Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:02 PM GMT

PDB ID	:	1RT1
Title	:	CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE COMPLEXED WITH MKC-442
Authors	:	Ren, J.; Esnouf, R.; Hopkins, A.; Willcox, B.; Jones, Y.; Ross, C.; Stammers, D.; Stuart, D.
Deposited on	:	1996-03-16
Resolution	:	2.55 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
http://wwpdb.org/validation/2016/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:

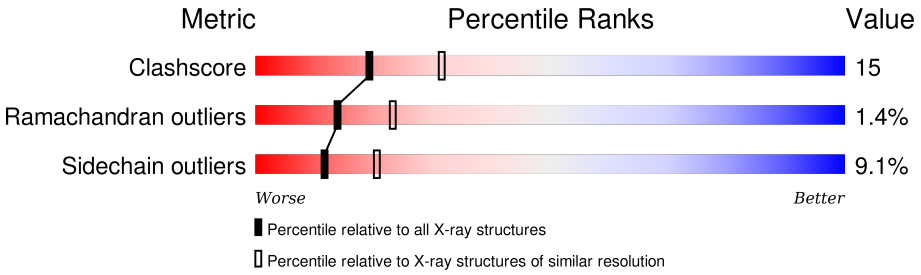
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	57% 33% 6% •
2	B	440	64% 27% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8272 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	539	4410	2853	734	815	8	0	0	0

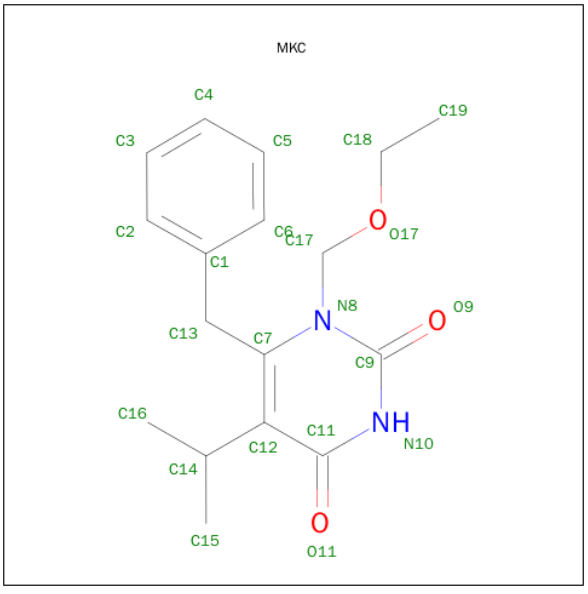
There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	415	3428	2230	568	623	7	0	0	0

- Molecule 3 is 6-BENZYL-1-ETHOXYMETHYL-5-ISOPROPYL URACIL (three-letter code: MKC) (formula: $C_{17}H_{22}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	17	2	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	253	Total	O	0	0
			253	253		
4	B	159	Total	O	0	0
			159	159		

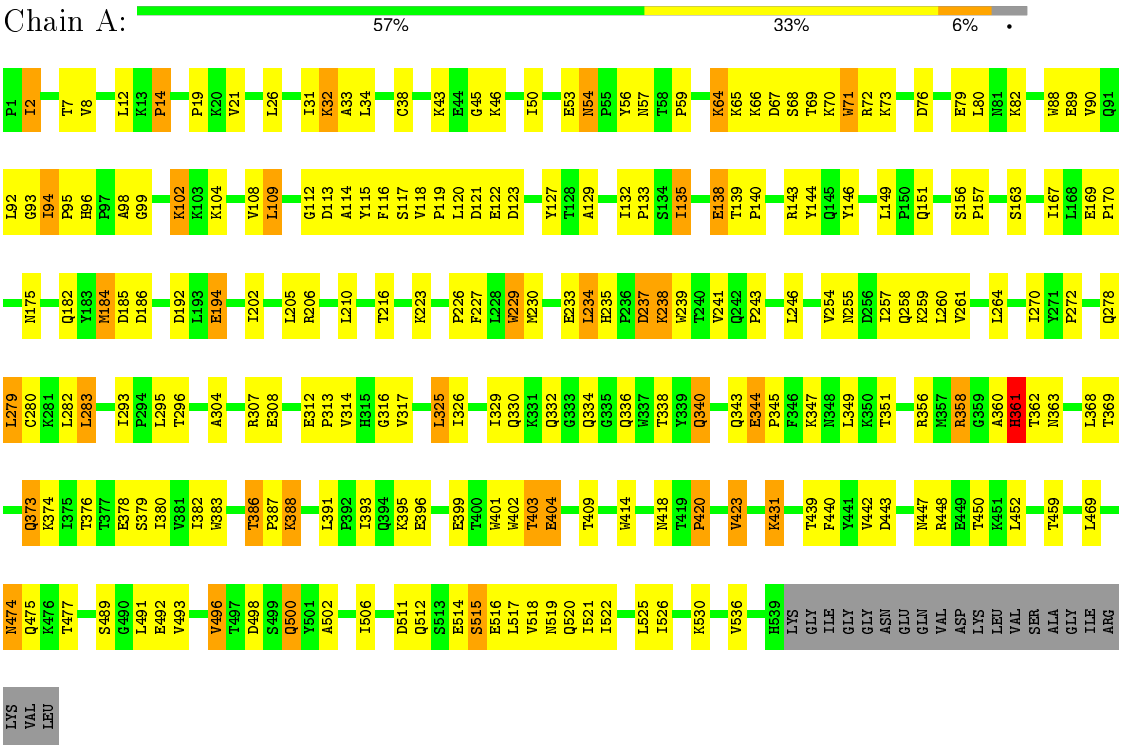
3 Residue-property plots (i)

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

Note EDS was not executed.

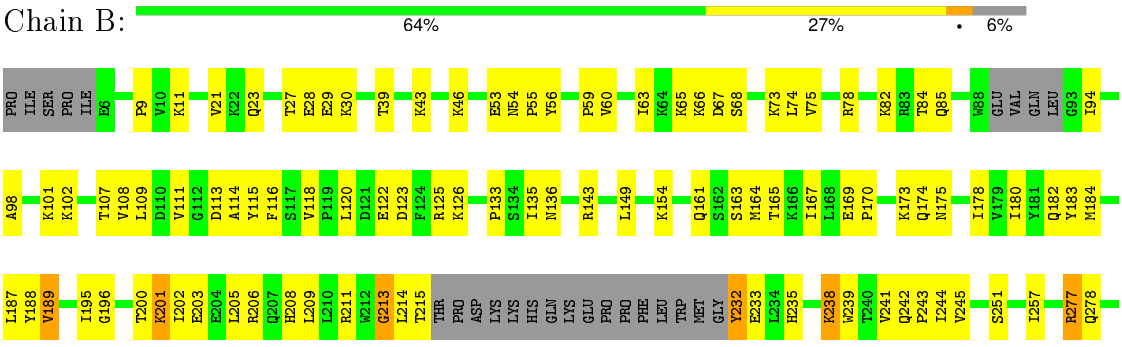
- Molecule 1: HIV-1 REVERSE TRANSCRIPTASE

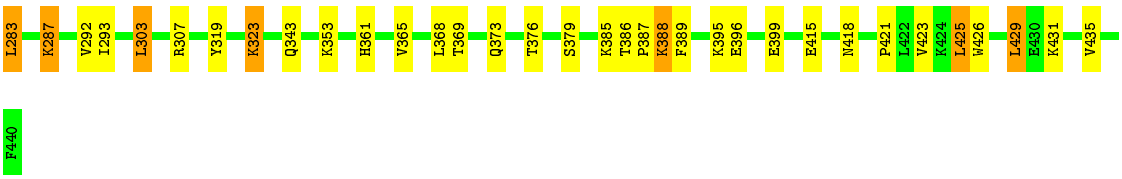
Chain A:



- Molecule 2: HIV-1 REVERSE TRANSCRIPTASE

Chain B:




L283
K287
V292
T293
L303
R307
Y319
K323
Q343
K353
H361
V365
L368
T369
Q373
T376
S379
K385
T386
P387
K388
F389
K395
E396
E399
E415
N418
P421
L422
V423
K424
L425
W426
L429
E430
K431
V435
F440

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	136.80Å 109.80Å 72.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.55	Depositor
% Data completeness (in resolution range)	95.5 (25.00-2.55)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8272	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0/4519	0.75	2/6143 (0.0%)
2	B	0.50	0/3524	0.73	0/4786
All	All	0.50	0/8043	0.74	2/10929 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	GLY	N-CA-C	-5.31	99.83	113.10
1	A	388	LYS	N-CA-C	-5.19	97.00	111.00

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	4410	0	4453	156	0
2	B	3428	0	3455	84	0
3	A	22	0	22	1	0
4	A	253	0	0	7	0
4	B	159	0	0	5	0
All	All	8272	0	7930	238	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 15.

All (238) 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:116:PHE:HE1	1:A:151:GLN:HG2	1.40	0.86
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.57	0.86
1:A:238:LYS:HB2	1:A:316:GLY:O	1.75	0.85
1:A:360:ALA:HA	1:A:514:GLU:HB3	1.58	0.85
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.57	0.84
1:A:358:ARG:HD3	1:A:358:ARG:H	1.45	0.79
1:A:94:ILE:H	1:A:94:ILE:HD13	1.46	0.79
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.18	0.78
2:B:163:SER:O	2:B:167:ILE:HG23	1.86	0.76
1:A:344:GLU:HG2	1:A:347:LYS:HB2	1.67	0.76
1:A:116:PHE:CE2	1:A:146:TYR:HE2	2.03	0.75
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.67	0.75
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.70	0.74
1:A:116:PHE:CE1	1:A:151:GLN:HG2	2.22	0.73
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.70	0.73
1:A:326:ILE:HG12	1:A:388:LYS:HE2	1.71	0.72
1:A:135:ILE:O	1:A:138:GLU:HG3	1.90	0.72
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.72	0.71
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.73	0.71
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.26	0.70
1:A:102:LYS:NZ	1:A:102:LYS:HB2	2.06	0.70
1:A:94:ILE:HB	1:A:229:TRP:HH2	1.55	0.70
2:B:84:THR:HB	2:B:154:LYS:HE2	1.76	0.68
1:A:312:GLU:HG2	1:A:313:PRO:HD2	1.75	0.68
1:A:380:ILE:CD1	1:A:386:THR:HG22	2.22	0.68
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.28	0.68
2:B:175:ASN:HD21	2:B:201:LYS:HD2	1.59	0.67
1:A:378:GLU:O	1:A:382:ILE:HG12	1.95	0.67
2:B:323:LYS:HB3	2:B:343:GLN:NE2	2.08	0.67
1:A:442:VAL:HG22	1:A:496:VAL:O	1.96	0.65
1:A:95:PRO:O	1:A:229:TRP:HZ3	1.80	0.64
1:A:64:LYS:H	1:A:64:LYS:HD2	1.61	0.64
1:A:206:ARG:O	1:A:210:LEU:HD23	1.97	0.64
1:A:115:TYR:HD2	1:A:156:SER:HB3	1.62	0.64
2:B:244:ILE:HG23	2:B:429:LEU:HB3	1.78	0.64
1:A:448:ARG:HE	1:A:474:ASN:H	1.44	0.64
1:A:304:ALA:O	1:A:308:GLU:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PHE:HE1	1:A:151:GLN:CG	2.09	0.63
1:A:255:ASN:O	1:A:259:LYS:HG2	1.98	0.63
1:A:96:HIS:HD2	1:A:98:ALA:H	1.47	0.62
2:B:78:ARG:O	2:B:82:LYS:HG3	1.98	0.62
2:B:175:ASN:ND2	2:B:201:LYS:HD2	2.14	0.62
1:A:94:ILE:HB	1:A:229:TRP:CH2	2.35	0.62
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.80	0.62
2:B:235:HIS:O	2:B:238:LYS:HG2	2.00	0.61
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.83	0.61
2:B:111:VAL:HA	2:B:214:LEU:HD22	1.83	0.61
1:A:50:ILE:HB	4:A:1047:HOH:O	2.01	0.60
1:A:243:PRO:HG3	4:A:1119:HOH:O	2.02	0.60
1:A:260:LEU:O	1:A:264:LEU:HD23	2.01	0.60
2:B:39:THR:O	2:B:43:LYS:HG2	2.02	0.60
1:A:114:ALA:HA	1:A:117:SER:OG	2.00	0.60
1:A:118:VAL:HB	1:A:149:LEU:HD22	1.83	0.60
2:B:23:GLN:HG2	2:B:133:PRO:HD3	1.82	0.59
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.84	0.59
1:A:116:PHE:HE2	1:A:146:TYR:HE2	1.46	0.59
2:B:169:GLU:O	2:B:173:LYS:HD3	2.01	0.59
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.84	0.59
2:B:213:GLY:O	2:B:214:LEU:HG	2.03	0.58
1:A:65:LYS:HB2	1:A:72:ARG:HD2	1.85	0.58
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.86	0.58
1:A:373:GLN:HG2	4:B:1363:HOH:O	2.03	0.58
2:B:426:TRP:O	2:B:429:LEU:HB2	2.05	0.57
1:A:376:THR:O	1:A:380:ILE:HG12	2.05	0.56
1:A:332:GLN:O	1:A:336:GLN:HB2	2.05	0.56
2:B:53:GLU:O	2:B:55:PRO:HD3	2.06	0.56
1:A:46:LYS:HE2	1:A:116:PHE:HB3	1.88	0.56
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.88	0.56
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.06	0.55
2:B:202:ILE:O	2:B:205:LEU:HB3	2.06	0.55
2:B:27:THR:HG22	2:B:29:GLU:H	1.70	0.55
1:A:129:ALA:HB1	1:A:143:ARG:HH12	1.71	0.55
1:A:68:SER:C	1:A:70:LYS:H	2.10	0.55
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.88	0.55
1:A:8:VAL:O	1:A:121:ASP:HB2	2.06	0.55
1:A:2:ILE:HD11	1:A:45:GLY:O	2.07	0.54
1:A:108:VAL:CG1	1:A:223:LYS:HB2	2.38	0.54
1:A:116:PHE:HE2	1:A:146:TYR:CE2	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:THR:HB	1:A:140:PRO:CD	2.38	0.54
2:B:365:VAL:O	2:B:369:THR:HG23	2.08	0.54
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.90	0.54
2:B:242:GLN:HB2	4:B:1406:HOH:O	2.08	0.54
1:A:94:ILE:H	1:A:94:ILE:CD1	2.19	0.54
2:B:369:THR:O	2:B:373:GLN:HG3	2.09	0.53
1:A:122:GLU:CD	1:A:122:GLU:H	2.10	0.53
1:A:516:GLU:O	1:A:520:GLN:HG3	2.08	0.53
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.91	0.53
2:B:169:GLU:HB2	2:B:170:PRO:CD	2.34	0.53
1:A:96:HIS:CD2	1:A:98:ALA:H	2.27	0.52
1:A:116:PHE:CE2	1:A:146:TYR:CE2	2.93	0.51
1:A:68:SER:C	1:A:70:LYS:N	2.64	0.51
1:A:226:PRO:HB3	1:A:235:HIS:ND1	2.25	0.51
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.50	0.51
1:A:293:ILE:N	1:A:293:ILE:HD12	2.25	0.51
1:A:418:ASN:OD1	1:A:420:PRO:HD3	2.11	0.51
1:A:358:ARG:HD3	1:A:358:ARG:N	2.21	0.50
1:A:308:GLU:HG2	4:A:1118:HOH:O	2.12	0.49
1:A:358:ARG:O	1:A:358:ARG:HG2	2.12	0.49
1:A:502:ALA:O	1:A:506:ILE:HG13	2.12	0.49
1:A:227:PHE:O	1:A:233:GLU:HA	2.12	0.49
1:A:102:LYS:HB2	1:A:102:LYS:HZ3	1.76	0.49
2:B:251:SER:HB3	2:B:292:VAL:CG1	2.42	0.49
1:A:515:SER:OG	1:A:518:VAL:HG23	2.13	0.49
1:A:516:GLU:O	1:A:519:ASN:HB2	2.13	0.49
2:B:54:ASN:O	2:B:143:ARG:NH2	2.46	0.49
1:A:108:VAL:HG11	1:A:223:LYS:HB2	1.94	0.48
1:A:82:LYS:HA	4:A:1037:HOH:O	2.11	0.48
1:A:257:ILE:HG23	1:A:279:LEU:HD12	1.93	0.48
1:A:521:ILE:O	1:A:525:LEU:HG	2.13	0.48
1:A:184:MET:HB3	1:A:185:ASP:H	1.51	0.48
1:A:46:LYS:HE2	1:A:116:PHE:CB	2.43	0.48
2:B:113:ASP:O	2:B:116:PHE:HD1	1.96	0.48
1:A:31:ILE:HG12	1:A:133:PRO:HG2	1.94	0.48
2:B:388:LYS:HE2	2:B:415:GLU:HB3	1.96	0.48
2:B:29:GLU:CG	2:B:30:LYS:N	2.77	0.48
2:B:245:VAL:HG13	2:B:431:LYS:HB2	1.95	0.48
2:B:170:PRO:O	2:B:174:GLN:HG3	2.13	0.48
2:B:122:GLU:HG3	2:B:123:ASP:N	2.29	0.47
1:A:330:GLN:HB2	1:A:338:THR:OG1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.96	0.47
1:A:115:TYR:CD2	1:A:156:SER:HB3	2.45	0.47
2:B:98:ALA:O	2:B:101:LYS:HG3	2.13	0.47
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.49	0.47
1:A:53:GLU:O	1:A:54:ASN:HB2	2.15	0.47
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.29	0.47
2:B:376:THR:CG2	2:B:386:THR:HG22	2.44	0.47
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.44	0.47
1:A:102:LYS:HB2	1:A:102:LYS:HZ2	1.78	0.47
2:B:379:SER:CB	2:B:387:PRO:HD3	2.45	0.47
2:B:178:ILE:CG2	2:B:189:VAL:HG12	2.45	0.47
2:B:232:TYR:HD1	2:B:233:GLU:H	1.63	0.47
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.96	0.47
1:A:33:ALA:HB1	1:A:71:TRP:HB3	1.97	0.47
1:A:234:LEU:HD12	1:A:239:TRP:HB3	1.97	0.46
2:B:257:ILE:HG22	2:B:283:LEU:HD21	1.97	0.46
1:A:65:LYS:HD3	1:A:67:ASP:OD2	2.15	0.46
1:A:65:LYS:HG2	1:A:66:LYS:H	1.80	0.46
2:B:287:LYS:HE2	2:B:293:ILE:HD11	1.97	0.46
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.97	0.46
1:A:43:LYS:HA	1:A:43:LYS:HD3	1.56	0.46
1:A:149:LEU:HG	1:A:156:SER:HA	1.98	0.46
1:A:254:VAL:O	1:A:258:GLN:HG3	2.15	0.46
2:B:114:ALA:HB2	2:B:214:LEU:HD11	1.98	0.46
2:B:46:LYS:HE2	2:B:116:PHE:CD2	2.51	0.46
1:A:237:ASP:O	1:A:238:LYS:HB3	2.16	0.46
1:A:254:VAL:HG22	1:A:293:ILE:CD1	2.46	0.46
1:A:272:PRO:HA	4:A:1148:HOH:O	2.15	0.46
1:A:34:LEU:HD21	1:A:73:LYS:HB2	1.98	0.46
2:B:27:THR:HG22	2:B:28:GLU:N	2.31	0.45
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.51	0.45
1:A:246:LEU:O	1:A:307:ARG:NH1	2.48	0.45
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.16	0.45
2:B:94:ILE:HD11	2:B:182:GLN:H	1.81	0.45
1:A:257:ILE:O	1:A:261:VAL:HG23	2.15	0.45
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.97	0.45
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.51	0.45
2:B:11:LYS:N	2:B:85:GLN:OE1	2.49	0.45
1:A:448:ARG:NE	1:A:474:ASN:H	2.11	0.45
2:B:107:THR:HA	2:B:232:TYR:O	2.16	0.45
2:B:353:LYS:HB2	2:B:353:LYS:HE3	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.97	0.45
1:A:511:ASP:OD1	1:A:512:GLN:HG2	2.17	0.45
2:B:118:VAL:HB	2:B:149:LEU:CD1	2.47	0.44
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.52	0.44
2:B:421:PRO:O	2:B:425:LEU:HD22	2.17	0.44
1:A:210:LEU:HD21	1:A:216:THR:HB	1.98	0.44
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.99	0.44
1:A:186:ASP:OD1	1:A:223:LYS:HE3	2.18	0.44
2:B:423:VAL:HG21	4:B:1408:HOH:O	2.16	0.44
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.53	0.44
1:A:401:TRP:CZ3	1:A:409:THR:HG21	2.53	0.44
1:A:26:LEU:HA	4:A:1040:HOH:O	2.17	0.44
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.53	0.44
1:A:226:PRO:HA	1:A:234:LEU:O	2.18	0.44
2:B:167:ILE:O	2:B:208:HIS:CE1	2.71	0.44
2:B:418:ASN:HB3	4:B:1378:HOH:O	2.17	0.44
2:B:277:ARG:HG2	2:B:278:GLN:N	2.33	0.44
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.48	0.44
1:A:522:ILE:O	1:A:526:ILE:HG13	2.18	0.44
1:A:102:LYS:NZ	1:A:102:LYS:CB	2.79	0.43
1:A:115:TYR:HE1	1:A:185:ASP:OD1	2.02	0.43
2:B:303:LEU:HD22	2:B:307:ARG:NE	2.33	0.43
2:B:66:LYS:O	2:B:67:ASP:HB3	2.18	0.43
2:B:188:TYR:CD1	2:B:188:TYR:N	2.85	0.43
1:A:32:LYS:HD3	1:A:32:LYS:HA	1.84	0.43
1:A:374:LYS:HE2	1:A:374:LYS:HB3	1.76	0.43
2:B:251:SER:HB3	2:B:292:VAL:HG11	1.99	0.43
1:A:431:LYS:HE3	1:A:431:LYS:HA	2.01	0.43
2:B:56:TYR:HE2	2:B:126:LYS:CE	2.32	0.43
1:A:340:GLN:CB	1:A:351:THR:HG22	2.49	0.43
2:B:107:THR:O	2:B:188:TYR:HA	2.19	0.43
2:B:241:VAL:HA	4:B:1410:HOH:O	2.19	0.43
1:A:282:LEU:HD21	1:A:295:LEU:HD22	2.01	0.43
2:B:196:GLY:O	2:B:200:THR:HG23	2.19	0.42
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.54	0.42
1:A:95:PRO:HA	2:B:136:ASN:O	2.19	0.42
1:A:109:LEU:HD11	1:A:206:ARG:HH11	1.84	0.42
2:B:28:GLU:HG3	2:B:135:ILE:HD11	2.02	0.42
1:A:399:GLU:O	1:A:403:THR:HB	2.18	0.42
1:A:194:GLU:HA	1:A:194:GLU:OE1	2.17	0.42
1:A:492:GLU:HA	1:A:530:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:CSD:O	1:A:283:LEU:HB2	2.19	0.42
1:A:241:VAL:CG2	1:A:314:VAL:HG23	2.50	0.42
2:B:232:TYR:HD1	2:B:233:GLU:N	2.17	0.42
2:B:395:LYS:O	2:B:399:GLU:HG3	2.19	0.42
1:A:99:GLY:HA3	2:B:136:ASN:ND2	2.35	0.42
1:A:373:GLN:NE2	2:B:396:GLU:HB3	2.34	0.42
2:B:102:LYS:HE3	2:B:102:LYS:HB2	1.81	0.42
2:B:319:TYR:OH	2:B:385:LYS:HD3	2.19	0.42
1:A:439:THR:O	1:A:459:THR:HB	2.19	0.42
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.48	0.42
1:A:50:ILE:HD11	1:A:143:ARG:HH11	1.85	0.41
1:A:69:THR:HG22	1:A:69:THR:O	2.20	0.41
1:A:202:ILE:HG22	1:A:206:ARG:NH2	2.35	0.41
2:B:277:ARG:HG2	2:B:278:GLN:H	1.84	0.41
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.88	0.41
1:A:360:ALA:O	1:A:361:HIS:HB3	2.19	0.41
2:B:205:LEU:O	2:B:208:HIS:HB3	2.19	0.41
1:A:56:TYR:O	1:A:57:ASN:HB2	2.20	0.41
2:B:203:GLU:HG2	2:B:206:ARG:NH2	2.35	0.41
1:A:379:SER:HA	1:A:383:TRP:CE3	2.55	0.41
2:B:161:GLN:O	2:B:165:THR:HG22	2.20	0.41
1:A:79:GLU:O	1:A:82:LYS:HG3	2.21	0.41
1:A:139:THR:HB	1:A:140:PRO:HD2	2.03	0.41
1:A:278:GLN:O	1:A:282:LEU:HD13	2.20	0.41
1:A:500:GLN:HE21	1:A:500:GLN:HB3	1.76	0.41
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.90	0.41
3:A:999:MKC:C6	3:A:999:MKC:H162	2.51	0.41
1:A:115:TYR:O	1:A:149:LEU:HB2	2.20	0.41
1:A:386:THR:HA	1:A:387:PRO:HD3	1.85	0.40
1:A:50:ILE:HG13	1:A:143:ARG:HB3	2.04	0.40
1:A:344:GLU:HG3	1:A:347:LYS:HD2	2.03	0.40
1:A:109:LEU:HA	1:A:109:LEU:HD12	1.96	0.40
1:A:404:GLU:HG3	4:A:1181:HOH:O	2.21	0.40
2:B:109:LEU:HD11	2:B:205:LEU:HD12	2.04	0.40
2:B:323:LYS:HB3	2:B:343:GLN:HE22	1.86	0.40
1:A:163:SER:O	1:A:167:ILE:HG13	2.21	0.40
1:A:498:ASP:HA	1:A:536:VAL:O	2.22	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	536/560 (96%)	476 (89%)	51 (10%)	9 (2%)	11 18
2	B	409/440 (93%)	382 (93%)	23 (6%)	4 (1%)	19 33
All	All	945/1000 (94%)	858 (91%)	74 (8%)	13 (1%)	14 23

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLY
1	A	361	HIS
2	B	195	ILE
2	B	213	GLY
1	A	14	PRO
1	A	230	MET
2	B	239	TRP
1	A	2	ILE
1	A	138	GLU
1	A	356	ARG
1	A	54	ASN
1	A	135	ILE
2	B	9	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	483/499 (97%)	428 (89%)	55 (11%)	7 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	376/400 (94%)	353 (94%)	23 (6%)	23 40
All	All	859/899 (96%)	781 (91%)	78 (9%)	12 20

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	21	VAL
1	A	32	LYS
1	A	64	LYS
1	A	71	TRP
1	A	89	GLU
1	A	90	VAL
1	A	92	LEU
1	A	94	ILE
1	A	102	LYS
1	A	109	LEU
1	A	113	ASP
1	A	120	LEU
1	A	123	ASP
1	A	175	ASN
1	A	182	GLN
1	A	184	MET
1	A	194	GLU
1	A	205	LEU
1	A	229	TRP
1	A	234	LEU
1	A	237	ASP
1	A	238	LYS
1	A	279	LEU
1	A	283	LEU
1	A	296	THR
1	A	325	LEU
1	A	334	GLN
1	A	340	GLN
1	A	344	GLU
1	A	345	PRO
1	A	358	ARG
1	A	361	HIS
1	A	362	THR
1	A	368	LEU
1	A	369	THR

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Mol	Chain	Res	Type
1	A	373	GLN
1	A	386	THR
1	A	396	GLU
1	A	402	TRP
1	A	403	THR
1	A	404	GLU
1	A	420	PRO
1	A	423	VAL
1	A	431	LYS
1	A	443	ASP
1	A	452	LEU
1	A	474	ASN
1	A	475	GLN
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL
1	A	500	GLN
1	A	515	SER
1	A	517	LEU
2	B	65	LYS
2	B	68	SER
2	B	73	LYS
2	B	164	MET
2	B	189	VAL
2	B	201	LYS
2	B	209	LEU
2	B	211	ARG
2	B	215	THR
2	B	232	TYR
2	B	238	LYS
2	B	243	PRO
2	B	277	ARG
2	B	283	LEU
2	B	287	LYS
2	B	303	LEU
2	B	323	LYS
2	B	361	HIS
2	B	368	LEU
2	B	388	LYS
2	B	425	LEU
2	B	429	LEU
2	B	435	VAL

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

Mol	Chain	Res	Type
1	A	57	ASN
1	A	91	GLN
1	A	221	HIS
1	A	278	GLN
1	A	334	GLN
1	A	361	HIS
1	A	474	ASN
1	A	475	GLN
1	A	500	GLN
2	B	57	ASN
2	B	161	GLN
2	B	175	ASN
2	B	182	GLN
2	B	197	GLN
2	B	235	HIS
2	B	255	ASN
2	B	269	GLN
2	B	332	GLN
2	B	334	GLN
2	B	394	GLN
2	B	428	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	0.59	0	3,8,10	3.57	1 (33%)

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	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	CSD	OD1-SG-CB	5.93	115.29	105.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	1	0

5.5 Carbohydrates (i)

There are no carbohydrates 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	MKC	A	999	-	15,23,23	1.04	1 (6%)	19,31,31	3.44	4 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MKC	A	999	-	-	0/10/12/12	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	MKC	C11-N10	3.21	1.39	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	999	MKC	C12-C11-N10	-6.37	115.00	125.18
3	A	999	MKC	C11-C12-C14	-3.12	112.99	122.83
3	A	999	MKC	C7-C12-C14	3.95	125.98	122.10
3	A	999	MKC	C11-N10-C9	12.40	125.97	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	MKC	1	0

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.