



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:31 AM GMT

PDB ID : 3IRX  
Title : Crystal Structure of HIV-1 reverse transcriptase (RT) in complex with the Non-nucleoside RT Inhibitor (E)-S-Methyl 5-(1-(3,7-Dimethyl-2-oxo-2,3-dihydrobenzo[d]oxazol-5-yl)-5-(5-methyl-1,3,4-oxadiazol-2-yl)pent-1-enyl)-2-methoxy-3-methylbenzothioate.  
Authors : Ho, W.C.; Arnold, E.  
Deposited on : 2009-08-24  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

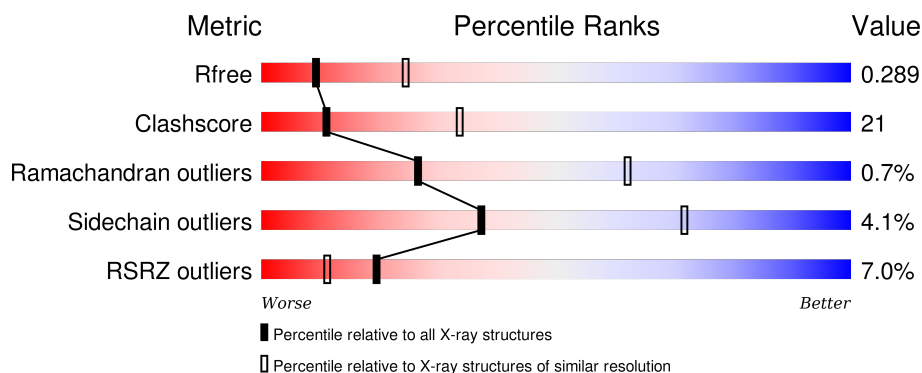
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	558	<div> <div>8%</div> <div>60%</div> <div>36%</div> <div>• •</div> </div>
2	B	428	<div> <div>6%</div> <div>65%</div> <div>31%</div> <div>• •</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7985 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	555	Total	C	N	O	S	0	0	0
			4508	2918	749	834	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P03366
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered	UNP P03366
A	173	ALA	LYS	engineered	UNP P03366
A	280	SER	CYS	engineered	UNP P03366

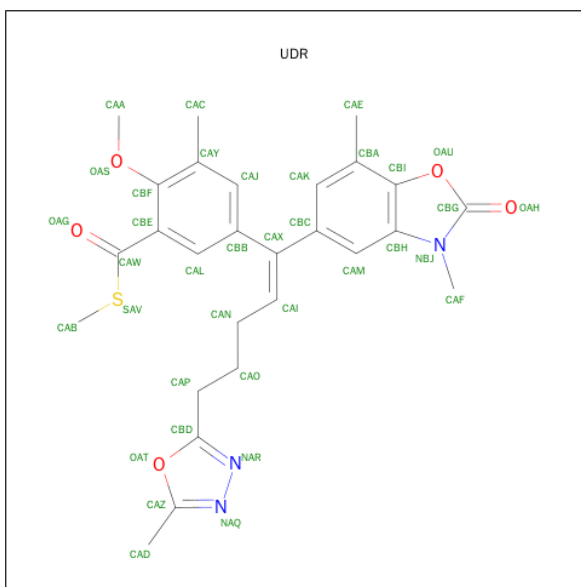
- Molecule 2 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	416	Total	C	N	O	S	0	0	0
			3441	2244	568	622	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered	UNP P03366

- Molecule 3 is (E)-S-METHYL 5-(1-(3,7-DIMETHYL-2-OXO-2,3-DIHYDROBENZO[D]OXAZOL-5-YL)-5-(5-METHYL-1,3,4-OXADIAZOL-2-YL)PENT-1-ENYL)-2-METHOXY-3-METHYLBENZOTHIOATE (three-letter code: UDR) (formula: C<sub>27</sub>H<sub>29</sub>N<sub>3</sub>O<sub>5</sub>S).

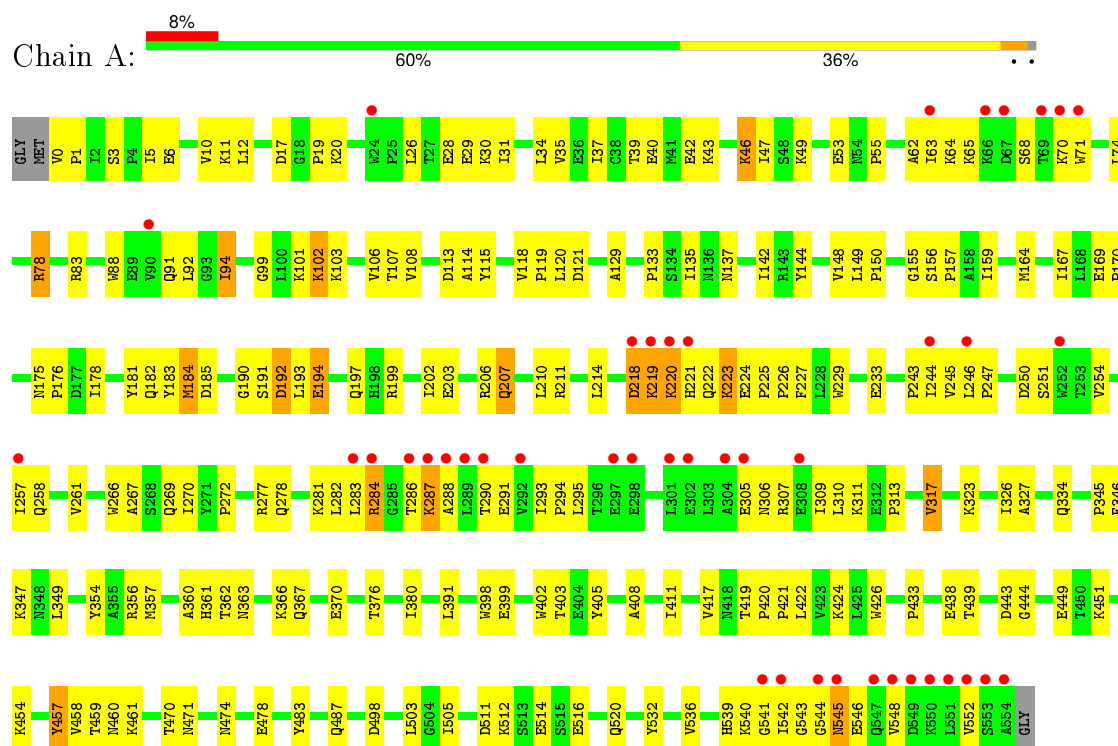


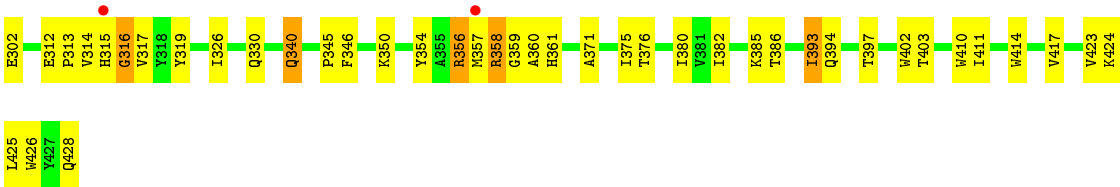
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			36	27	3	5	1		

### 3 Residue-property plots

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.

#### • Molecule 1: Reverse transcriptase/ribonuclease H





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.64Å 75.39Å 110.66Å 90.00° 100.08° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 35.64 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.1 (50.00-2.80) 87.2 (35.64-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.236 , 0.289 0.237 , 0.289	Depositor DCC
$R_{free}$ test set	1414 reflections (4.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	72.7	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 61.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 28872 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7985	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: UDR

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	0.46	0/4626	0.64	0/6289
2	B	0.44	0/3541	0.62	0/4810
All	All	0.46	0/8167	0.63	0/11099

There are no bond length outliers.

There are no bond angle outliers.

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	4508	0	4563	217	0
2	B	3441	0	3476	130	0
3	A	36	0	29	8	0
All	All	7985	0	8068	335	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 21.

All (335) 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:420:PRO:HB2	1:A:421:PRO:HD3	1.18	1.17
1:A:224:GLU:C	1:A:226:PRO:HD2	1.66	1.15
1:A:218:ASP:O	1:A:219:LYS:HD2	1.58	1.03
1:A:106:VAL:HG21	3:A:556:UDR:HAAB	1.42	0.99
2:B:315:HIS:O	2:B:317:VAL:HG23	1.65	0.96
1:A:420:PRO:HB2	1:A:421:PRO:CD	1.95	0.94
1:A:421:PRO:O	1:A:422:LEU:HD23	1.68	0.94
1:A:106:VAL:HG21	3:A:556:UDR:CAA	1.98	0.93
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.51	0.92
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.04	0.92
1:A:222:GLN:O	1:A:222:GLN:HG3	1.67	0.92
1:A:223:LYS:O	1:A:224:GLU:CD	2.10	0.90
1:A:408:ALA:O	2:B:393:ILE:HD12	1.72	0.89
1:A:419:THR:HB	1:A:420:PRO:CD	2.03	0.88
2:B:358:ARG:CZ	2:B:358:ARG:H	1.88	0.86
1:A:103:LYS:HA	1:A:192:ASP:OD1	1.74	0.86
1:A:543:GLY:HA2	1:A:546:GLU:HB2	1.56	0.86
1:A:26:LEU:HB2	1:A:31:ILE:HD11	1.58	0.85
1:A:317:VAL:HG23	1:A:349:LEU:HD23	1.59	0.84
1:A:219:LYS:HE3	1:A:219:LYS:HA	1.60	0.83
1:A:223:LYS:O	1:A:224:GLU:OE1	1.95	0.82
1:A:225:PRO:N	1:A:226:PRO:HD2	1.94	0.82
1:A:543:GLY:H	1:A:546:GLU:CG	1.93	0.82
1:A:254:VAL:HB	1:A:290:THR:HA	1.64	0.78
1:A:543:GLY:H	1:A:546:GLU:HG2	1.49	0.78
2:B:66:LYS:HG3	2:B:67:ASP:H	1.49	0.78
2:B:170:PRO:HB2	2:B:208:HIS:CE1	2.19	0.77
2:B:33:ALA:O	2:B:37:ILE:HG12	1.85	0.76
1:A:225:PRO:N	1:A:226:PRO:CD	2.48	0.76
2:B:5:ILE:HD13	2:B:5:ILE:O	1.86	0.75
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.68	0.75
1:A:419:THR:HB	1:A:420:PRO:HD3	1.69	0.75
1:A:399:GLU:HG3	1:A:402:TRP:HE1	1.53	0.74
1:A:439:THR:H	1:A:460:ASN:ND2	1.85	0.74
1:A:419:THR:CB	1:A:420:PRO:CD	2.65	0.74
1:A:219:LYS:CE	1:A:219:LYS:HA	2.16	0.73
2:B:94:ILE:HD12	2:B:94:ILE:O	1.88	0.73
1:A:142:ILE:H	1:A:142:ILE:HD12	1.53	0.73
2:B:402:TRP:NE1	2:B:403:THR:HG23	2.03	0.73
2:B:31:ILE:HD11	2:B:133:PRO:HG2	1.71	0.72
1:A:516:GLU:O	1:A:520:GLN:HG3	1.90	0.71
1:A:539:HIS:O	1:A:540:LYS:HG2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:C	1:A:226:PRO:CD	2.54	0.71
1:A:541:GLY:HA2	1:A:546:GLU:HG3	1.72	0.71
1:A:114:ALA:HB1	1:A:214:LEU:HD22	1.72	0.70
1:A:458:VAL:HG23	2:B:286:THR:HG21	1.74	0.70
1:A:420:PRO:CB	1:A:421:PRO:HD3	2.09	0.70
1:A:142:ILE:N	1:A:142:ILE:HD12	2.06	0.70
2:B:402:TRP:CE2	2:B:403:THR:CG2	2.74	0.69
2:B:209:LEU:O	2:B:214:LEU:HB2	1.92	0.69
2:B:402:TRP:CZ2	2:B:403:THR:HG22	2.28	0.69
2:B:240:THR:O	2:B:350:LYS:HD2	1.93	0.68
1:A:399:GLU:HA	1:A:402:TRP:HD1	1.59	0.68
2:B:183:TYR:CD2	2:B:380:ILE:HD13	2.29	0.68
2:B:270:ILE:HD12	2:B:270:ILE:N	2.09	0.67
2:B:402:TRP:CE2	2:B:403:THR:HG23	2.29	0.67
1:A:419:THR:HB	1:A:420:PRO:HD2	1.77	0.66
2:B:170:PRO:HB2	2:B:208:HIS:HE1	1.61	0.66
1:A:539:HIS:C	1:A:540:LYS:HG2	2.17	0.65
2:B:210:LEU:O	2:B:210:LEU:HD23	1.96	0.65
1:A:543:GLY:HA3	2:B:284:ARG:HA	1.79	0.65
1:A:458:VAL:CG2	2:B:286:THR:HG21	2.26	0.65
2:B:5:ILE:HG23	2:B:6:GLU:HG3	1.79	0.64
1:A:94:ILE:H	1:A:94:ILE:HD13	1.62	0.64
1:A:541:GLY:O	2:B:280:SER:HB3	1.99	0.63
2:B:423:VAL:HG12	2:B:426:TRP:CE3	2.33	0.63
1:A:164:MET:HG2	1:A:182:GLN:NE2	2.14	0.63
1:A:317:VAL:CG2	1:A:349:LEU:HD23	2.27	0.62
2:B:85:GLN:O	2:B:85:GLN:HG3	1.99	0.62
1:A:544:GLY:HA2	2:B:286:THR:CG2	2.30	0.62
2:B:10:VAL:HG13	2:B:85:GLN:HE21	1.64	0.62
2:B:163:SER:O	2:B:167:ILE:HG13	2.00	0.62
1:A:402:TRP:CE2	1:A:403:THR:HG23	2.35	0.61
1:A:233:GLU:OE1	1:A:243:PRO:HD3	1.99	0.61
2:B:393:ILE:HG13	2:B:394:GLN:N	2.14	0.61
1:A:354:TYR:OH	1:A:370:GLU:HB3	2.00	0.61
1:A:540:LYS:O	1:A:546:GLU:CD	2.39	0.61
2:B:238:LYS:HG2	2:B:239:TRP:N	2.16	0.60
1:A:202:ILE:O	1:A:206:ARG:HG3	2.00	0.60
2:B:108:VAL:O	2:B:231:GLY:HA2	2.01	0.60
1:A:181:TYR:CD2	3:A:556:UDR:HAPA	2.36	0.60
1:A:457:TYR:C	1:A:457:TYR:CD1	2.74	0.60
1:A:399:GLU:HA	1:A:402:TRP:NE1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:GLY:HA2	1:A:552:VAL:HG11	1.84	0.59
1:A:103:LYS:HD3	1:A:192:ASP:OD1	2.03	0.59
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.37	0.59
1:A:102:LYS:HE3	1:A:102:LYS:N	2.16	0.59
1:A:203:GLU:OE1	1:A:206:ARG:HD3	2.00	0.59
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.02	0.59
1:A:220:LYS:O	1:A:221:HIS:ND1	2.35	0.59
2:B:402:TRP:CE2	2:B:403:THR:HG22	2.37	0.59
2:B:206:ARG:HB2	2:B:206:ARG:NH1	2.18	0.59
2:B:156:SER:N	2:B:157:PRO:HD2	2.18	0.59
1:A:257:ILE:O	1:A:261:VAL:HG23	2.02	0.59
1:A:361:HIS:NE2	1:A:505:ILE:HD12	2.17	0.59
1:A:305:GLU:O	1:A:309:ILE:HD13	2.02	0.59
1:A:65:LYS:HE3	1:A:68:SER:OG	2.02	0.58
1:A:419:THR:CB	1:A:420:PRO:HD2	2.32	0.58
1:A:323:LYS:HA	1:A:323:LYS:HE2	1.84	0.58
2:B:113:ASP:HB2	2:B:228:LEU:HD21	1.84	0.58
1:A:424:LYS:HE2	1:A:426:TRP:CZ3	2.39	0.58
2:B:423:VAL:HG12	2:B:426:TRP:CZ3	2.39	0.58
1:A:62:ALA:C	1:A:63:ILE:HD12	2.23	0.58
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.39	0.58
2:B:358:ARG:CZ	2:B:358:ARG:N	2.64	0.58
1:A:64:LYS:HB2	1:A:71:TRP:CD2	2.39	0.58
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.85	0.58
1:A:417:VAL:O	1:A:417:VAL:HG13	2.04	0.57
1:A:28:GLU:HG3	1:A:135:ILE:HD12	1.86	0.57
2:B:31:ILE:CD1	2:B:133:PRO:HG2	2.34	0.57
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.86	0.57
2:B:357:MET:O	2:B:357:MET:HG3	2.04	0.56
1:A:498:ASP:HB3	1:A:545:ASN:HD21	1.69	0.56
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.21	0.56
1:A:107:THR:HG22	1:A:108:VAL:N	2.20	0.56
1:A:266:TRP:O	1:A:269:GLN:HG2	2.06	0.56
1:A:278:GLN:O	1:A:282:LEU:HG	2.06	0.55
1:A:246:LEU:HD21	1:A:310:LEU:HD12	1.87	0.55
1:A:366:LYS:HE2	1:A:405:TYR:OH	2.06	0.55
1:A:543:GLY:CA	1:A:546:GLU:HB2	2.33	0.55
1:A:542:ILE:O	2:B:283:LEU:HB3	2.08	0.55
2:B:402:TRP:CG	2:B:403:THR:N	2.75	0.55
1:A:246:LEU:HD21	1:A:310:LEU:CD1	2.37	0.54
2:B:376:THR:CG2	2:B:386:THR:HG22	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LYS:HB3	1:A:471:ASN:HA	1.89	0.54
1:A:17:ASP:O	1:A:83:ARG:HD3	2.07	0.54
1:A:10:VAL:HG12	1:A:11:LYS:N	2.21	0.54
1:A:222:GLN:O	1:A:222:GLN:CG	2.48	0.54
1:A:363:ASN:HD21	1:A:366:LYS:HG3	1.73	0.54
1:A:219:LYS:O	1:A:220:LYS:HB2	2.07	0.54
2:B:356:ARG:HG2	2:B:356:ARG:O	2.08	0.54
1:A:39:THR:O	1:A:43:LYS:HG2	2.08	0.54
1:A:498:ASP:HB3	1:A:545:ASN:ND2	2.23	0.53
2:B:315:HIS:O	2:B:317:VAL:CG2	2.50	0.53
2:B:118:VAL:HB	2:B:149:LEU:HD12	1.89	0.53
1:A:345:PRO:O	1:A:346:PHE:HB2	2.09	0.53
2:B:76:ASP:OD1	2:B:76:ASP:C	2.47	0.53
1:A:31:ILE:O	1:A:35:VAL:HG23	2.09	0.52
2:B:91:GLN:O	2:B:92:LEU:HB2	2.09	0.52
1:A:420:PRO:CB	1:A:421:PRO:CD	2.71	0.52
1:A:29:GLU:HG3	1:A:30:LYS:N	2.24	0.52
1:A:376:THR:O	1:A:380:ILE:HG12	2.10	0.52
2:B:193:LEU:HB3	2:B:197:GLN:HG3	1.92	0.52
1:A:398:TRP:CZ2	1:A:411:ILE:HG12	2.44	0.52
1:A:183:TYR:O	1:A:184:MET:HB2	2.10	0.52
2:B:393:ILE:HD11	2:B:397:THR:CG2	2.39	0.52
2:B:183:TYR:CE2	2:B:184:MET:HG2	2.45	0.52
2:B:115:TYR:OH	2:B:157:PRO:HA	2.10	0.52
1:A:284:ARG:H	1:A:284:ARG:HD3	1.75	0.52
1:A:258:GLN:HB2	1:A:283:LEU:HD22	1.92	0.52
1:A:543:GLY:C	1:A:545:ASN:H	2.13	0.52
2:B:85:GLN:O	2:B:87:PHE:N	2.43	0.52
2:B:376:THR:HG23	2:B:386:THR:HG22	1.90	0.52
1:A:536:VAL:HG21	1:A:542:ILE:HG21	1.92	0.51
1:A:175:ASN:N	1:A:176:PRO:HD3	2.25	0.51
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.91	0.51
1:A:65:LYS:HE3	1:A:68:SER:CB	2.39	0.51
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.10	0.51
1:A:53:GLU:O	1:A:55:PRO:HD3	2.11	0.51
1:A:277:ARG:NH1	1:A:334:GLN:O	2.44	0.51
1:A:540:LYS:HE3	2:B:265:ASN:OD1	2.11	0.51
2:B:183:TYR:CD2	2:B:184:MET:HG2	2.45	0.51
1:A:470:THR:O	1:A:471:ASN:HB3	2.11	0.50
1:A:483:TYR:CE2	1:A:487:GLN:NE2	2.80	0.50
2:B:270:ILE:N	2:B:270:ILE:CD1	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LYS:O	1:A:313:PRO:HD3	2.11	0.50
2:B:345:PRO:O	2:B:346:PHE:HB2	2.11	0.50
1:A:317:VAL:HG23	1:A:349:LEU:CD2	2.38	0.50
1:A:155:GLY:O	1:A:159:ILE:HG12	2.10	0.50
1:A:544:GLY:O	1:A:548:VAL:HG12	2.10	0.50
2:B:125:ARG:O	2:B:145:GLN:HG3	2.12	0.50
1:A:106:VAL:HG21	3:A:556:UDR:HAAA	1.90	0.50
2:B:410:TRP:O	2:B:411:ILE:HD13	2.12	0.49
1:A:207:GLN:O	1:A:210:LEU:HB3	2.11	0.49
1:A:106:VAL:CG2	3:A:556:UDR:HAAB	2.27	0.49
2:B:425:LEU:HD12	2:B:428:GLN:HB2	1.94	0.49
1:A:245:VAL:O	1:A:247:PRO:HD3	2.10	0.49
2:B:101:LYS:HD3	2:B:382:ILE:HG23	1.94	0.49
2:B:142:ILE:CG2	2:B:144:TYR:CE1	2.96	0.49
1:A:443:ASP:HB2	1:A:548:VAL:HG13	1.94	0.49
1:A:65:LYS:O	1:A:68:SER:HB2	2.13	0.49
1:A:31:ILE:HD12	1:A:133:PRO:HG2	1.95	0.49
2:B:10:VAL:O	2:B:11:LYS:HD3	2.13	0.49
2:B:233:GLU:CD	2:B:233:GLU:H	2.16	0.49
1:A:326:ILE:HG22	1:A:327:ALA:N	2.28	0.49
1:A:224:GLU:HB3	1:A:226:PRO:HD2	1.94	0.49
1:A:224:GLU:O	1:A:226:PRO:HD2	2.07	0.49
1:A:129:ALA:HA	1:A:144:TYR:O	2.13	0.49
2:B:278:GLN:HB2	2:B:302:GLU:OE1	2.13	0.49
1:A:541:GLY:O	2:B:280:SER:O	2.29	0.48
2:B:281:LYS:HD2	2:B:284:ARG:NH1	2.28	0.48
2:B:315:HIS:O	2:B:316:GLY:C	2.52	0.48
2:B:206:ARG:HH11	2:B:206:ARG:HB2	1.77	0.48
1:A:78:ARG:HB2	1:A:78:ARG:HH11	1.78	0.48
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.48	0.48
2:B:312:GLU:HB3	2:B:313:PRO:HD2	1.96	0.48
2:B:287:LYS:HD3	2:B:293:ILE:HD11	1.96	0.48
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.49	0.48
1:A:63:ILE:N	1:A:63:ILE:HD12	2.29	0.47
1:A:229:TRP:CE2	3:A:556:UDR:HAO	2.50	0.47
1:A:224:GLU:O	1:A:227:PHE:CE2	2.67	0.47
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.49	0.47
1:A:426:TRP:HD1	1:A:511:ASP:HB2	1.80	0.47
1:A:142:ILE:H	1:A:142:ILE:CD1	2.23	0.47
2:B:167:ILE:HG12	2:B:212:TRP:CE3	2.49	0.47
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.80	0.47
1:A:244:ILE:HG13	1:A:267:ALA:HB2	1.97	0.47
2:B:359:GLY:C	2:B:361:HIS:H	2.18	0.47
1:A:536:VAL:HB	1:A:542:ILE:HG13	1.96	0.47
1:A:284:ARG:HD3	1:A:284:ARG:N	2.30	0.47
1:A:356:ARG:HG2	1:A:357:MET:O	2.15	0.47
1:A:439:THR:H	1:A:460:ASN:HD22	1.61	0.46
1:A:295:LEU:HD12	1:A:295:LEU:N	2.30	0.46
1:A:31:ILE:CD1	1:A:133:PRO:HG2	2.44	0.46
1:A:544:GLY:CA	2:B:286:THR:HG22	2.44	0.46
2:B:314:VAL:HG22	2:B:315:HIS:N	2.31	0.46
2:B:277:ARG:NH1	2:B:281:LYS:HZ2	2.13	0.46
1:A:167:ILE:O	1:A:170:PRO:HD2	2.15	0.46
2:B:47:ILE:HD12	2:B:144:TYR:CD2	2.50	0.46
1:A:449:GLU:N	1:A:449:GLU:CD	2.69	0.46
3:A:556:UDR:HANA	3:A:556:UDR:CAL	2.44	0.46
2:B:8:VAL:O	2:B:10:VAL:HG23	2.16	0.46
1:A:246:LEU:CD1	1:A:307:ARG:HG2	2.45	0.46
2:B:208:HIS:O	2:B:211:ARG:HG2	2.16	0.46
1:A:270:ILE:O	1:A:272:PRO:HD3	2.16	0.46
1:A:293:ILE:HG23	1:A:294:PRO:HD2	1.97	0.46
1:A:457:TYR:HD1	1:A:457:TYR:C	2.19	0.46
1:A:148:VAL:O	1:A:150:PRO:HD3	2.16	0.46
1:A:424:LYS:HE2	1:A:426:TRP:CE3	2.51	0.45
2:B:116:PHE:CD2	2:B:148:VAL:HG21	2.51	0.45
1:A:426:TRP:CD1	1:A:511:ASP:HB2	2.51	0.45
1:A:363:ASN:ND2	1:A:366:LYS:HG3	2.31	0.45
1:A:46:LYS:N	1:A:46:LYS:HE3	2.32	0.45
1:A:543:GLY:C	1:A:545:ASN:N	2.70	0.45
2:B:169:GLU:OE2	2:B:169:GLU:HA	2.16	0.45
2:B:207:GLN:OE1	2:B:210:LEU:HD13	2.17	0.45
2:B:423:VAL:C	2:B:425:LEU:H	2.19	0.45
2:B:115:TYR:HE2	2:B:156:SER:O	1.99	0.45
2:B:105:SER:O	2:B:190:GLY:HA2	2.16	0.45
1:A:101:LYS:HG3	1:A:103:LYS:NZ	2.32	0.45
2:B:8:VAL:HB	2:B:159:ILE:HD12	1.98	0.45
2:B:326:ILE:N	2:B:326:ILE:HD12	2.31	0.45
1:A:250:ASP:OD2	1:A:251:SER:N	2.50	0.45
2:B:340:GLN:HE21	2:B:340:GLN:HB2	1.60	0.45
1:A:287:LYS:O	1:A:288:ALA:HB3	2.15	0.45
1:A:224:GLU:CB	1:A:226:PRO:HD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:HD3	1:A:367:GLN:NE2	2.32	0.45
2:B:371:ALA:O	2:B:375:ILE:HG13	2.17	0.45
1:A:120:LEU:HD12	1:A:121:ASP:H	1.82	0.45
1:A:19:PRO:O	1:A:20:LYS:HD3	2.17	0.45
1:A:474:ASN:O	1:A:478:GLU:HG3	2.16	0.45
1:A:417:VAL:O	1:A:417:VAL:CG1	2.65	0.44
2:B:11:LYS:H	2:B:85:GLN:NE2	2.15	0.44
1:A:199:ARG:CZ	1:A:199:ARG:HB2	2.47	0.44
1:A:118:VAL:HG11	1:A:149:LEU:HD11	1.98	0.44
1:A:542:ILE:O	1:A:542:ILE:HG22	2.16	0.44
2:B:169:GLU:N	2:B:170:PRO:CD	2.81	0.44
1:A:74:LEU:C	1:A:74:LEU:HD13	2.38	0.44
1:A:70:LYS:HG2	1:A:71:TRP:H	1.82	0.44
2:B:66:LYS:HG3	2:B:67:ASP:N	2.24	0.44
1:A:64:LYS:HB2	1:A:71:TRP:CE2	2.53	0.44
2:B:234:LEU:HD12	2:B:234:LEU:O	2.18	0.44
1:A:281:LYS:O	1:A:281:LYS:HD3	2.17	0.44
1:A:42:GLU:OE1	1:A:49:LYS:HG3	2.18	0.44
1:A:398:TRP:CH2	1:A:411:ILE:HG12	2.53	0.44
2:B:358:ARG:NE	2:B:358:ARG:N	2.66	0.44
2:B:108:VAL:HG22	2:B:188:TYR:CE2	2.53	0.44
1:A:194:GLU:HG3	1:A:197:GLN:NE2	2.33	0.44
2:B:402:TRP:CZ2	2:B:403:THR:CG2	2.98	0.43
1:A:5:ILE:O	1:A:6:GLU:C	2.56	0.43
1:A:194:GLU:HA	1:A:194:GLU:OE1	2.18	0.43
2:B:191:SER:OG	2:B:198:HIS:ND1	2.44	0.43
1:A:102:LYS:HD2	1:A:102:LYS:O	2.18	0.43
1:A:0:VAL:N	1:A:1:PRO:CD	2.82	0.43
2:B:314:VAL:CG2	2:B:315:HIS:N	2.81	0.43
1:A:156:SER:N	1:A:157:PRO:CD	2.82	0.43
1:A:254:VAL:HG23	1:A:291:GLU:N	2.33	0.43
2:B:85:GLN:CG	2:B:85:GLN:O	2.65	0.43
2:B:151:GLN:HB3	2:B:151:GLN:HE21	1.61	0.43
1:A:99:GLY:HA3	2:B:136:ASN:ND2	2.32	0.43
2:B:354:TYR:OH	2:B:357:MET:HG2	2.19	0.43
2:B:154:LYS:HG2	2:B:154:LYS:O	2.18	0.43
2:B:27:THR:OG1	2:B:30:LYS:HG3	2.18	0.43
1:A:449:GLU:N	1:A:449:GLU:OE2	2.51	0.43
2:B:116:PHE:HD2	2:B:148:VAL:HG21	1.83	0.42
1:A:438:GLU:HG3	1:A:461:LYS:HD3	2.01	0.42
2:B:37:ILE:HG22	2:B:41:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:LYS:HB2	1:A:552:VAL:HG13	2.02	0.42
1:A:115:TYR:OH	1:A:156:SER:HB3	2.19	0.42
1:A:224:GLU:CA	1:A:226:PRO:HD2	2.46	0.42
2:B:239:TRP:O	2:B:242:GLN:NE2	2.52	0.42
1:A:190:GLY:O	1:A:191:SER:HB3	2.19	0.42
2:B:358:ARG:HA	2:B:358:ARG:NH1	2.34	0.42
1:A:543:GLY:N	1:A:546:GLU:HG2	2.27	0.42
1:A:284:ARG:H	1:A:284:ARG:CD	2.33	0.42
1:A:194:GLU:HG3	1:A:197:GLN:HE21	1.85	0.42
1:A:360:ALA:O	1:A:514:GLU:HG2	2.20	0.42
2:B:194:GLU:HG2	2:B:197:GLN:HG2	2.02	0.42
1:A:107:THR:HG22	1:A:108:VAL:H	1.85	0.41
1:A:246:LEU:HD11	1:A:310:LEU:HD12	2.02	0.41
1:A:354:TYR:CZ	1:A:370:GLU:HB3	2.54	0.41
1:A:516:GLU:O	1:A:516:GLU:HG2	2.19	0.41
1:A:70:LYS:HG2	1:A:71:TRP:N	2.35	0.41
1:A:37:ILE:O	1:A:40:GLU:HG2	2.21	0.41
2:B:13:LYS:HD2	2:B:16:MET:CE	2.50	0.41
1:A:218:ASP:O	1:A:219:LYS:CD	2.48	0.41
1:A:542:ILE:H	1:A:546:GLU:CG	2.34	0.41
2:B:330:GLN:HE21	2:B:330:GLN:HB2	1.70	0.41
1:A:206:ARG:CZ	1:A:218:ASP:CB	2.99	0.41
1:A:399:GLU:CA	1:A:402:TRP:CD1	2.92	0.41
2:B:205:LEU:O	2:B:209:LEU:HG	2.20	0.41
1:A:102:LYS:HD2	1:A:102:LYS:C	2.41	0.41
1:A:29:GLU:CG	1:A:30:LYS:N	2.84	0.41
1:A:287:LYS:NZ	1:A:287:LYS:HB3	2.36	0.41
1:A:503:LEU:HA	1:A:503:LEU:HD23	1.64	0.41
2:B:99:GLY:O	2:B:103:LYS:HG2	2.21	0.41
2:B:5:ILE:C	2:B:5:ILE:HD13	2.41	0.41
2:B:156:SER:N	2:B:157:PRO:CD	2.84	0.41
1:A:118:VAL:HA	1:A:119:PRO:HD2	1.95	0.41
1:A:283:LEU:HA	1:A:286:THR:HG23	2.03	0.40
2:B:260:LEU:HD12	2:B:260:LEU:HA	1.83	0.40
1:A:223:LYS:HB3	1:A:223:LYS:HE2	1.72	0.40
1:A:181:TYR:CD2	3:A:556:UDR:CAP	3.05	0.40
1:A:306:ASN:O	1:A:310:LEU:HB2	2.21	0.40
1:A:293:ILE:CG2	1:A:294:PRO:HD2	2.52	0.40
2:B:360:ALA:O	2:B:361:HIS:CG	2.74	0.40
2:B:103:LYS:HE2	2:B:179:VAL:HG23	2.04	0.40
2:B:58:THR:HG21	2:B:77:PHE:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LYS:NZ	1:A:223:LYS:HB3	2.30	0.40
2:B:393:ILE:HD11	2:B:397:THR:HG21	2.03	0.40
1:A:542:ILE:H	1:A:546:GLU:HG2	1.86	0.40
1:A:12:LEU:HD22	1:A:83:ARG:O	2.21	0.40
1:A:391:LEU:O	1:A:417:VAL:HG12	2.22	0.40
1:A:175:ASN:HB3	1:A:178:ILE:HG12	2.03	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	553/558 (99%)	482 (87%)	68 (12%)	3 (0%)	34	69
2	B	412/428 (96%)	362 (88%)	46 (11%)	4 (1%)	19	52
All	All	965/986 (98%)	844 (88%)	114 (12%)	7 (1%)	26	62

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	424	LYS
1	A	194	GLU
1	A	184	MET
2	B	86	ASP
2	B	316	GLY
1	A	317	VAL
2	B	195	ILE

### 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	494/495 (100%)	468 (95%)	26 (5%)	28	61
2	B	378/390 (97%)	368 (97%)	10 (3%)	54	86
All	All	872/885 (98%)	836 (96%)	36 (4%)	37	72

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	46	LYS
1	A	78	ARG
1	A	91	GLN
1	A	92	LEU
1	A	94	ILE
1	A	102	LYS
1	A	113	ASP
1	A	137	ASN
1	A	185	ASP
1	A	192	ASP
1	A	193	LEU
1	A	207	GLN
1	A	211	ARG
1	A	218	ASP
1	A	219	LYS
1	A	220	LYS
1	A	223	LYS
1	A	284	ARG
1	A	287	LYS
1	A	347	LYS
1	A	362	THR
1	A	457	TYR
1	A	459	THR
1	A	512	LYS
1	A	545	ASN
2	B	5	ILE

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Mol	Chain	Res	Type
2	B	88	TRP
2	B	233	GLU
2	B	248	GLU
2	B	340	GLN
2	B	356	ARG
2	B	358	ARG
2	B	393	ILE
2	B	414	TRP
2	B	417	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	151	GLN
1	A	197	GLN
1	A	222	GLN
1	A	242	GLN
1	A	255	ASN
1	A	306	ASN
1	A	336	GLN
1	A	394	GLN
1	A	460	ASN
1	A	475	GLN
1	A	487	GLN
1	A	507	GLN
1	A	524	GLN
2	B	85	GLN
2	B	151	GLN
2	B	174	GLN
2	B	197	GLN
2	B	208	HIS
2	B	255	ASN
2	B	278	GLN
2	B	330	GLN
2	B	340	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	UDR	A	556	-	29,39,39	2.94	8 (27%)	33,56,56	1.00	2 (6%)

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	UDR	A	556	-	-	0/21/23/23	0/2/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	556	UDR	CBB-CAX	-7.83	1.38	1.49
3	A	556	UDR	NAQ-NAR	-6.84	1.23	1.37
3	A	556	UDR	CBC-CAX	-6.32	1.40	1.49
3	A	556	UDR	CAN-CAI	-3.85	1.39	1.50
3	A	556	UDR	CBE-CAW	2.81	1.53	1.50
3	A	556	UDR	OAH-CBG	3.53	1.23	1.19
3	A	556	UDR	CAI-CAX	4.49	1.39	1.34
3	A	556	UDR	CAP-CBD	6.00	1.53	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	556	UDR	CAA-OAS-CBF	-2.16	109.14	114.82
3	A	556	UDR	CBB-CAX-CBC	2.09	119.65	116.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	556	UDR	8	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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	555/558 (99%)	0.16	43 (7%) 16 8	40, 90, 158, 175	0
2	B	416/428 (97%)	0.16	25 (6%) 25 15	49, 81, 149, 182	0
All	All	971/986 (98%)	0.16	68 (7%) 19 11	40, 86, 154, 182	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	227	PHE	11.9
2	B	2	ILE	11.4
2	B	1	PRO	10.9
2	B	3	SER	8.8
1	A	553	SER	7.7
1	A	554	ALA	7.4
1	A	287	LYS	6.7
1	A	552	VAL	6.2
1	A	220	LYS	5.8
1	A	547	GLN	5.7
2	B	4	PRO	5.6
1	A	549	ASP	5.3
2	B	92	LEU	5.3
1	A	286	THR	5.1
1	A	67	ASP	5.0
1	A	292	VAL	4.9
1	A	551	LEU	4.6
2	B	93	GLY	4.5
1	A	297	GLU	4.4
1	A	548	VAL	4.3
2	B	173	LYS	4.3
1	A	219	LYS	4.3
2	B	230	MET	4.1
2	B	90	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	69	THR	4.0
1	A	545	ASN	3.9
2	B	91	GLN	3.6
2	B	228	LEU	3.6
1	A	24	TRP	3.5
1	A	301	LEU	3.5
1	A	283	LEU	3.5
1	A	218	ASP	3.5
1	A	284	ARG	3.4
1	A	298	GLU	3.3
1	A	550	LYS	3.3
2	B	315	HIS	3.2
2	B	16	MET	3.1
1	A	308	GLU	3.0
1	A	541	GLY	2.9
2	B	85	GLN	2.8
2	B	357	MET	2.8
2	B	232	TYR	2.8
1	A	66	LYS	2.7
1	A	63	ILE	2.7
2	B	186	ASP	2.7
1	A	304	ALA	2.5
1	A	70	LYS	2.5
1	A	252	TRP	2.5
1	A	221	HIS	2.5
1	A	71	TRP	2.4
2	B	231	GLY	2.3
2	B	88	TRP	2.3
1	A	289	LEU	2.2
1	A	542	ILE	2.1
2	B	185	ASP	2.1
1	A	90	VAL	2.1
1	A	305	GLU	2.1
2	B	166	LYS	2.1
2	B	94	ILE	2.1
2	B	5	ILE	2.1
1	A	290	THR	2.1
1	A	302	GLU	2.1
1	A	244	ILE	2.1
2	B	151	GLN	2.1
1	A	288	ALA	2.1
1	A	257	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	246	LEU	2.0
1	A	544	GLY	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	UDR	A	556	36/36	0.91	0.23	0.50	69,76,79,81	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.