



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 12:50 am BST

PDB ID : 5UV5
Title : Crystal Structure of a 2-Hydroxyisoquinoline-1,3-dione RNase H Active Site Inhibitor with Multiple Binding Modes to HIV Reverse Transcriptase
Authors : Kirby, K.A.; Sarafianos, S.G.
Deposited on : 2017-02-19
Resolution : 3.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

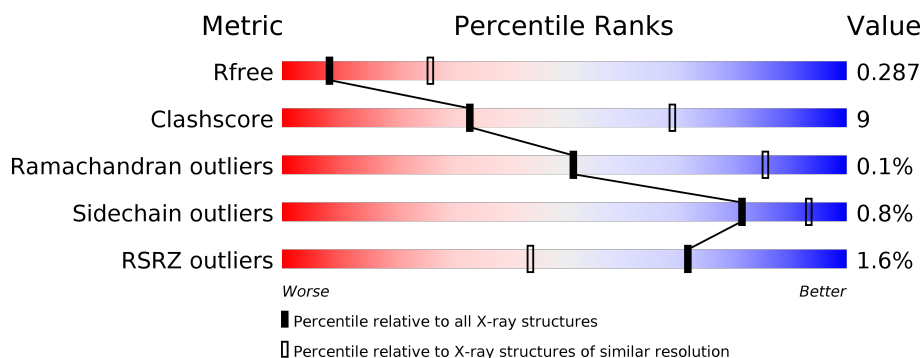
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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 $\leq 5\%$. 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	557	<div> <div>4%</div> <div>68% 27% . .</div> </div>
1	C	557	<div> <div>%</div> <div>82% 16% .</div> </div>
2	B	429	<div> <div>%</div> <div>76% 17% 7%</div> </div>
2	D	429	<div> <div>%</div> <div>73% 18% 8%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15370 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
1	A	534	Total	C	N	O	S	0	0	0
			4351	2819	723	802	7			
1	C	546	Total	C	N	O	S	0	0	0
			4442	2877	734	825	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
C	-1	MET	-	initiating methionine	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	400	Total	C	N	O	S	0	0	0
			3291	2138	547	600	6			
2	D	393	Total	C	N	O	S	0	0	0
			3246	2115	537	588	6			

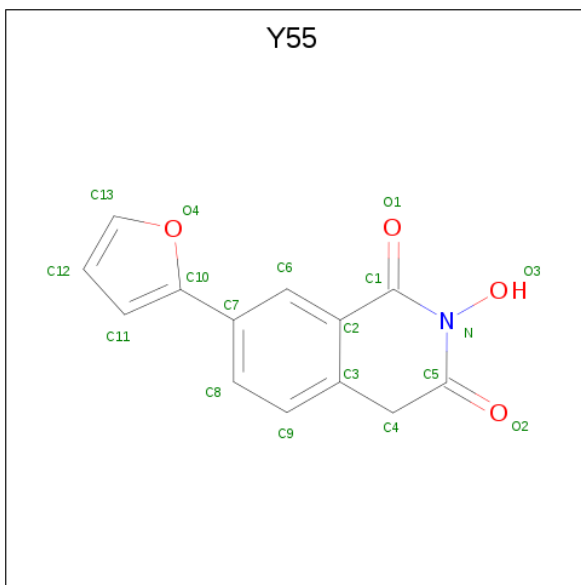
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366
D	0	GLY	-	expression tag	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mn 2 2	0	0
3	C	2	Total Mn 2 2	0	0

- Molecule 4 is 7-(furan-2-yl)-2-hydroxyisoquinoline-1,3(2H,4H)-dione (three-letter code: Y55) (formula: C₁₃H₉NO₄).

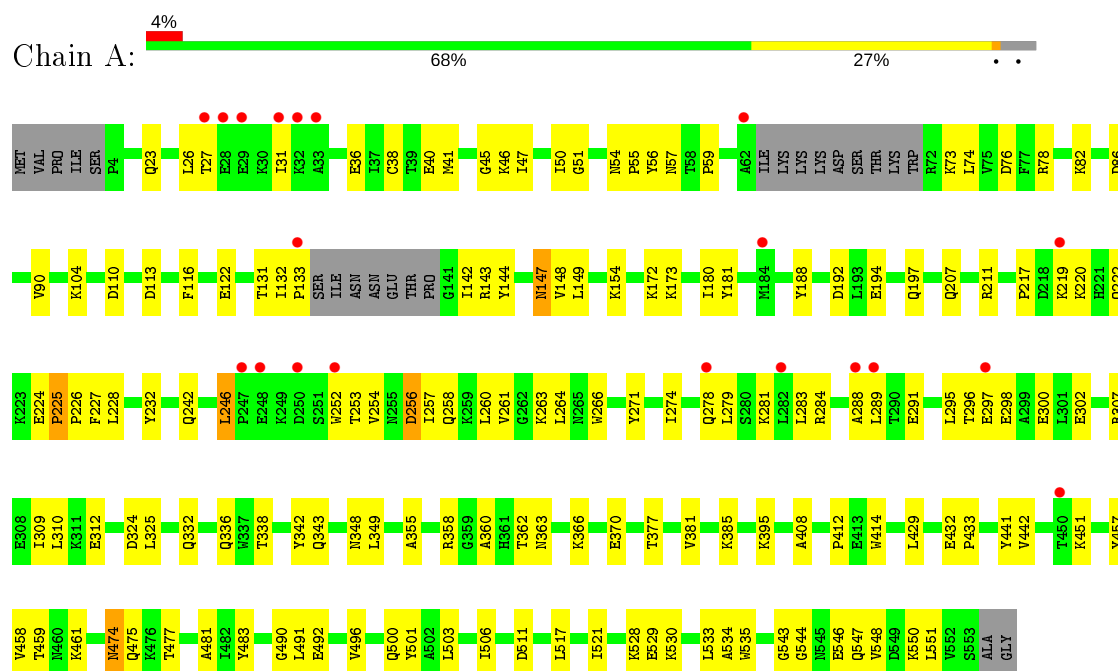


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 18 13 1 4	0	0
4	C	1	Total C N O 18 13 1 4	0	0

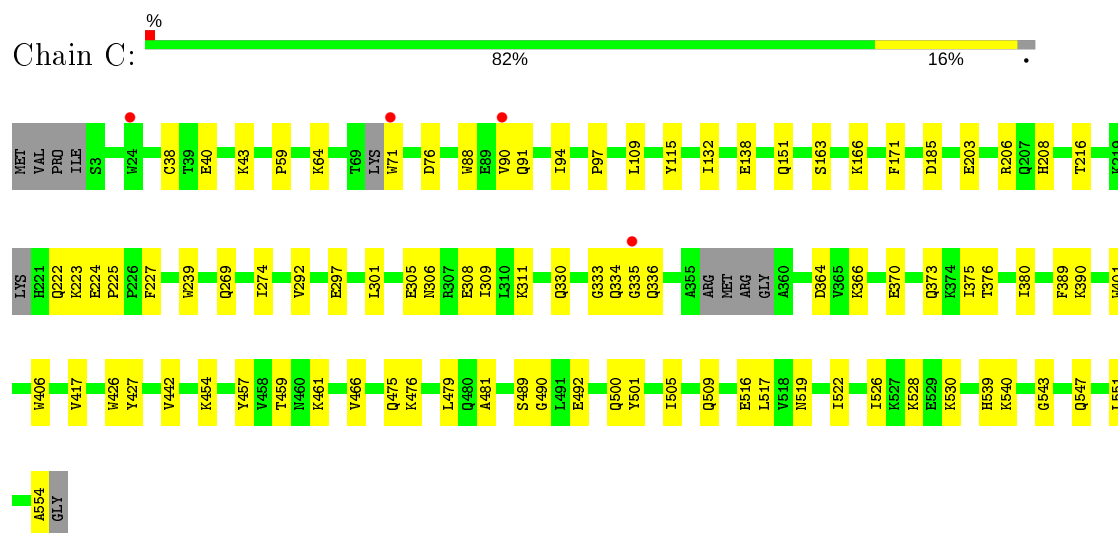
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

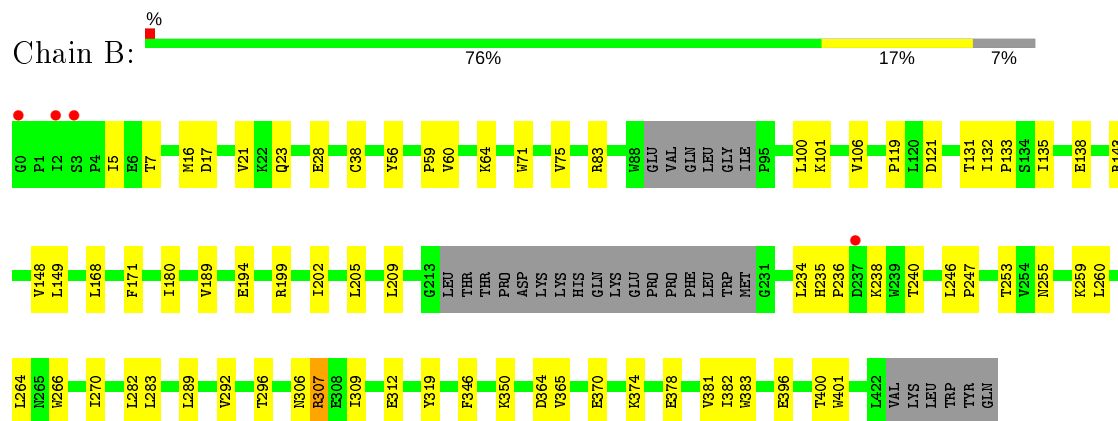
• Molecule 1: Reverse transcriptase/ribonuclease H



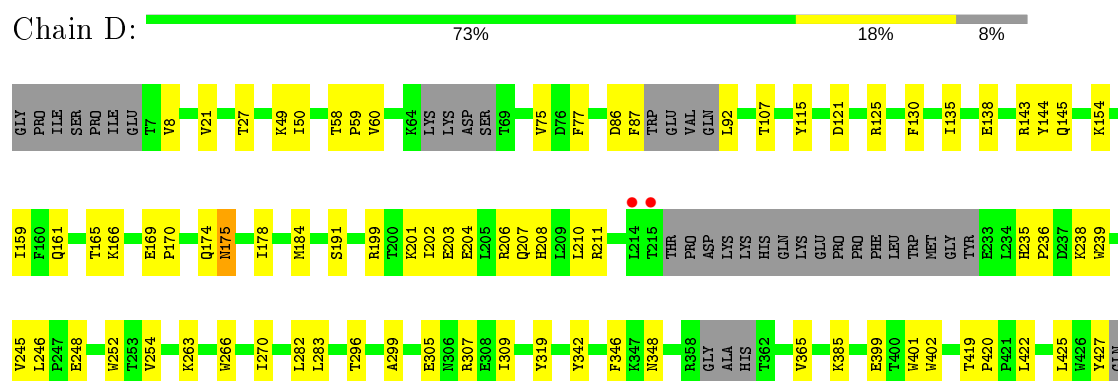
• Molecule 1: Reverse transcriptase/ribonuclease H



• Molecule 2: p51 RT



• Molecule 2: p51 RT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.99Å 88.67Å 108.86Å 105.53° 93.41° 110.13°	Depositor
Resolution (Å)	62.43 – 3.00 62.43 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (62.43-3.00) 98.0 (62.43-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.11.1	Depositor
R, R_{free}	0.232 , 0.287 0.232 , 0.287	Depositor DCC
R_{free} test set	2174 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15370	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MN, Y55

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	0.30	0/4463	0.50	0/6060
1	C	0.28	0/4556	0.45	0/6190
2	B	0.28	0/3384	0.45	0/4595
2	D	0.27	0/3334	0.45	0/4526
All	All	0.28	0/15737	0.46	0/21371

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	GLU	Peptide
1	A	225	PRO	Peptide
1	A	246	LEU	Peptide

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	4351	0	4401	109	0
1	C	4442	0	4482	60	0
2	B	3291	0	3321	54	0
2	D	3246	0	3288	54	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
4	A	18	0	0	0	0
4	C	18	0	0	1	0
All	All	15370	0	15492	264	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 9.

All (264) 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:297:GLU:HA	1:A:300:GLU:HG3	1.68	0.76
1:C:459:THR:HG22	1:C:461:LYS:H	1.51	0.76
1:A:222:GLN:OE1	1:A:228:LEU:N	2.19	0.76
2:B:189:VAL:HG21	2:B:202:ILE:HD11	1.67	0.75
1:A:459:THR:HG22	1:A:461:LYS:H	1.51	0.75
1:C:427:TYR:O	1:C:509:GLN:NE2	2.20	0.75
2:D:248:GLU:OE1	2:D:307:ARG:NH2	2.21	0.74
1:A:254:VAL:HA	1:A:257:ILE:HB	1.68	0.74
1:A:27:THR:O	1:A:31:ILE:HG12	1.87	0.74
1:A:23:GLN:NE2	1:A:57:ASN:OD1	2.21	0.73
2:D:246:LEU:O	2:D:307:ARG:NH1	2.21	0.73
2:D:170:PRO:HG2	2:D:208:HIS:CE1	2.26	0.71
1:A:288:ALA:HB3	1:A:291:GLU:HG2	1.74	0.70
1:A:110:ASP:HB3	1:A:220:LYS:HG2	1.74	0.69
2:B:306:ASN:HA	2:B:309:ILE:HG22	1.72	0.69
1:C:516:GLU:HA	1:C:519:ASN:HB2	1.74	0.69
1:A:475:GLN:HB3	1:A:501:TYR:CE1	2.28	0.69
1:C:489:SER:O	1:C:528:LYS:NZ	2.26	0.68
1:C:88:TRP:HD1	1:C:90:VAL:HG12	1.58	0.68
2:B:7:THR:HG21	2:B:121:ASP:HA	1.77	0.67
1:C:206:ARG:HD3	1:C:216:THR:HB	1.77	0.66
2:D:422:LEU:HB2	2:D:425:LEU:HD22	1.77	0.66
1:A:491:LEU:HB3	1:A:529:GLU:HB2	1.78	0.66
1:A:74:LEU:HD21	1:A:289:LEU:HD23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LYS:HA	1:A:266:TRP:HD1	1.62	0.65
1:A:500:GLN:CD	1:A:500:GLN:H	2.00	0.65
1:C:274:ILE:HG13	1:C:306:ASN:HB2	1.78	0.65
1:A:143:ARG:NH1	1:A:143:ARG:HB3	2.12	0.64
1:A:260:LEU:HD23	1:A:264:LEU:HD12	1.79	0.64
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.79	0.64
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.79	0.64
2:D:245:VAL:O	2:D:263:LYS:NZ	2.31	0.64
1:A:45:GLY:O	1:A:147:ASN:ND2	2.26	0.64
2:B:106:VAL:HG12	2:B:236:PRO:HD3	1.80	0.63
1:A:358:ARG:HE	1:A:360:ALA:HB3	1.63	0.63
1:A:503:LEU:HD12	1:A:533:LEU:HG	1.80	0.63
1:A:271:TYR:OH	1:A:312:GLU:O	2.12	0.63
1:A:432:GLU:HG3	1:A:433:PRO:HD2	1.81	0.63
2:B:180:ILE:HG12	2:B:189:VAL:HG12	1.80	0.61
1:A:50:ILE:HG21	1:A:54:ASN:OD1	2.00	0.61
1:C:223:LYS:HG3	1:C:224:GLU:OE1	2.01	0.61
2:B:101:LYS:HD3	2:B:382:ILE:HD12	1.84	0.60
1:C:375:ILE:HD11	1:C:389:PHE:HE2	1.67	0.59
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.84	0.59
2:D:201:LYS:HA	2:D:204:GLU:HB2	1.85	0.59
2:D:87:PHE:HD2	2:D:92:LEU:HD23	1.67	0.59
2:D:207:GLN:HA	2:D:210:LEU:HB2	1.86	0.58
2:D:86:ASP:OD1	2:D:154:LYS:NZ	2.35	0.58
1:A:252:TRP:CZ3	1:A:295:LEU:HD11	2.39	0.58
1:A:254:VAL:HG21	1:A:283:LEU:HD13	1.85	0.58
2:D:296:THR:HG23	2:D:299:ALA:H	1.68	0.57
1:A:254:VAL:HG13	1:A:289:LEU:HD12	1.86	0.57
1:A:358:ARG:HB2	1:A:362:THR:HB	1.87	0.57
2:D:8:VAL:HG21	2:D:159:ILE:HD13	1.87	0.56
1:A:547:GLN:HA	1:A:550:LYS:HE2	1.88	0.56
1:A:256:ASP:O	1:A:260:LEU:HB2	2.06	0.56
1:A:281:LYS:O	1:A:284:ARG:HG2	2.05	0.56
1:C:308:GLU:HG3	1:C:311:LYS:HD2	1.86	0.56
1:A:23:GLN:NE2	1:A:131:THR:H	2.04	0.56
1:C:308:GLU:CG	1:C:311:LYS:HD2	2.36	0.56
2:B:16:MET:HG2	1:C:292:VAL:HG21	1.87	0.55
1:C:376:THR:O	1:C:380:ILE:HG12	2.06	0.55
1:A:143:ARG:HH11	1:A:143:ARG:HB3	1.69	0.55
2:D:282:LEU:HD21	2:D:296:THR:H	1.71	0.55
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:ARG:HA	2:D:202:ILE:HB	1.88	0.54
1:C:64:LYS:HD3	1:C:71:TRP:HA	1.89	0.54
2:B:378:GLU:O	2:B:382:ILE:HG12	2.08	0.54
1:A:23:GLN:HE22	1:A:131:THR:H	1.55	0.53
2:B:106:VAL:HG13	2:B:234:LEU:HB2	1.89	0.53
2:D:107:THR:HG21	2:D:202:ILE:HD11	1.91	0.53
2:D:135:ILE:O	2:D:138:GLU:HG3	2.08	0.53
1:C:88:TRP:CD1	1:C:90:VAL:HG12	2.42	0.52
2:D:282:LEU:HD21	2:D:296:THR:HG22	1.91	0.52
1:A:475:GLN:HB3	1:A:501:TYR:CD1	2.43	0.52
2:B:5:ILE:CD1	2:B:119:PRO:HD3	2.39	0.52
1:A:143:ARG:HH11	1:A:143:ARG:CB	2.23	0.52
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.45	0.52
1:A:172:LYS:HG2	1:A:180:ILE:HD12	1.92	0.51
1:A:260:LEU:HD22	1:A:279:LEU:HD13	1.92	0.51
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.92	0.51
2:B:56:TYR:O	2:B:143:ARG:NH2	2.42	0.51
2:B:235:HIS:HB2	2:B:238:LYS:NZ	2.25	0.51
2:B:282:LEU:HD21	2:B:296:THR:HB	1.92	0.51
1:A:412:PRO:HD3	2:B:401:TRP:CZ2	2.45	0.51
2:B:240:THR:O	2:B:350:LYS:NZ	2.43	0.51
1:C:163:SER:HA	1:C:166:LYS:HE3	1.92	0.51
2:D:254:VAL:HG13	2:D:283:LEU:HD22	1.93	0.51
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.92	0.51
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.92	0.51
1:A:260:LEU:CD2	1:A:264:LEU:HD12	2.40	0.51
1:C:40:GLU:HA	1:C:43:LYS:HG2	1.93	0.51
1:C:115:TYR:HD2	1:C:151:GLN:HA	1.76	0.51
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.93	0.50
1:C:406:TRP:NE1	2:D:419:THR:O	2.44	0.50
1:C:442:VAL:HG12	1:C:457:TYR:HB3	1.93	0.50
1:A:51:GLY:O	1:A:143:ARG:HD3	2.10	0.50
1:C:426:TRP:CE3	1:C:526:ILE:HD13	2.47	0.50
1:A:90:VAL:HG13	2:B:131:THR:HG21	1.93	0.50
1:A:263:LYS:HA	1:A:266:TRP:CD1	2.43	0.50
1:A:534:ALA:HB1	2:B:259:LYS:NZ	2.27	0.50
1:A:86:ASP:OD1	1:A:154:LYS:NZ	2.37	0.50
1:C:203:GLU:OE2	1:C:206:ARG:NH2	2.44	0.50
2:D:175:ASN:ND2	2:D:178:ILE:HG13	2.26	0.50
1:A:217:PRO:HG2	1:A:220:LYS:HB3	1.93	0.50
1:C:185:ASP:OD1	1:C:185:ASP:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:166:LYS:HA	2:D:169:GLU:HG2	1.94	0.49
1:C:171:PHE:HB2	1:C:208:HIS:CD2	2.47	0.49
2:D:270:ILE:HG12	2:D:346:PHE:HB3	1.94	0.49
1:A:31:ILE:HG23	1:A:133:PRO:HG2	1.94	0.49
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.95	0.48
1:A:23:GLN:HG2	1:A:57:ASN:HD21	1.76	0.48
1:A:246:LEU:O	1:A:307:ARG:NH2	2.47	0.48
2:B:135:ILE:O	2:B:138:GLU:HG2	2.12	0.48
2:D:130:PHE:CZ	2:D:144:TYR:HB2	2.49	0.48
1:A:56:TYR:O	1:A:143:ARG:NH2	2.45	0.48
1:A:534:ALA:HB1	2:B:259:LYS:HZ1	1.79	0.48
2:B:100:LEU:HG	2:B:381:VAL:HG13	1.95	0.48
2:B:168:LEU:HD22	2:B:205:LEU:HD11	1.96	0.48
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.94	0.48
1:A:173:LYS:N	1:A:173:LYS:HD2	2.28	0.48
1:C:500:GLN:H	1:C:500:GLN:CD	2.17	0.47
2:B:148:VAL:HG12	2:B:149:LEU:H	1.78	0.47
2:D:319:TYR:OH	2:D:385:LYS:HE2	2.13	0.47
1:A:228:LEU:HD21	1:A:242:GLN:OE1	2.14	0.47
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.49	0.47
1:A:543:GLY:O	1:A:547:GLN:HG2	2.14	0.47
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.95	0.47
1:A:76:ASP:OD1	1:A:78:ARG:NE	2.48	0.47
2:D:248:GLU:HG3	2:D:252:TRP:HZ2	1.80	0.47
2:D:60:VAL:HG23	2:D:75:VAL:HG22	1.97	0.47
1:A:309:ILE:O	1:A:312:GLU:HG2	2.14	0.47
2:B:266:TRP:HE1	1:C:138:GLU:HG2	1.79	0.47
2:B:266:TRP:NE1	1:C:138:GLU:HG2	2.29	0.47
1:A:271:TYR:HB3	1:A:274:ILE:HD13	1.96	0.47
1:A:441:TYR:CD1	1:A:544:GLY:HA3	2.50	0.47
1:C:476:LYS:HD2	1:C:517:LEU:HD13	1.96	0.46
1:C:64:LYS:HZ3	1:C:71:TRP:N	2.13	0.46
2:D:170:PRO:O	2:D:174:GLN:HG2	2.15	0.46
2:D:248:GLU:HB2	2:D:307:ARG:HH22	1.81	0.46
2:B:396:GLU:O	2:B:400:THR:OG1	2.26	0.46
2:D:203:GLU:HA	2:D:206:ARG:HG2	1.98	0.46
2:D:342:TYR:HB3	2:D:348:ASN:HA	1.98	0.46
2:B:17:ASP:O	2:B:83:ARG:HD3	2.15	0.46
2:B:64:LYS:HE3	2:B:71:TRP:CE2	2.50	0.46
1:A:483:TYR:HB2	1:A:521:ILE:HG12	1.98	0.46
2:D:170:PRO:HG2	2:D:208:HIS:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:CYS:O	1:A:47:ILE:HD11	2.16	0.46
1:A:181:TYR:CD1	2:B:138:GLU:HB3	2.50	0.46
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.56	0.46
1:C:366:LYS:HG3	1:C:401:TRP:CZ2	2.51	0.46
1:C:459:THR:HG22	1:C:461:LYS:N	2.26	0.46
1:A:342:TYR:HB3	1:A:348:ASN:HA	1.98	0.46
1:C:59:PRO:HG2	1:C:76:ASP:HB3	1.98	0.46
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.98	0.45
1:C:301:LEU:O	1:C:305:GLU:HG2	2.17	0.45
2:D:235:HIS:O	2:D:238:LYS:HG2	2.15	0.45
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.98	0.45
1:C:522:ILE:O	1:C:526:ILE:HG13	2.16	0.45
1:A:263:LYS:HD2	1:A:266:TRP:HE1	1.82	0.45
1:A:451:LYS:O	1:A:451:LYS:HG2	2.17	0.45
2:B:247:PRO:O	2:B:307:ARG:NH2	2.47	0.45
1:C:38:CYS:SG	1:C:132:ILE:HD11	2.57	0.45
1:C:225:PRO:HG3	1:C:227:PHE:CE1	2.52	0.45
2:D:87:PHE:HB3	2:D:92:LEU:HB3	1.98	0.45
1:A:490:GLY:O	1:A:528:LYS:NZ	2.38	0.45
2:B:370:GLU:O	2:B:374:LYS:HG3	2.16	0.45
1:A:296:THR:HG22	1:A:298:GLU:HG2	2.00	0.44
2:B:253:THR:HA	2:B:292:VAL:HA	1.98	0.44
2:B:199:ARG:O	2:B:202:ILE:HG22	2.17	0.44
1:A:194:GLU:HG3	1:A:197:GLN:H	1.82	0.44
2:B:270:ILE:HG12	2:B:346:PHE:HB3	2.00	0.44
1:A:336:GLN:HG2	1:A:355:ALA:HB2	2.00	0.44
1:A:54:ASN:HA	1:A:55:PRO:HD3	1.66	0.44
1:C:297:GLU:OE2	1:C:301:LEU:HB2	2.17	0.44
2:B:202:ILE:HA	2:B:202:ILE:HD12	1.73	0.44
1:C:334:GLN:HG2	1:C:335:GLY:N	2.33	0.44
1:C:492:GLU:HG2	1:C:530:LYS:HB2	2.00	0.44
1:C:543:GLY:HA3	2:D:283:LEU:O	2.18	0.44
2:D:50:ILE:HD13	2:D:145:GLN:HB3	1.99	0.44
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.88	0.44
1:A:332:GLN:HG3	1:A:338:THR:HG23	2.00	0.44
2:B:119:PRO:HA	2:B:148:VAL:HA	1.99	0.44
2:B:255:ASN:HB2	2:B:289:LEU:HB3	1.99	0.44
1:C:543:GLY:O	1:C:547:GLN:HG2	2.18	0.43
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.99	0.43
1:C:390:LYS:HB3	1:C:417:VAL:HG21	1.99	0.43
1:A:278:GLN:HB2	1:A:302:GLU:CD	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:GLU:HA	1:C:373:GLN:HG2	1.99	0.43
2:D:121:ASP:O	2:D:125:ARG:HG3	2.19	0.43
1:A:132:ILE:HD11	1:A:142:ILE:HG12	2.00	0.43
2:B:171:PHE:CG	2:B:205:LEU:HD13	2.54	0.43
1:C:380:ILE:HD12	2:D:27:THR:HG22	2.01	0.43
2:B:312:GLU:H	2:B:312:GLU:CD	2.19	0.43
1:C:306:ASN:O	1:C:309:ILE:HG22	2.19	0.43
1:C:97:PRO:HB2	1:C:239:TRP:CG	2.53	0.43
1:A:207:GLN:O	1:A:211:ARG:HG3	2.19	0.43
1:A:543:GLY:HA3	2:B:283:LEU:O	2.19	0.43
1:A:23:GLN:CD	1:A:57:ASN:HD21	2.21	0.43
2:B:235:HIS:HB2	2:B:238:LYS:HZ2	1.84	0.43
1:C:466:VAL:HG21	1:C:551:LEU:HB3	2.00	0.43
1:C:519:ASN:HA	1:C:522:ILE:HD12	2.01	0.43
2:D:399:GLU:HA	2:D:402:TRP:HD1	1.83	0.43
1:A:496:VAL:HG22	1:A:534:ALA:HB3	2.00	0.42
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.19	0.42
1:A:41:MET:HE1	1:A:73:LYS:HD3	2.00	0.42
2:B:319:TYR:CZ	2:B:383:TRP:HB3	2.54	0.42
2:B:23:GLN:HG2	2:B:133:PRO:HD3	2.00	0.42
1:C:500:GLN:OE1	1:C:500:GLN:N	2.42	0.42
2:D:266:TRP:CD2	2:D:425:LEU:HD23	2.54	0.42
1:C:490:GLY:O	1:C:528:LYS:NZ	2.32	0.42
1:A:148:VAL:HG22	1:A:149:LEU:H	1.85	0.42
1:A:458:VAL:HG12	1:A:548:VAL:HB	2.01	0.42
2:B:168:LEU:HD13	2:B:180:ILE:HG21	2.01	0.42
1:C:222:GLN:HG2	1:C:227:PHE:HA	2.00	0.42
1:C:333:GLY:H	1:C:336:GLN:HB2	1.85	0.42
1:C:539:HIS:CD2	4:C:603:Y55:C6	3.02	0.42
2:B:28:GLU:HA	2:B:135:ILE:HD11	2.01	0.42
2:D:107:THR:HG21	2:D:202:ILE:CD1	2.49	0.42
1:C:479:LEU:HD11	1:C:505:ILE:HD12	2.00	0.42
1:A:253:THR:HG22	1:A:256:ASP:OD2	2.19	0.42
1:A:23:GLN:CG	1:A:57:ASN:HD21	2.32	0.42
2:D:248:GLU:HB2	2:D:307:ARG:NH2	2.33	0.42
2:D:263:LYS:HD2	2:D:427:TYR:CE1	2.55	0.42
1:A:297:GLU:HG2	1:A:297:GLU:H	1.68	0.42
1:A:377:THR:O	1:A:381:VAL:HG23	2.20	0.42
1:A:517:LEU:O	1:A:521:ILE:HG13	2.20	0.41
2:D:266:TRP:CG	2:D:425:LEU:HD23	2.55	0.41
1:A:547:GLN:O	1:A:551:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:VAL:HB	1:C:481:ALA:HB1	2.02	0.41
2:D:58:THR:HG21	2:D:77:PHE:CD1	2.56	0.41
2:D:207:GLN:O	2:D:211:ARG:HG3	2.20	0.41
1:A:113:ASP:HB3	1:A:116:PHE:HB2	2.02	0.41
1:A:219:LYS:HA	1:A:219:LYS:HD2	1.60	0.41
1:A:474:ASN:O	1:A:477:THR:OG1	2.36	0.41
1:C:454:LYS:NZ	1:C:554:ALA:HB3	2.35	0.41
2:D:305:GLU:O	2:D:309:ILE:HG13	2.20	0.41
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.55	0.41
1:A:271:TYR:CD2	1:A:310:LEU:HD23	2.55	0.41
1:C:540:LYS:HA	1:C:540:LYS:HD3	1.69	0.41
2:B:205:LEU:O	2:B:209:LEU:HG	2.21	0.41
2:D:178:ILE:HD13	2:D:191:SER:HB3	2.01	0.41
2:D:115:TYR:OH	2:D:184:MET:O	2.32	0.41
2:D:399:GLU:HA	2:D:402:TRP:CD1	2.55	0.41
1:A:40:GLU:OE1	1:A:40:GLU:HA	2.21	0.41
1:A:78:ARG:O	1:A:82:LYS:HG3	2.21	0.41
2:B:246:LEU:HD11	2:B:264:LEU:HD21	2.02	0.41
1:A:46:LYS:NZ	1:A:116:PHE:O	2.24	0.41
1:A:222:GLN:HB3	1:A:227:PHE:CD1	2.55	0.41
2:B:148:VAL:HG12	2:B:149:LEU:N	2.36	0.41
2:B:60:VAL:HG23	2:B:75:VAL:HG22	2.02	0.41
2:D:420:PRO:C	2:D:422:LEU:H	2.25	0.41
1:A:366:LYS:O	1:A:370:GLU:HG3	2.21	0.40
1:A:546:GLU:O	1:A:550:LYS:HG3	2.21	0.40
2:D:236:PRO:HA	2:D:239:TRP:CD2	2.57	0.40
1:A:258:GLN:HA	1:A:261:VAL:HG22	2.03	0.40
1:A:325:LEU:HD12	1:A:385:LYS:HG3	2.04	0.40
2:B:7:THR:CG2	2:B:121:ASP:HA	2.48	0.40
1:C:94:ILE:HG23	1:C:269:GLN:OE1	2.21	0.40
1:C:476:LYS:HD3	1:C:476:LYS:HA	1.81	0.40
2:D:161:GLN:O	2:D:165:THR:HG23	2.21	0.40
2:D:49:LYS:HA	2:D:143:ARG:O	2.22	0.40
1:A:228:LEU:HA	1:A:232:TYR:O	2.21	0.40
2:B:5:ILE:HD12	2:B:119:PRO:HD3	2.04	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	528/557 (95%)	501 (95%)	25 (5%)	2 (0%)	34	72
1	C	538/557 (97%)	520 (97%)	18 (3%)	0	100	100
2	B	394/429 (92%)	380 (96%)	14 (4%)	0	100	100
2	D	383/429 (89%)	364 (95%)	19 (5%)	0	100	100
All	All	1843/1972 (94%)	1765 (96%)	76 (4%)	2 (0%)	51	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	PRO
1	A	226	PRO

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	476/497 (96%)	470 (99%)	6 (1%)	69	89
1	C	488/497 (98%)	484 (99%)	4 (1%)	81	93
2	B	362/390 (93%)	359 (99%)	3 (1%)	81	93
2	D	358/390 (92%)	357 (100%)	1 (0%)	92	97
All	All	1684/1774 (95%)	1670 (99%)	14 (1%)	81	93

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	122	GLU
1	A	147	ASN
1	A	256	ASP
1	A	324	ASP
1	A	474	ASN
2	B	194	GLU
2	B	260	LEU
2	B	307	ARG
1	C	91	GLN
1	C	109	LEU
1	C	330	GLN
1	C	364	ASP
2	D	175	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	57	ASN
1	A	306	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	Y55	C	603	3	15,20,20	3.01	8 (53%)	19,29,29	1.86	5 (26%)
4	Y55	A	603	3	15,20,20	3.00	8 (53%)	19,29,29	1.63	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
4	Y55	C	603	3	-	2/2/20/20	0/3/3/3
4	Y55	A	603	3	-	0/2/20/20	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	Y55	C7-C10	-6.23	1.35	1.46
4	C	603	Y55	C7-C10	-6.13	1.36	1.46
4	A	603	Y55	C2-C1	-5.17	1.37	1.47
4	C	603	Y55	C2-C1	-5.11	1.37	1.47
4	C	603	Y55	O3-N	-4.48	1.32	1.38
4	A	603	Y55	O3-N	-4.40	1.32	1.38
4	C	603	Y55	C2-C3	-4.17	1.35	1.40
4	A	603	Y55	C2-C3	-3.91	1.35	1.40
4	C	603	Y55	C6-C2	-3.14	1.34	1.39
4	C	603	Y55	C6-C7	-2.81	1.34	1.39
4	A	603	Y55	C6-C2	-2.78	1.35	1.39
4	A	603	Y55	C9-C3	-2.74	1.35	1.39
4	A	603	Y55	C6-C7	-2.59	1.35	1.39
4	C	603	Y55	C9-C3	-2.45	1.35	1.39
4	A	603	Y55	C9-C8	-2.43	1.34	1.38
4	C	603	Y55	C9-C8	-2.01	1.35	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	Y55	O3-N-C5	-4.66	111.71	116.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	Y55	O3-N-C5	-4.44	111.95	116.81
4	C	603	Y55	C8-C7-C10	3.39	124.70	120.42
4	A	603	Y55	C11-C12-C13	-2.63	103.57	112.92
4	C	603	Y55	C11-C12-C13	-2.58	103.75	112.92
4	A	603	Y55	C4-C5-N	-2.28	115.25	116.99
4	C	603	Y55	C2-C6-C7	2.15	125.02	120.97
4	A	603	Y55	C2-C1-N	2.08	117.52	114.88
4	C	603	Y55	C2-C1-N	2.03	117.46	114.88

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	603	Y55	C11-C10-C7-C6
4	C	603	Y55	C11-C10-C7-C8

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	603	Y55	1	0

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	534/557 (95%)	-0.01	20 (3%) 41 17	29, 69, 130, 155	0
1	C	546/557 (98%)	-0.16	4 (0%) 87 69	34, 67, 102, 125	0
2	B	400/429 (93%)	-0.21	4 (1%) 82 59	26, 56, 101, 117	0
2	D	393/429 (91%)	-0.30	2 (0%) 91 75	27, 56, 101, 133	0
All	All	1873/1972 (94%)	-0.16	30 (1%) 72 44	26, 63, 115, 155	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	0	GLY	6.4
2	D	215	THR	5.4
1	A	288	ALA	4.3
2	B	3	SER	4.1
1	A	28	GLU	3.4
1	A	133	PRO	3.2
1	A	62	ALA	3.2
1	A	297	GLU	3.2
2	D	214	LEU	2.8
1	A	219	LYS	2.7
1	C	335	GLY	2.7
1	A	278	GLN	2.6
1	A	32	LYS	2.6
2	B	2	ILE	2.6
2	B	237	ASP	2.5
1	C	24	TRP	2.5
1	A	248	GLU	2.4
1	A	282	LEU	2.4
1	A	31	ILE	2.4
1	A	250	ASP	2.3
1	A	33	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	71	TRP	2.2
1	A	184	MET	2.2
1	A	450	THR	2.1
1	A	252	TRP	2.1
1	A	289	LEU	2.1
1	A	27	THR	2.0
1	A	29	GLU	2.0
1	C	90	VAL	2.0
1	A	247	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates 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	MN	C	602	1/1	0.79	0.12	75,75,75,75	0
4	Y55	C	603	18/18	0.90	0.20	91,97,114,114	0
3	MN	C	601	1/1	0.91	0.22	93,93,93,93	0
4	Y55	A	603	18/18	0.91	0.25	75,85,89,98	0
3	MN	A	602	1/1	0.93	0.20	61,61,61,61	0
3	MN	A	601	1/1	0.96	0.10	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.