



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:26 PM UTC

PDB ID : 5UV5 / pdb_00005uv5
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

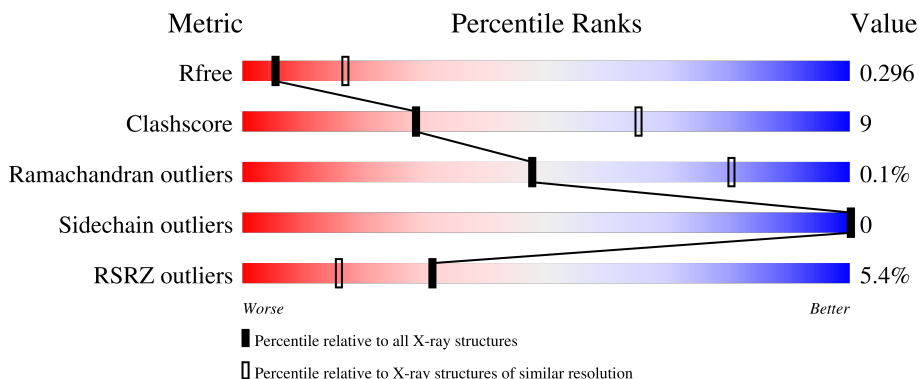
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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 $\leq 5\%$. 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	9% 68% 28% .
1	C	557	4% 82% 16% .
2	B	429	4% 76% 17% 7%
2	D	429	3% 73% 19% 8%

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			

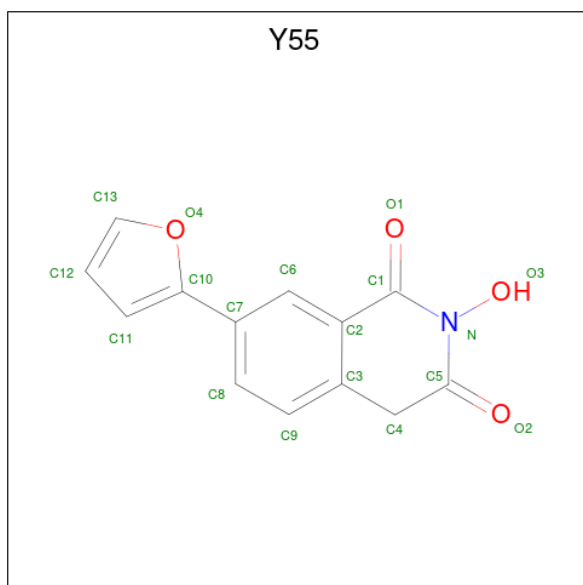
There are 4 discrepancies between the modelled and reference sequences:

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 (CCD ID: MN) (formula: Mn).

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

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

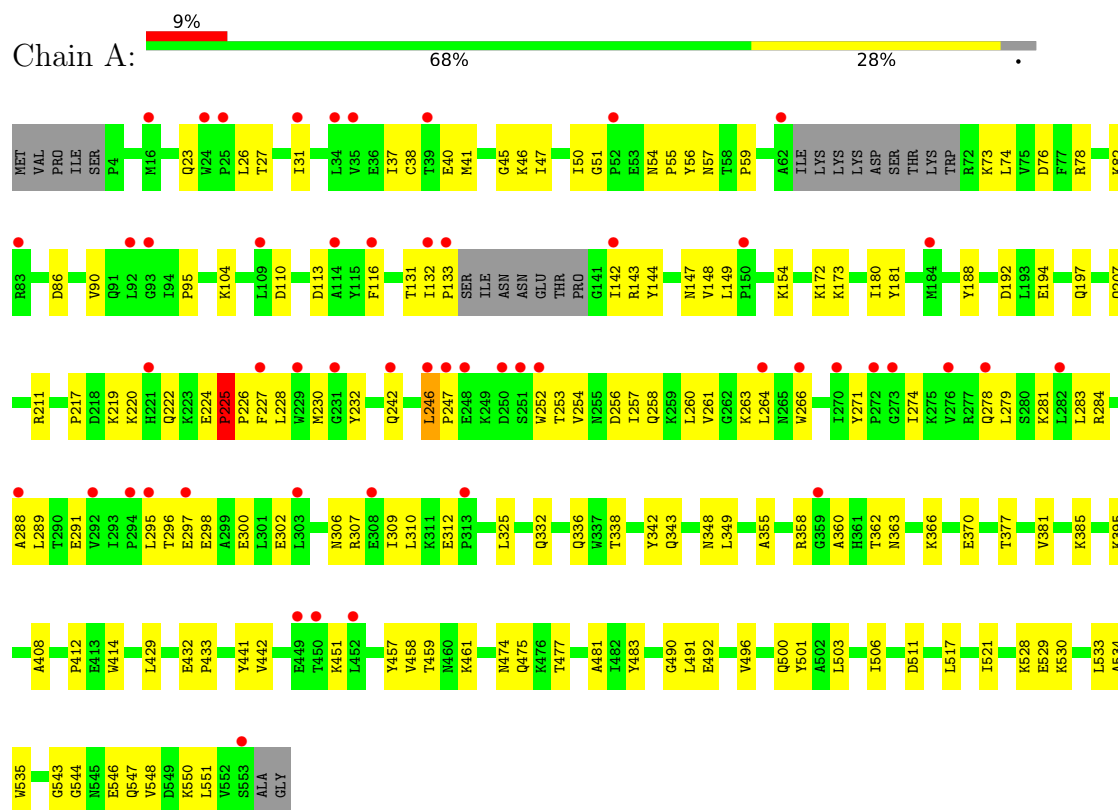


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			18	13	1	4		
4	C	1	Total	C	N	O	0	0
			18	13	1	4		

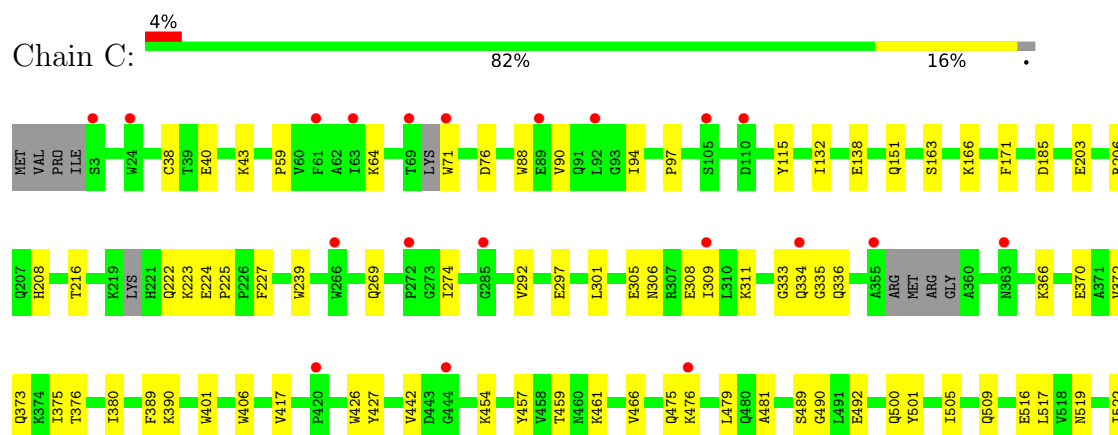
3 Residue-property plots [i](#)

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

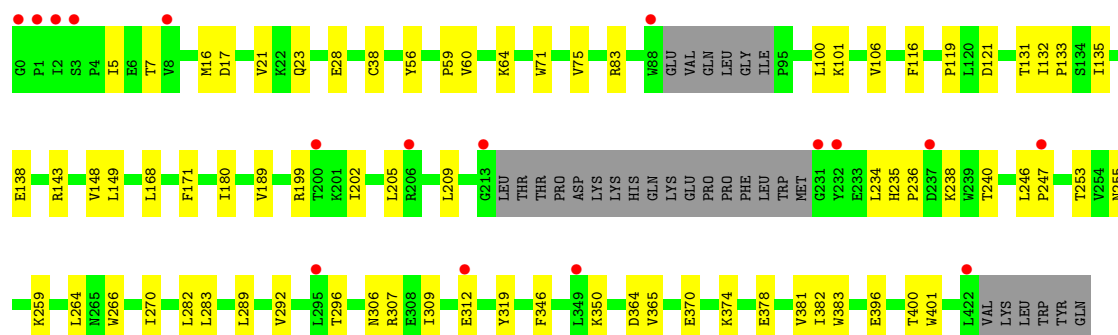
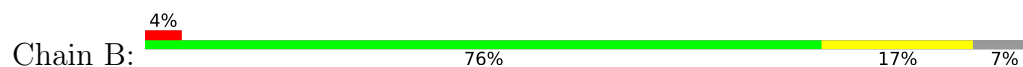


• Molecule 1: Reverse transcriptase/ribonuclease H

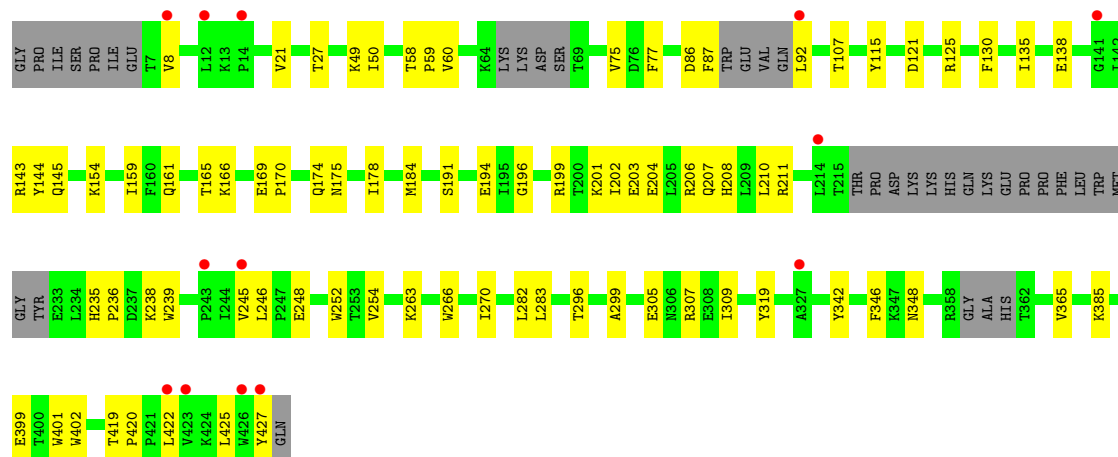
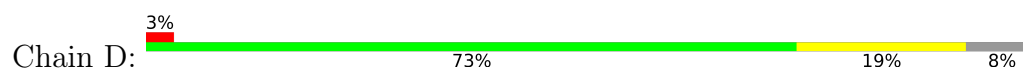




• Molecule 2: p51 RT



• 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 0.238 , 0.296	Depositor DCC
R_{free} test set	2174 reflections (4.72%)	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)	0.31 , 61.1	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y55, MN

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	0.21	0/4463	0.46	2/6060 (0.0%)
1	C	0.16	0/4556	0.34	0/6190
2	B	0.17	0/3384	0.35	0/4595
2	D	0.16	0/3334	0.33	0/4526
All	All	0.18	0/15737	0.38	2/21371 (0.0%)

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.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	PRO	CA-C-N	-9.74	107.67	119.84
1	A	225	PRO	C-N-CA	-9.74	107.67	119.84

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 ⓘ

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	115	0
1	C	4442	0	4482	60	0
2	B	3291	0	3321	55	0
2	D	3246	0	3288	55	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	272	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 (272) 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
1:A:37:ILE:HG22	1:A:41:MET:HE2	1.72	0.71
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:500:GLN:CD	1:A:500:GLN:H	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:263:LYS:HA	1:A:266:TRP:HD1	1.62	0.65
1:C:274:ILE:HG13	1:C:306:ASN:HB2	1.78	0.65
1:A:143:ARG:HB3	1:A:143:ARG:NH1	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
1:A:41:MET:HE1	1:A:73:LYS:HZ3	1.66	0.60
2:B:101:LYS:HD3	2:B:382:ILE:HD12	1.84	0.60
2:D:86:ASP:OD1	2:D:154:LYS:NZ	2.35	0.59
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:87:PHE:HD2	2:D:92:LEU:HD23	1.67	0.59
2:D:201:LYS:HA	2:D:204:GLU:HB2	1.85	0.59
2:D:207:GLN:HA	2:D:210:LEU:HB2	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB3	1:A:143:ARG:HH11	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
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
1:A:534:ALA:HB1	2:B:259:LYS:HZ1	1.73	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
1:C:500:GLN:H	1:C:500:GLN:CD	2.17	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
2:B:312:GLU:H	2:B:312:GLU:CD	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:278:GLN:HB2	1:A:302:GLU:CD	2.38	0.48
1:A:23:GLN:HG2	1:A:57:ASN:HD21	1.76	0.48
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.95	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
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:A:46:LYS:NZ	1:A:116:PHE:O	2.24	0.47
1:A:23:GLN:CD	1:A:57:ASN:HD21	2.21	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:59:PRO:HG2	1:A:76:ASP:HB3	1.95	0.47
1:A:543:GLY:O	1:A:547:GLN:HG2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:GLY:O	1:A:528:LYS:NZ	2.38	0.47
1:C:372:VAL:O	1:C:376:THR:OG1	2.31	0.47
1:C:476:LYS:HD2	1:C:517:LEU:HD13	1.96	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
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
2:D:420:PRO:C	2:D:422:LEU:H	2.25	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
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
1:A:95:PRO:HD2	1:A:230:MET:HE1	2.00	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:54:ASN:HA	1:A:55:PRO:HD3	1.66	0.44
1:A:336:GLN:HG2	1:A:355:ALA:HB2	2.00	0.44
1:C:297:GLU:OE2	1:C:301:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ILE:HD12	2:B:202:ILE:HA	1.73	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:334:GLN:HG2	1:C:335:GLY:N	2.33	0.43
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
2:B:116:PHE:C	2:B:148:VAL:HG11	2.43	0.43
1:C:390:LYS:HB3	1:C:417:VAL:HG21	1.99	0.43
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
1:C:97:PRO:HB2	1:C:239:TRP:CG	2.53	0.43
1:C:306:ASN:O	1:C:309:ILE:HG22	2.19	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
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:363:ASN:HA	1:A:511:ASP:OD1	2.19	0.42
1:A:496:VAL:HG22	1:A:534:ALA:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:247:PRO:C	1:A:307:ARG:HH22	2.26	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:38:CYS:HA	1:A:41:MET:HE3	2.02	0.42
1:A:297:GLU:H	1:A:297:GLU:HG2	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
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:194:GLU:CD	2:D:196:GLY:H	2.27	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:HD2	1:A:219:LYS:HA	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
1:A:274:ILE:HG13	1:A:306:ASN:CG	2.46	0.41
1:A:475:GLN:CD	1:A:475:GLN:H	2.28	0.41
2:B:205:LEU:O	2:B:209:LEU:HG	2.21	0.41
2:D:115:TYR:OH	2:D:184:MET:O	2.32	0.41
2:D:178:ILE:HD13	2:D:191:SER:HB3	2.01	0.41
2:D:399:GLU:HA	2:D:402:TRP:CD1	2.55	0.41
1:A:40:GLU:HA	1:A:40:GLU:OE1	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:222:GLN:HB3	1:A:227:PHE:CD1	2.55	0.41
2:B:60:VAL:HG23	2:B:75:VAL:HG22	2.02	0.41
2:B:148:VAL:HG12	2:B:149:LEU:N	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:C:476:LYS:HD3	1.81	0.40
2:D:49:LYS:HA	2:D:143:ARG:O	2.22	0.40
2:D:161:GLN:O	2:D:165:THR:HG23	2.21	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%)	30	65
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%)	48	80

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%)	476 (100%)	0	100	100
1	C	488/497 (98%)	488 (100%)	0	100	100
2	B	362/390 (93%)	362 (100%)	0	100	100
2	D	358/390 (92%)	358 (100%)	0	100	100
All	All	1684/1774 (95%)	1684 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	57	ASN
1	A	373	GLN
1	A	407	GLN
1	A	500	GLN
2	B	182	GLN
2	B	255	ASN
1	C	242	GLN
1	C	474	ASN
2	D	269	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	18,20,20	3.49	11 (61%)	23,29,29	1.84	5 (21%)
4	Y55	A	603	3	18,20,20	3.49	11 (61%)	23,29,29	1.69	5 (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	-	4/4/20/20	0/3/3/3
4	Y55	A	603	3	-	0/4/20/20	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	Y55	O4-C10	-7.83	1.24	1.37
4	C	603	Y55	O4-C10	-7.79	1.24	1.37
4	A	603	Y55	C7-C10	-5.38	1.35	1.48
4	C	603	Y55	C7-C10	-5.31	1.36	1.48
4	A	603	Y55	C2-C1	-5.23	1.37	1.47
4	C	603	Y55	C2-C1	-5.17	1.37	1.47
4	C	603	Y55	O3-N	-5.00	1.32	1.38
4	A	603	Y55	O3-N	-4.90	1.32	1.38
4	A	603	Y55	O4-C13	-4.51	1.23	1.37
4	C	603	Y55	O4-C13	-4.51	1.23	1.37
4	C	603	Y55	C2-C3	-4.07	1.35	1.40
4	A	603	Y55	C2-C3	-3.82	1.35	1.40
4	C	603	Y55	C6-C2	-3.15	1.34	1.39
4	C	603	Y55	C6-C7	-3.08	1.34	1.39
4	A	603	Y55	C9-C3	-2.86	1.35	1.39
4	A	603	Y55	C8-C7	-2.83	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	Y55	C6-C7	-2.82	1.35	1.39
4	A	603	Y55	C6-C2	-2.79	1.35	1.39
4	A	603	Y55	C9-C8	-2.76	1.34	1.38
4	C	603	Y55	C8-C7	-2.64	1.35	1.39
4	C	603	Y55	C9-C3	-2.56	1.35	1.39
4	C	603	Y55	C9-C8	-2.29	1.35	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	Y55	O3-N-C5	-5.47	111.71	116.82
4	A	603	Y55	O3-N-C5	-5.21	111.95	116.82
4	C	603	Y55	C8-C7-C6	-2.84	115.96	119.25
4	C	603	Y55	C2-C6-C7	2.62	125.02	120.70
4	C	603	Y55	C13-O4-C10	2.60	110.20	106.02
4	A	603	Y55	C13-O4-C10	2.57	110.15	106.02
4	C	603	Y55	C8-C7-C10	2.48	124.70	120.77
4	A	603	Y55	C8-C7-C6	-2.46	116.40	119.25
4	A	603	Y55	C4-C5-N	-2.06	115.25	116.94
4	A	603	Y55	C11-C12-C13	-2.00	103.57	106.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	603	Y55	C11-C10-C7-C8
4	C	603	Y55	O4-C10-C7-C6
4	C	603	Y55	O4-C10-C7-C8
4	C	603	Y55	C11-C10-C7-C6

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

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%)	0.67	52 (9%) 13 7	29, 69, 130, 155	0
1	C	546/557 (98%)	0.55	20 (3%) 45 25	34, 67, 102, 125	0
2	B	400/429 (93%)	0.42	17 (4%) 40 21	26, 56, 101, 117	0
2	D	393/429 (91%)	0.39	13 (3%) 49 28	27, 56, 101, 133	0
All	All	1873/1972 (94%)	0.52	102 (5%) 31 16	26, 63, 115, 155	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	ALA	4.9
1	A	246	LEU	4.7
2	B	0	GLY	4.3
1	A	282	LEU	4.0
1	C	444	GLY	4.0
2	B	3	SER	3.4
2	D	327	ALA	3.4
1	A	272	PRO	3.4
1	A	93	GLY	3.4
1	A	294	PRO	3.4
2	B	2	ILE	3.3
2	B	422	LEU	3.2
2	B	1	PRO	3.2
2	B	247	PRO	3.1
1	A	278	GLN	3.0
1	A	133	PRO	3.0
1	C	69	THR	3.0
2	D	141	GLY	3.0
1	A	450	THR	3.0
1	A	266	TRP	2.9
1	A	264	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	88	TRP	2.9
2	D	8	VAL	2.9
1	C	363	ASN	2.9
1	C	24	TRP	2.9
1	A	116	PHE	2.8
1	A	132	ILE	2.8
2	D	427	TYR	2.8
1	C	272	PRO	2.8
1	A	92	LEU	2.7
1	C	71	TRP	2.7
1	C	355	ALA	2.7
2	B	237	ASP	2.6
1	A	273	GLY	2.6
2	B	231	GLY	2.6
1	A	248	GLU	2.6
1	A	303	LEU	2.6
2	B	295	LEU	2.6
1	A	231	GLY	2.6
1	A	24	TRP	2.5
2	D	14	PRO	2.5
1	A	295	LEU	2.5
1	C	309	ILE	2.5
1	A	31	ILE	2.5
1	A	184	MET	2.5
1	A	34	LEU	2.5
2	D	422	LEU	2.5
1	A	252	TRP	2.4
2	D	92	LEU	2.4
1	A	247	PRO	2.4
1	C	285	GLY	2.4
1	A	35	VAL	2.4
2	D	245	VAL	2.4
1	C	92	LEU	2.4
1	A	52	PRO	2.4
2	D	243	PRO	2.4
1	A	297	GLU	2.4
1	C	476	LYS	2.3
1	C	3	SER	2.3
1	A	109	LEU	2.3
1	A	313	PRO	2.3
1	A	288	ALA	2.3
1	A	16	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	553	SER	2.3
2	D	426	TRP	2.3
2	B	232	TYR	2.2
1	A	250	ASP	2.2
1	C	110	ASP	2.2
1	A	142	ILE	2.2
1	C	63	ILE	2.2
2	B	312	GLU	2.2
2	B	213	GLY	2.2
1	C	105	SER	2.2
1	A	292	VAL	2.2
1	A	270	ILE	2.2
1	A	452	LEU	2.2
2	B	349	LEU	2.2
1	A	308	GLU	2.1
1	A	449	GLU	2.1
1	A	227	PHE	2.1
1	A	221	HIS	2.1
1	C	61	PHE	2.1
1	C	266	TRP	2.1
2	D	12	LEU	2.1
2	B	206	ARG	2.1
1	A	114	ALA	2.1
1	C	334	GLN	2.1
1	A	359	GLY	2.1
1	A	25	PRO	2.1
1	A	150	PRO	2.1
1	C	89	GLU	2.1
1	A	251	SER	2.1
1	A	83	ARG	2.1
1	A	229	TRP	2.1
1	A	39	THR	2.1
1	C	420	PRO	2.1
2	B	8	VAL	2.0
2	B	200	THR	2.0
1	A	242	GLN	2.0
1	A	276	VAL	2.0
2	D	423	VAL	2.0
2	D	214	LEU	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	Y55	A	603	18/18	0.81	0.13	75,85,89,98	0
4	Y55	C	603	18/18	0.83	0.14	91,97,114,114	0
3	MN	A	602	1/1	0.93	0.11	61,61,61,61	0
3	MN	C	602	1/1	0.93	0.07	75,75,75,75	0
3	MN	C	601	1/1	0.97	0.10	93,93,93,93	0
3	MN	A	601	1/1	0.99	0.04	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.