MET	3.2
2	B	104	LYS	3.2
1	A	217	PRO	3.1
2	B	423	VAL	3.1
1	A	16	MET	3.1
1	A	64	LYS	3.1
1	A	218	ASP	3.1
1	A	29	GLU	3.0
1	A	360	ALA	3.0
1	A	448	ARG	3.0
2	B	214	LEU	2.9
1	A	28	GLU	2.9
2	B	43	LYS	2.8
1	A	446	ALA	2.8
1	A	17	ASP	2.8
1	A	63	ILE	2.8
1	A	215	THR	2.7
2	B	207	GLN	2.7
1	A	402	TRP	2.7
2	B	68	SER	2.6
1	A	501	TYR	2.5
2	B	7	THR	2.5
2	B	356	ARG	2.5
1	A	14	PRO	2.5
2	B	5	ILE	2.4
2	B	427	TYR	2.4
2	B	97	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	445	ALA	2.3
2	B	172	ARG	2.3
1	A	222	GLN	2.3
1	A	454	LYS	2.2
1	A	473	THR	2.2
2	B	198	HIS	2.2
2	B	425	LEU	2.2
2	B	102	LYS	2.1
1	A	112	GLY	2.1
2	B	122	GLU	2.1
1	A	50	ILE	2.1
1	A	93	GLY	2.1
1	A	197	GLN	2.1
2	B	211	ARG	2.1
2	B	355	ALA	2.1
1	A	359	GLY	2.0
2	B	212	TRP	2.0
1	A	82	LYS	2.0
1	A	32	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSD	A	280	8/9	0.91	0.18	49,53,65,66	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

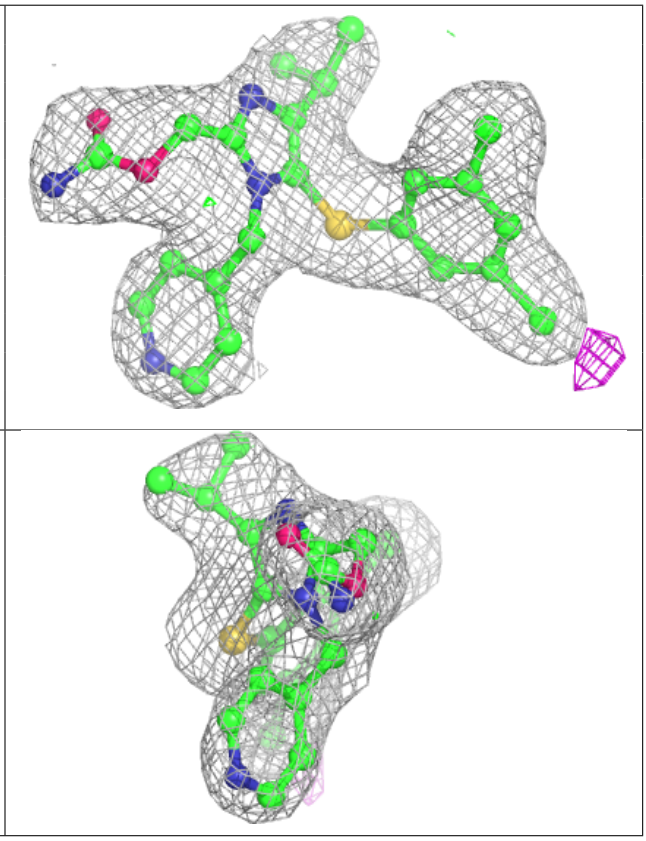
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	S11	A	999	29/29	0.95	0.19	42,50,60,69	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 S11 A 999:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.