Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 12:12 PM EDT

PDB ID	:	2OPS
Title	:	Crystal Structure of Y188C Mutant HIV-1 Reverse Transcriptase in Complex with GW420867X.
Authors	:	Ren, J.; Nichols, C.E.; Chamberlain, P.P.; Weaver, K.L.; Short, S.A.; Chan, J.H.; Kleim, J.; Stammers, D.K.
Deposited on	:	2007-01-30
Resolution	:	2.30 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 following versions of software and data (see references (i)) were used in the production of this report:

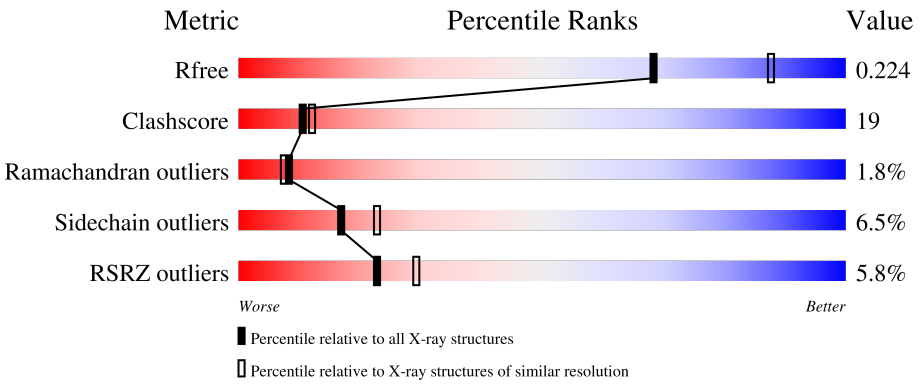
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	542	6% 65% 30% • •
2	B	435	6% 61% 29% • 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7928 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	536	4374	2829	729	807	9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	CYS	TYR	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

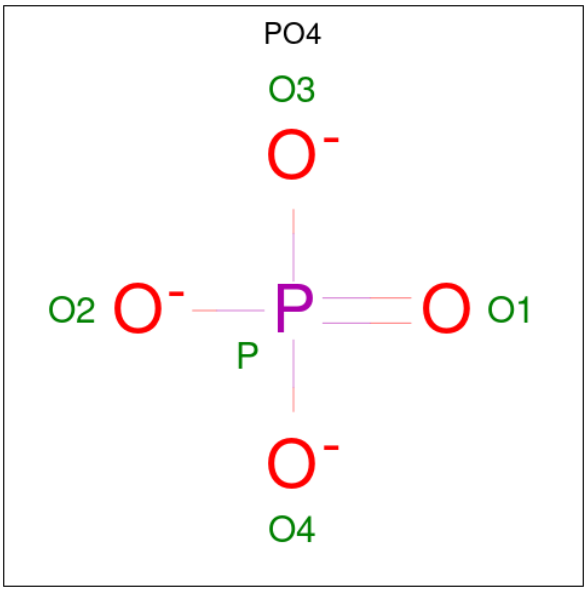
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	409	3373	2190	561	614	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

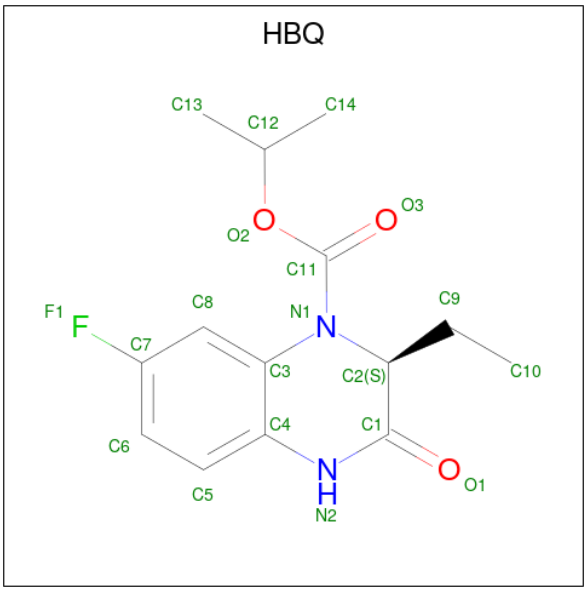
Chain	Residue	Modelled	Actual	Comment	Reference
B	188	CYS	TYR	engineered mutation	UNP P04585

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



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

- Molecule 4 is ISOPROPYL (2S)-2-ETHYL-7-FLUORO-3-OXO-3,4-DIHYDROQUINOXALINE-1(2H)-CARBOXYLATE (three-letter code: HBQ) (formula: $C_{14}H_{17}FN_2O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
4	A	1	20	14	1	2	3	0	0

- Molecule 5 is water.

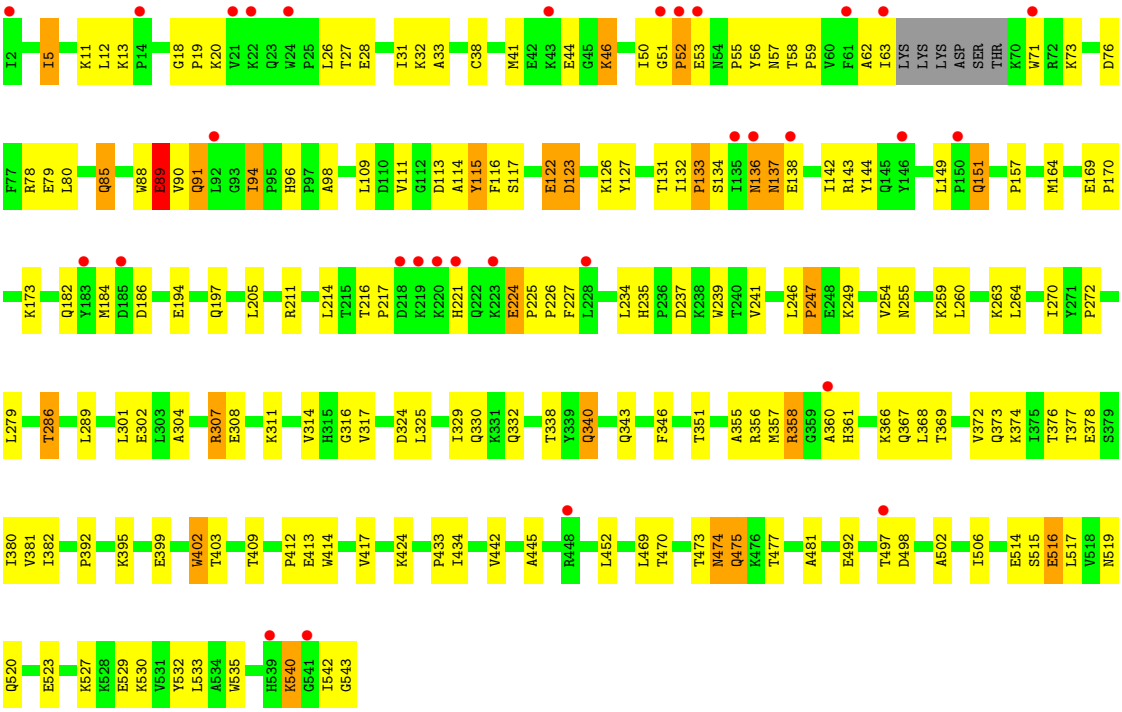
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	93	93	93	0	0
			Total	O		
5	B	58	58	58	0	0

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.

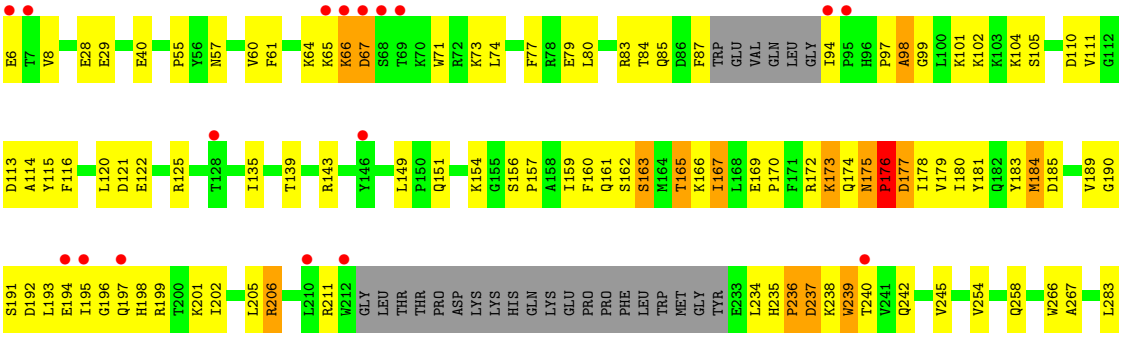
• Molecule 1: Reverse transcriptase/ribonuclease H

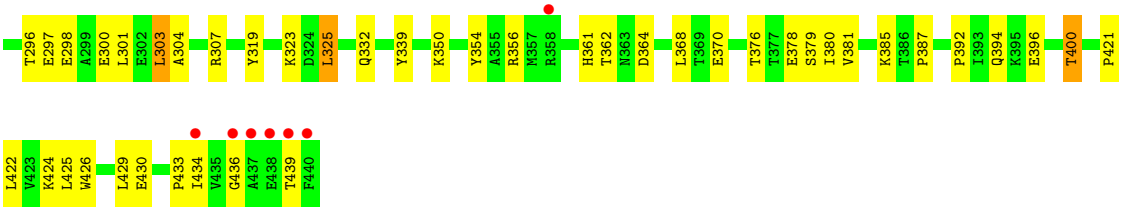
Chain A: 6% 65% 30%



• Molecule 2: p51 RT

Chain B: 6% 61% 29% 6%




T296
E297
E298
A299
E300
L301
E302
L303
A304
R307
Y319
K323
D324
L325
Q332
Y339
K350
Y354
A355
R356
M357
R358
H361
T362
N363
D364
L368
T369
E370
T376
T377
E378
S379
I380
V381
K385
T386
P387
P392
I393
Q394
K395
E396
T400
P421
L422
V423
K424
L425
W426
L429
E430
P433
I434
V435
G436
A437
E438
T439
F440

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	138.50Å 110.30Å 72.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.45 – 2.30 24.45 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (24.45-2.30) 98.7 (24.45-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.301 0.203 , 0.224	Depositor DCC
R_{free} test set	2472 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	46.3	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7928	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: PO4, CSD, HBQ

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	0.50	0/4480	0.71	0/6089
2	B	0.50	0/3465	0.72	1/4703 (0.0%)
All	All	0.50	0/7945	0.72	1/10792 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	325	LEU	CA-CB-CG	5.44	127.82	115.30

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	4374	0	4414	173	1
2	B	3373	0	3408	121	1
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	20	0	17	0	0
5	A	93	0	0	6	0
5	B	58	0	0	3	0
All	All	7928	0	7839	289	1

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 19.

All (289) 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:172:ARG:O	2:B:176:PRO:HD3	1.56	1.06
1:A:96:HIS:HD2	1:A:98:ALA:H	1.14	0.94
1:A:51:GLY:H	1:A:52:PRO:HD2	1.36	0.91
1:A:225:PRO:HG3	1:A:227:PHE:CZ	2.05	0.91
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.53	0.90
2:B:195:ILE:HD11	2:B:199:ARG:NH2	1.90	0.87
2:B:163:SER:O	2:B:167:ILE:HG23	1.76	0.85
2:B:175:ASN:O	2:B:177:ASP:N	2.11	0.84
2:B:169:GLU:HA	2:B:173:LYS:HZ3	1.42	0.83
1:A:96:HIS:CD2	1:A:98:ALA:H	1.97	0.82
2:B:296:THR:HG22	2:B:298:GLU:H	1.43	0.82
1:A:357:MET:HB2	1:A:367:GLN:NE2	1.95	0.81
1:A:109:LEU:HG	1:A:216:THR:HG21	1.61	0.81
1:A:94:ILE:HD13	1:A:94:ILE:H	1.45	0.81
2:B:161:GLN:O	2:B:165:THR:HG22	1.82	0.79
1:A:57:ASN:HD22	1:A:143:ARG:NH2	1.80	0.79
1:A:136:ASN:ND2	1:A:138:GLU:HB3	1.98	0.79
2:B:180:ILE:HG12	2:B:189:VAL:HG12	1.65	0.78
1:A:50:ILE:HG13	1:A:51:GLY:H	1.50	0.77
1:A:32:LYS:HA	1:A:32:LYS:HE2	1.67	0.76
2:B:433:PRO:HB2	2:B:436:GLY:HA2	1.69	0.73
1:A:90:VAL:HG21	1:A:157:PRO:HB2	1.68	0.73
1:A:136:ASN:O	1:A:138:GLU:N	2.21	0.73
1:A:57:ASN:HD21	1:A:131:THR:HG22	1.53	0.73
1:A:182:GLN:HB2	5:A:1015:HOH:O	1.87	0.72
1:A:226:PRO:HG3	1:A:235:HIS:ND1	2.06	0.71
2:B:332:GLN:NE2	2:B:424:LYS:HE2	2.05	0.70
1:A:225:PRO:HG3	1:A:227:PHE:HZ	1.56	0.70
1:A:516:GLU:O	1:A:520:GLN:HG3	1.92	0.70
1:A:132:ILE:HB	1:A:142:ILE:HB	1.74	0.70
1:A:378:GLU:O	1:A:382:ILE:HG12	1.91	0.69
2:B:379:SER:OG	2:B:387:PRO:HD3	1.91	0.69
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.75	0.69
1:A:226:PRO:HA	1:A:234:LEU:O	1.93	0.69
1:A:514:GLU:HG3	1:A:515:SER:H	1.58	0.69
1:A:270:ILE:CG2	1:A:314:VAL:HG11	2.23	0.68
1:A:332:GLN:HG3	5:A:1030:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:PRO:HB3	1:A:221:HIS:HB2	1.74	0.68
2:B:350:LYS:HE2	2:B:378:GLU:OE2	1.94	0.68
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.29	0.67
1:A:41:MET:HG2	1:A:46:LYS:HE3	1.76	0.67
2:B:396:GLU:O	2:B:400:THR:HG23	1.94	0.67
1:A:51:GLY:N	1:A:52:PRO:HD2	2.09	0.67
1:A:51:GLY:H	1:A:52:PRO:CD	2.08	0.66
2:B:254:VAL:O	2:B:258:GLN:HG3	1.96	0.66
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.31	0.66
1:A:360:ALA:HA	1:A:514:GLU:HG2	1.78	0.66
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.31	0.65
1:A:308:GLU:OE1	1:A:311:LYS:HE2	1.96	0.65
2:B:193:LEU:HD13	2:B:201:LYS:HE3	1.79	0.65
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.63	0.64
1:A:57:ASN:HD21	1:A:131:THR:CG2	2.09	0.64
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.27	0.64
2:B:194:GLU:OE1	2:B:197:GLN:HG3	1.98	0.64
2:B:193:LEU:HD13	2:B:201:LYS:CE	2.28	0.64
2:B:421:PRO:O	2:B:425:LEU:HD13	1.98	0.64
2:B:193:LEU:HD13	2:B:201:LYS:CD	2.29	0.63
2:B:239:TRP:O	2:B:240:THR:HG23	1.98	0.63
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.81	0.63
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.34	0.63
1:A:57:ASN:HD22	1:A:143:ARG:HH21	1.44	0.63
1:A:96:HIS:HD2	1:A:98:ALA:N	1.93	0.63
2:B:79:GLU:O	2:B:83:ARG:HG3	1.99	0.63
1:A:122:GLU:H	1:A:122:GLU:CD	2.02	0.62
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.80	0.62
1:A:51:GLY:N	1:A:52:PRO:CD	2.61	0.62
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.33	0.62
2:B:239:TRP:CD1	2:B:239:TRP:N	2.67	0.61
1:A:542:ILE:HG22	1:A:543:GLY:N	2.15	0.61
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.61	0.61
1:A:324:ASP:O	1:A:343:GLN:HG2	2.00	0.61
1:A:50:ILE:HG13	1:A:51:GLY:N	2.14	0.60
2:B:396:GLU:O	2:B:400:THR:CG2	2.50	0.60
1:A:217:PRO:CB	1:A:221:HIS:HB2	2.32	0.60
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.84	0.59
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.01	0.59
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.67	0.59
2:B:172:ARG:C	2:B:174:GLN:H	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:SER:O	2:B:190:GLY:HA2	2.02	0.59
1:A:211:ARG:HG2	1:A:211:ARG:NH1	2.16	0.59
2:B:29:GLU:CD	2:B:71:TRP:HZ2	2.06	0.59
2:B:170:PRO:O	2:B:174:GLN:HB2	2.03	0.59
1:A:57:ASN:ND2	1:A:143:ARG:HH21	2.01	0.58
1:A:117:SER:HB2	1:A:214:LEU:HD23	1.85	0.58
1:A:123:ASP:O	1:A:126:LYS:HE3	2.02	0.58
1:A:357:MET:HB2	1:A:367:GLN:HE22	1.67	0.58
1:A:346:PHE:N	1:A:346:PHE:CD2	2.70	0.58
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.68	0.58
2:B:169:GLU:HA	2:B:173:LYS:NZ	2.15	0.58
1:A:33:ALA:HB1	1:A:71:TRP:HB2	1.84	0.57
1:A:19:PRO:O	1:A:56:TYR:HA	2.04	0.57
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.39	0.57
1:A:540:LYS:HB3	1:A:542:ILE:HG13	1.87	0.57
2:B:6:GLU:HG2	2:B:6:GLU:O	2.05	0.57
1:A:44:GLU:OE1	1:A:46:LYS:HE2	2.06	0.56
1:A:57:ASN:ND2	1:A:131:THR:HG22	2.21	0.56
2:B:169:GLU:HG2	2:B:173:LYS:NZ	2.20	0.56
2:B:197:GLN:HB3	2:B:201:LYS:HE2	1.87	0.56
1:A:32:LYS:HE2	1:A:32:LYS:CA	2.35	0.56
1:A:11:LYS:O	1:A:85:GLN:HB3	2.06	0.56
1:A:136:ASN:C	1:A:138:GLU:N	2.59	0.56
1:A:194:GLU:HB2	1:A:197:GLN:HE21	1.71	0.56
1:A:409:THR:O	2:B:364:ASP:HB2	2.07	0.55
2:B:339:TYR:OH	2:B:350:LYS:HE3	2.07	0.55
1:A:542:ILE:HG22	1:A:543:GLY:H	1.72	0.55
1:A:358:ARG:HG2	1:A:358:ARG:NH1	2.22	0.55
2:B:172:ARG:O	2:B:174:GLN:N	2.39	0.55
1:A:116:PHE:CZ	1:A:151:GLN:HB2	2.42	0.54
1:A:62:ALA:C	1:A:63:ILE:HD12	2.27	0.54
2:B:84:THR:HB	2:B:154:LYS:HE2	1.89	0.54
1:A:301:LEU:HD23	1:A:302:GLU:N	2.23	0.54
1:A:28:GLU:O	1:A:32:LYS:HG2	2.07	0.54
2:B:60:VAL:HG21	2:B:73:LYS:HZ2	1.73	0.54
2:B:376:THR:O	2:B:380:ILE:HG13	2.08	0.54
2:B:122:GLU:HA	2:B:122:GLU:OE2	2.07	0.53
2:B:169:GLU:HG2	2:B:173:LYS:HZ1	1.72	0.53
2:B:195:ILE:O	2:B:199:ARG:HG3	2.09	0.53
1:A:301:LEU:HD23	1:A:301:LEU:C	2.29	0.52
2:B:193:LEU:HD22	2:B:201:LYS:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:HG23	1:A:76:ASP:O	2.09	0.52
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.91	0.52
2:B:97:PRO:O	2:B:99:GLY:N	2.43	0.52
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.92	0.52
1:A:116:PHE:HZ	1:A:151:GLN:HB2	1.74	0.52
1:A:20:LYS:HE3	1:A:55:PRO:CB	2.40	0.52
1:A:402:TRP:CH2	2:B:362:THR:HA	2.45	0.52
1:A:376:THR:O	1:A:380:ILE:HG12	2.09	0.51
2:B:175:ASN:N	2:B:176:PRO:CD	2.72	0.51
1:A:63:ILE:HD12	1:A:63:ILE:N	2.25	0.51
2:B:354:TYR:OH	2:B:370:GLU:HB3	2.11	0.51
1:A:473:THR:HB	5:A:1072:HOH:O	2.10	0.51
1:A:117:SER:CB	1:A:214:LEU:HD23	2.41	0.51
1:A:279:LEU:HD23	1:A:302:GLU:OE1	2.10	0.51
1:A:301:LEU:O	1:A:304:ALA:HB3	2.10	0.51
1:A:357:MET:HE1	1:A:374:LYS:HE2	1.92	0.51
1:A:502:ALA:O	1:A:506:ILE:HG13	2.11	0.51
1:A:514:GLU:HG3	1:A:515:SER:N	2.24	0.51
1:A:225:PRO:CG	1:A:227:PHE:CZ	2.89	0.51
1:A:519:ASN:O	1:A:523:GLU:HG2	2.11	0.51
2:B:195:ILE:HG23	2:B:196:GLY:H	1.74	0.51
1:A:237:ASP:OD2	1:A:237:ASP:N	2.43	0.51
1:A:246:LEU:O	1:A:307:ARG:NH1	2.44	0.50
1:A:114:ALA:HB1	1:A:214:LEU:HD22	1.93	0.50
2:B:424:LYS:HD2	2:B:425:LEU:HD12	1.94	0.50
1:A:19:PRO:HG2	1:A:80:LEU:HB2	1.94	0.50
1:A:217:PRO:HB3	1:A:221:HIS:CB	2.42	0.50
1:A:270:ILE:HG22	1:A:314:VAL:HG11	1.94	0.50
1:A:279:LEU:CD2	1:A:302:GLU:OE1	2.60	0.49
2:B:245:VAL:HG22	2:B:429:LEU:O	2.12	0.49
2:B:361:HIS:HB3	5:B:1153:HOH:O	2.11	0.49
2:B:193:LEU:HD13	2:B:201:LYS:HD3	1.94	0.49
1:A:19:PRO:HG3	1:A:80:LEU:HA	1.94	0.49
1:A:88:TRP:O	1:A:89:GLU:CB	2.60	0.49
1:A:164:MET:HB3	1:A:182:GLN:NE2	2.28	0.49
1:A:260:LEU:O	1:A:264:LEU:HD23	2.13	0.49
1:A:368:LEU:O	1:A:372:VAL:HG23	2.12	0.49
2:B:97:PRO:HG3	2:B:181:TYR:HB2	1.94	0.49
2:B:111:VAL:HG23	2:B:111:VAL:O	2.12	0.49
1:A:329:ILE:O	1:A:392:PRO:HD3	2.12	0.49
1:A:492:GLU:HA	1:A:530:LYS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LEU:HD23	1:A:470:THR:HG22	1.94	0.48
1:A:402:TRP:CD1	1:A:402:TRP:C	2.87	0.48
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.95	0.48
2:B:301:LEU:O	2:B:304:ALA:HB3	2.13	0.48
1:A:50:ILE:O	1:A:143:ARG:HB2	2.14	0.48
2:B:97:PRO:HB2	2:B:179:VAL:HG11	1.96	0.48
2:B:198:HIS:O	2:B:202:ILE:HG12	2.13	0.48
1:A:226:PRO:CG	1:A:235:HIS:ND1	2.76	0.48
2:B:297:GLU:O	2:B:300:GLU:HB3	2.13	0.48
2:B:235:HIS:O	2:B:237:ASP:N	2.47	0.47
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.37	0.47
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.44	0.47
1:A:5:ILE:H	1:A:5:ILE:HG12	1.41	0.47
1:A:211:ARG:HH11	1:A:211:ARG:CG	2.28	0.47
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.95	0.47
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.49	0.47
2:B:94:ILE:HG13	2:B:94:ILE:O	2.15	0.47
1:A:51:GLY:HA2	1:A:143:ARG:HD3	1.96	0.47
1:A:117:SER:HB2	1:A:214:LEU:CD2	2.45	0.47
1:A:366:LYS:NZ	2:B:394:GLN:NE2	2.62	0.46
2:B:98:ALA:O	2:B:101:LYS:HG2	2.14	0.46
1:A:12:LEU:O	1:A:13:LYS:C	2.54	0.46
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.45	0.46
1:A:94:ILE:H	1:A:94:ILE:CD1	2.24	0.46
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.15	0.46
2:B:433:PRO:HB2	2:B:436:GLY:CA	2.43	0.46
2:B:159:ILE:HG22	2:B:159:ILE:O	2.14	0.46
1:A:523:GLU:O	1:A:527:LYS:HG3	2.15	0.46
1:A:373:GLN:HG2	5:A:1038:HOH:O	2.16	0.46
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.34	0.46
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.51	0.46
1:A:330:GLN:HB2	1:A:338:THR:OG1	2.15	0.46
2:B:28:GLU:HA	2:B:135:ILE:HD11	1.97	0.46
2:B:206:ARG:HG3	2:B:206:ARG:HH11	1.81	0.46
1:A:239:TRP:CH2	1:A:316:GLY:HA3	2.51	0.45
2:B:434:ILE:HD12	2:B:434:ILE:N	2.31	0.45
2:B:161:GLN:HB3	5:B:1142:HOH:O	2.15	0.45
1:A:109:LEU:CG	1:A:216:THR:HG21	2.40	0.45
1:A:498:ASP:C	1:A:498:ASP:OD1	2.55	0.45
2:B:235:HIS:C	2:B:237:ASP:H	2.20	0.45
1:A:346:PHE:N	1:A:346:PHE:HD2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:CG2	1:A:76:ASP:O	2.63	0.45
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.31	0.45
1:A:109:LEU:HG	1:A:216:THR:CG2	2.40	0.45
1:A:136:ASN:C	1:A:138:GLU:H	2.19	0.44
2:B:376:THR:O	2:B:379:SER:HB3	2.17	0.44
1:A:260:LEU:HG	1:A:264:LEU:CD2	2.47	0.44
1:A:239:TRP:CD2	1:A:316:GLY:HA3	2.53	0.44
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.52	0.44
2:B:65:LYS:NZ	2:B:110:ASP:OD1	2.51	0.44
1:A:241:VAL:HG23	1:A:314:VAL:O	2.17	0.44
2:B:64:LYS:HE2	2:B:71:TRP:CE2	2.53	0.44
2:B:303:LEU:O	2:B:307:ARG:HG3	2.18	0.44
2:B:325:LEU:HB2	2:B:385:LYS:HE3	2.00	0.44
2:B:439:THR:HG22	2:B:439:THR:O	2.17	0.44
1:A:44:GLU:HB2	1:A:46:LYS:HD3	2.00	0.44
1:A:417:VAL:O	1:A:417:VAL:HG13	2.18	0.44
2:B:66:LYS:O	2:B:67:ASP:O	2.36	0.43
2:B:175:ASN:N	2:B:176:PRO:HD3	2.33	0.43
1:A:366:LYS:NZ	2:B:394:GLN:HE21	2.15	0.43
1:A:445:ALA:HA	1:A:474:ASN:HD21	1.84	0.43
2:B:120:LEU:O	2:B:121:ASP:C	2.56	0.43
1:A:41:MET:SD	1:A:73:LYS:HE3	2.58	0.43
1:A:50:ILE:HG13	1:A:52:PRO:HD2	2.00	0.43
1:A:254:VAL:HB	1:A:289:LEU:O	2.18	0.43
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.16	0.43
2:B:113:ASP:O	2:B:116:PHE:CD2	2.71	0.43
2:B:77:PHE:CD2	2:B:80:LEU:HD23	2.54	0.43
2:B:195:ILE:HG23	2:B:196:GLY:N	2.33	0.43
1:A:434:ILE:HG23	5:A:1062:HOH:O	2.19	0.43
1:A:26:LEU:CD1	1:A:133:PRO:HG2	2.48	0.43
1:A:254:VAL:HG22	1:A:286:THR:HG21	2.00	0.43
2:B:245:VAL:O	2:B:245:VAL:HG23	2.19	0.43
1:A:26:LEU:HD12	1:A:133:PRO:HG2	2.00	0.43
2:B:172:ARG:C	2:B:174:GLN:N	2.72	0.43
2:B:183:TYR:O	2:B:184:MET:C	2.57	0.43
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.84	0.42
1:A:434:ILE:HD11	1:A:530:LYS:HB3	1.98	0.42
2:B:154:LYS:O	2:B:157:PRO:HD2	2.18	0.42
1:A:88:TRP:O	1:A:89:GLU:HB3	2.19	0.42
1:A:357:MET:HE2	1:A:374:LYS:HE3	2.01	0.42
1:A:90:VAL:O	1:A:91:GLN:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:SER:CB	2:B:387:PRO:HD3	2.49	0.42
1:A:90:VAL:O	1:A:91:GLN:C	2.58	0.42
2:B:85:GLN:NE2	2:B:87:PHE:CE1	2.88	0.42
2:B:98:ALA:O	2:B:101:LYS:HE3	2.19	0.42
1:A:224:GLU:HA	1:A:225:PRO:HD3	1.62	0.42
2:B:162:SER:N	5:B:1142:HOH:O	2.31	0.42
2:B:197:GLN:HB3	2:B:201:LYS:CE	2.49	0.42
1:A:111:VAL:O	1:A:114:ALA:HB3	2.19	0.42
2:B:195:ILE:CD1	2:B:199:ARG:HH21	2.31	0.42
1:A:377:THR:O	1:A:381:VAL:HG23	2.19	0.42
2:B:156:SER:N	2:B:157:PRO:HD2	2.34	0.42
2:B:6:GLU:O	2:B:6:GLU:CG	2.67	0.42
2:B:175:ASN:C	2:B:177:ASP:H	2.21	0.42
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.54	0.42
1:A:38:CYS:HB3	1:A:144:TYR:CE1	2.55	0.41
1:A:255:ASN:O	1:A:259:LYS:HG2	2.19	0.41
1:A:272:PRO:HA	5:A:1020:HOH:O	2.20	0.41
1:A:314:VAL:O	1:A:314:VAL:HG12	2.19	0.41
2:B:85:GLN:NE2	2:B:87:PHE:HE1	2.18	0.41
2:B:239:TRP:O	2:B:240:THR:CG2	2.68	0.41
2:B:240:THR:O	2:B:350:LYS:HG3	2.20	0.41
2:B:242:GLN:HB2	2:B:430:GLU:CD	2.41	0.41
2:B:332:GLN:HE21	2:B:424:LYS:HE2	1.81	0.41
1:A:366:LYS:HZ2	2:B:394:GLN:NE2	2.17	0.41
2:B:113:ASP:O	2:B:116:PHE:HD2	2.03	0.41
2:B:101:LYS:O	2:B:236:PRO:HB3	2.20	0.41
1:A:53:GLU:O	1:A:55:PRO:HD3	2.20	0.41
1:A:136:ASN:O	1:A:137:ASN:C	2.58	0.41
2:B:242:GLN:HA	2:B:242:GLN:OE1	2.19	0.41
1:A:497:THR:O	1:A:535:TRP:HA	2.21	0.41
2:B:120:LEU:HD23	2:B:125:ARG:HG2	2.02	0.41
2:B:165:THR:HG23	2:B:166:LYS:H	1.85	0.41
2:B:180:ILE:HG12	2:B:189:VAL:CG1	2.44	0.41
1:A:27:THR:O	1:A:31:ILE:HG13	2.21	0.41
1:A:247:PRO:O	1:A:307:ARG:NH1	2.49	0.41
1:A:115:TYR:CE1	1:A:151:GLN:NE2	2.88	0.41
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.03	0.41
2:B:101:LYS:HG3	2:B:102:LYS:HG3	2.03	0.41
2:B:267:ALA:HB2	2:B:426:TRP:CH2	2.56	0.41
2:B:211:ARG:HE	2:B:211:ARG:HB3	1.65	0.41
1:A:399:GLU:O	1:A:403:THR:HB	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:GLN:O	2:B:201:LYS:HG3	2.21	0.40
1:A:412:PRO:O	1:A:413:GLU:C	2.60	0.40
1:A:169:GLU:O	1:A:173:LYS:HD3	2.20	0.40
1:A:475:GLN:HE21	1:A:475:GLN:HB3	1.57	0.40
1:A:78:ARG:CG	1:A:79:GLU:N	2.85	0.40
2:B:234:LEU:CD1	2:B:381:VAL:HG21	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ALA:N	2:B:297:GLU:OE1[2_555]	2.17	0.03

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	531/542 (98%)	494 (93%)	29 (6%)	8 (2%)	10 10
2	B	403/435 (93%)	365 (91%)	29 (7%)	9 (2%)	6 5
All	All	934/977 (96%)	859 (92%)	58 (6%)	17 (2%)	8 7

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	91	GLN
1	A	137	ASN
2	B	67	ASP
2	B	173	LYS
2	B	176	PRO
1	A	52	PRO

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Mol	Chain	Res	Type
1	A	85	GLN
2	B	66	LYS
2	B	98	ALA
1	A	133	PRO
1	A	247	PRO
1	A	361	HIS
2	B	236	PRO
2	B	238	LYS
2	B	184	MET
2	B	175	ASN

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	478/484 (99%)	444 (93%)	34 (7%)	14 19
2	B	372/395 (94%)	351 (94%)	21 (6%)	21 29
All	All	850/879 (97%)	795 (94%)	55 (6%)	17 23

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	46	LYS
1	A	89	GLU
1	A	94	ILE
1	A	113	ASP
1	A	115	TYR
1	A	122	GLU
1	A	123	ASP
1	A	134	SER
1	A	136	ASN
1	A	149	LEU
1	A	151	GLN
1	A	184	MET

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Mol	Chain	Res	Type
1	A	186	ASP
1	A	205	LEU
1	A	224	GLU
1	A	249	LYS
1	A	263	LYS
1	A	286	THR
1	A	307	ARG
1	A	317	VAL
1	A	325	LEU
1	A	340	GLN
1	A	358	ARG
1	A	369	THR
1	A	402	TRP
1	A	424	LYS
1	A	474	ASN
1	A	475	GLN
1	A	516	GLU
1	A	517	LEU
1	A	529	GLU
1	A	533	LEU
1	A	540	LYS
2	B	8	VAL
2	B	40	GLU
2	B	55	PRO
2	B	139	THR
2	B	163	SER
2	B	165	THR
2	B	167	ILE
2	B	176	PRO
2	B	177	ASP
2	B	205	LEU
2	B	206	ARG
2	B	237	ASP
2	B	239	TRP
2	B	283	LEU
2	B	303	LEU
2	B	323	LYS
2	B	356	ARG
2	B	368	LEU
2	B	392	PRO
2	B	400	THR
2	B	422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	96	HIS
1	A	136	ASN
1	A	174	GLN
1	A	182	GLN
1	A	197	GLN
1	A	207	GLN
1	A	208	HIS
1	A	222	GLN
1	A	242	GLN
1	A	278	GLN
1	A	332	GLN
1	A	334	GLN
1	A	474	ASN
1	A	475	GLN
2	B	57	ASN
2	B	174	GLN
2	B	197	GLN
2	B	332	GLN
2	B	394	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CSD	A	280	1	3,7,8	1.07	0	1,8,10	0.06	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
1	CSD	A	280	1	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

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)

3 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	B	1302	-	4,4,4	1.68	0	6,6,6	0.43	0
4	HBQ	A	999	-	21,21,21	1.67	6 (28%)	28,30,30	1.07	3 (10%)
3	PO4	A	1301	-	4,4,4	1.62	0	6,6,6	0.45	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	HBQ	A	999	-	-	0/10/26/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	HBQ	C11-N1	3.77	1.43	1.37
4	A	999	HBQ	C2-N1	3.24	1.51	1.47
4	A	999	HBQ	C4-C3	3.05	1.44	1.40
4	A	999	HBQ	C3-N1	2.81	1.46	1.42
4	A	999	HBQ	C6-C5	2.09	1.42	1.38
4	A	999	HBQ	O3-C11	2.06	1.24	1.21

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	999	HBQ	O2-C11-N1	2.40	113.62	110.81
4	A	999	HBQ	O3-C11-N1	-2.36	120.13	124.09
4	A	999	HBQ	O2-C12-C13	-2.25	101.17	107.14

There are no chirality outliers.

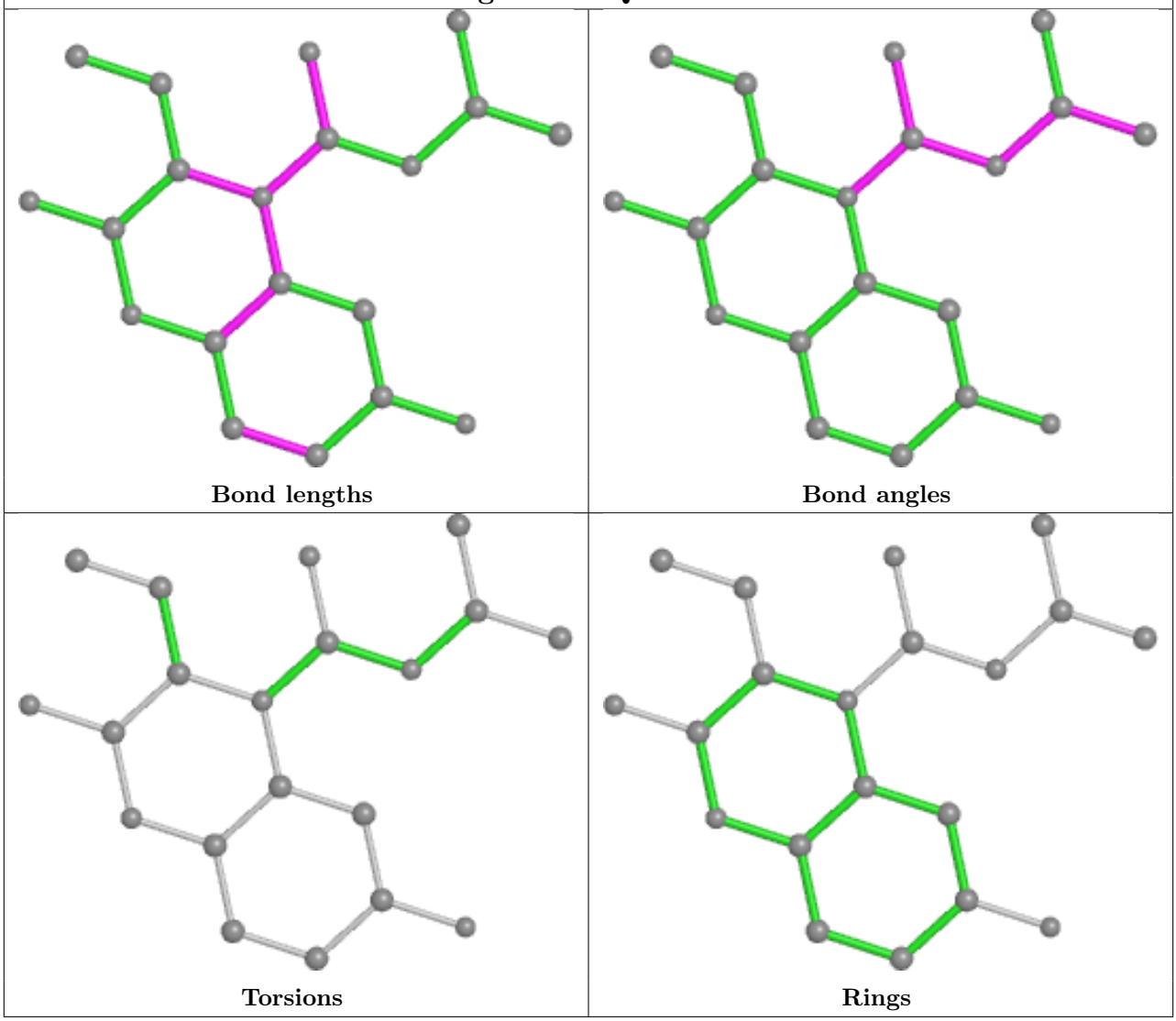
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 HBQ A 999



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	535/542 (98%)	0.02	31 (5%)	23	29	25, 52, 104, 143	0
2	B	409/435 (94%)	0.02	24 (5%)	22	28	27, 52, 107, 150	0
All	All	944/977 (96%)	0.02	55 (5%)	23	29	25, 52, 106, 150	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	440	PHE	7.9
2	B	195	ILE	5.6
1	A	92	LEU	5.6
2	B	67	ASP	5.3
2	B	94	ILE	5.2
1	A	138	GLU	4.9
2	B	439	THR	4.9
2	B	434	ILE	4.7
2	B	68	SER	4.5
1	A	135	ILE	4.5
1	A	2	ILE	4.4
2	B	240	THR	4.4
2	B	69	THR	4.3
1	A	52	PRO	4.1
2	B	212	TRP	3.6
1	A	53	GLU	3.5
1	A	223	LYS	3.5
2	B	66	LYS	3.4
1	A	228	LEU	3.4
1	A	220	LYS	3.1
1	A	218	ASP	3.1
2	B	210	LEU	2.9
1	A	43	LYS	2.9
1	A	541	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	95	PRO	2.8
2	B	437	ALA	2.8
2	B	436	GLY	2.7
2	B	197	GLN	2.6
1	A	71	TRP	2.5
2	B	358	ARG	2.4
2	B	146	TYR	2.4
1	A	360	ALA	2.4
1	A	219	LYS	2.4
1	A	150	PRO	2.4
1	A	24	TRP	2.3
2	B	7	THR	2.3
2	B	6	GLU	2.3
1	A	21	VAL	2.3
2	B	438	GLU	2.3
1	A	14	PRO	2.3
1	A	183	TYR	2.2
1	A	185	ASP	2.2
1	A	497	THR	2.2
1	A	221	HIS	2.2
1	A	146	TYR	2.2
1	A	22	LYS	2.1
1	A	63	ILE	2.1
1	A	51	GLY	2.1
1	A	539	HIS	2.1
2	B	128	THR	2.1
1	A	61	PHE	2.1
2	B	194	GLU	2.0
1	A	448	ARG	2.0
1	A	136	ASN	2.0
2	B	65	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	0.95	0.14	44,52,75,76	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

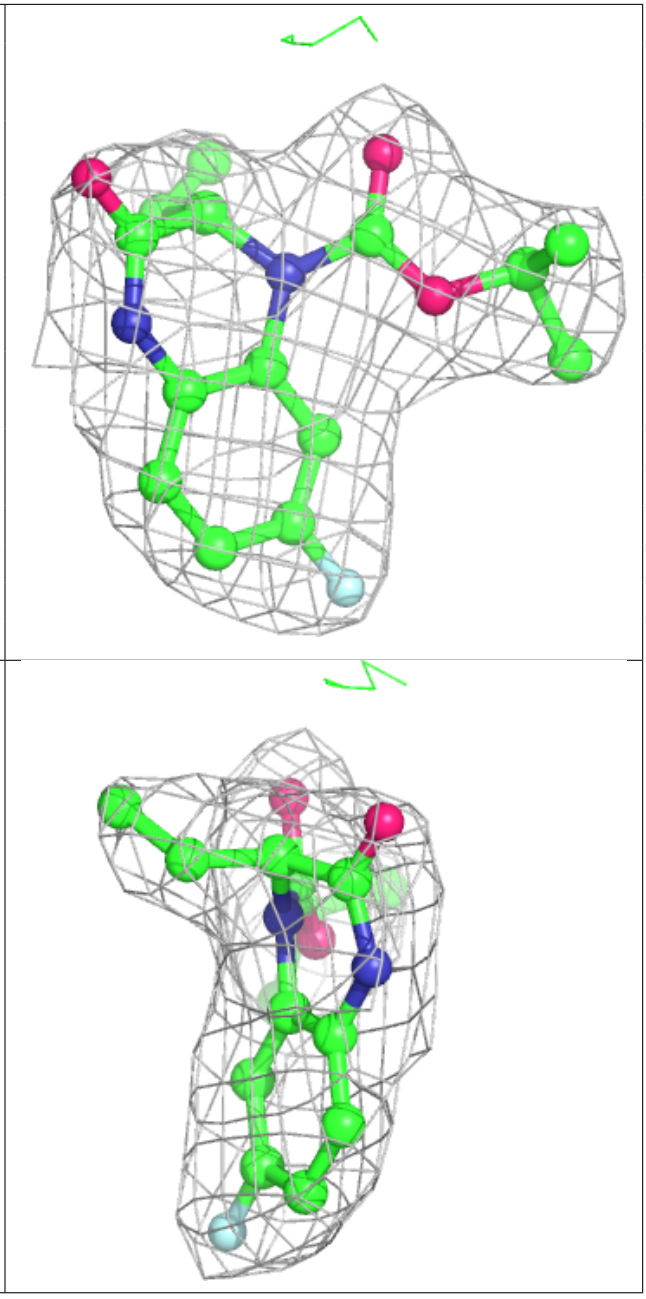
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PO4	B	1302	5/5	0.84	0.14	94,107,112,114	0
3	PO4	A	1301	5/5	0.90	0.17	90,127,129,137	0
4	HBQ	A	999	20/20	0.98	0.16	29,38,61,69	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 HBQ 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.