



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:02 PM GMT

PDB ID : 1RT4
Title : HIV-1 REVERSE TRANSCRIPTASE COMPLEXED WITH UC781
Authors : Ren, J.; Stammers, D.K.; Stuart, D.I.
Deposited on : 1998-07-29
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

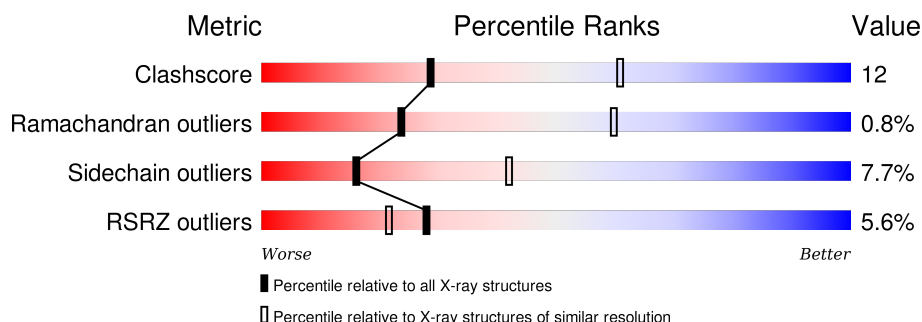
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	560	
2	B	440	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	1003	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7766 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4396	2847	732	809	8			

There is a discrepancy between the modelled and reference sequences:

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

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

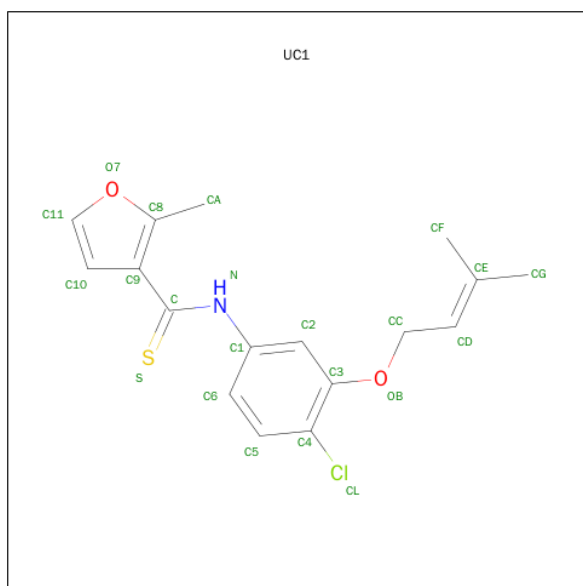
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3340	2170	556	607	7			

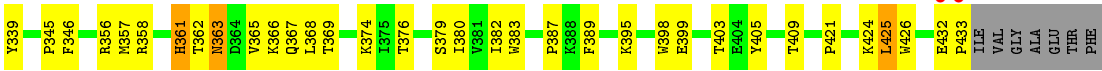
- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is 2-METHYL-FURAN-3-CARBOTHIOIC ACID [4-CHLORO-3-(3-METHYL-BUT-2-ENYLOXY)-PHENYL]-AMIDE (three-letter code: UC1) (formula: C₁₇H₁₈ClNO₂S).





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	140.40 Å 111.20 Å 73.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.6 (30.00-2.90) 93.6 (29.93-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 2.90 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.237 , 0.295 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 87.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 24458 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7766	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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, 0.375 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: CSD, PO4, UC1

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	0.33	0/4503	0.59	0/6117
2	B	0.32	0/3432	0.61	1/4659 (0.0%)
All	All	0.33	0/7935	0.60	1/10776 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	236	PRO	N-CA-C	5.07	125.27	112.10

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	4396	0	4451	105	0
2	B	3340	0	3376	73	0
3	A	5	0	0	0	0
4	A	22	0	18	7	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
All	All	7766	0	7845	180	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 12.

All (180) 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:278:GLN:HG2	1:A:298:GLU:HB3	1.54	0.89
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.61	0.82
1:A:410:TRP:CD1	2:B:363:ASN:HB2	2.16	0.80
1:A:21:VAL:HG11	1:A:59:PRO:HD3	1.68	0.75
2:B:158:ALA:O	2:B:161:GLN:HB2	1.90	0.72
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.21	0.71
2:B:101:LYS:HE2	2:B:382:ILE:HG23	1.74	0.69
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.75	0.69
1:A:244:ILE:HG23	1:A:310:LEU:HD13	1.74	0.68
1:A:109:LEU:HD23	1:A:216:THR:HG21	1.76	0.67
1:A:26:LEU:HD22	1:A:30:LYS:HE2	1.75	0.67
1:A:92:LEU:H	1:A:92:LEU:HD23	1.60	0.66
2:B:101:LYS:HG2	2:B:382:ILE:HA	1.76	0.66
2:B:157:PRO:HG2	2:B:184:MET:HA	1.78	0.66
2:B:395:LYS:O	2:B:399:GLU:HG2	1.95	0.66
1:A:358:ARG:HB3	1:A:358:ARG:NH1	2.11	0.65
1:A:474:ASN:ND2	1:A:474:ASN:H	1.95	0.64
1:A:235:HIS:HB2	1:A:238:LYS:O	1.97	0.64
2:B:242:GLN:HE21	2:B:242:GLN:HA	1.63	0.63
1:A:461:ARG:HH11	1:A:461:ARG:HG3	1.63	0.63
1:A:356:ARG:HH22	1:A:371:ALA:HB2	1.63	0.63
1:A:23:GLN:HE22	1:A:60:VAL:H	1.46	0.62
1:A:197:GLN:HE21	1:A:197:GLN:HA	1.65	0.62
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.35	0.61
2:B:13:LYS:HE2	2:B:82:LYS:O	2.01	0.61
1:A:340:GLN:CB	1:A:351:THR:HG22	2.31	0.60
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.84	0.59
2:B:295:LEU:HD12	2:B:295:LEU:H	1.66	0.59
1:A:171:PHE:HB2	1:A:208:HIS:HD2	1.66	0.59
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.02	0.58
1:A:27:THR:HB	1:A:30:LYS:HG3	1.86	0.58
1:A:34:LEU:HB3	1:A:132:ILE:HD12	1.85	0.58
2:B:363:ASN:ND2	2:B:366:LYS:HB2	2.19	0.58
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.86	0.58
2:B:421:PRO:O	2:B:425:LEU:HD22	2.04	0.57
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.87	0.57
1:A:122:GLU:CD	1:A:122:GLU:H	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:LYS:HE2	2:B:374:LYS:HA	1.86	0.56
1:A:381:VAL:HG22	2:B:25:PRO:HB3	1.88	0.56
2:B:72:ARG:HH21	2:B:409:THR:HG22	1.71	0.56
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.39	0.56
2:B:197:GLN:O	2:B:201:LYS:HB2	2.06	0.56
1:A:64:LYS:HD2	1:A:68:SER:HA	1.89	0.55
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.41	0.55
1:A:489:SER:HB2	1:A:493:VAL:HG22	1.88	0.55
2:B:206:ARG:O	2:B:210:LEU:HD13	2.06	0.55
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.89	0.54
1:A:240:THR:OG1	1:A:315:HIS:HB3	2.08	0.54
2:B:163:SER:O	2:B:167:ILE:HG13	2.08	0.54
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.07	0.53
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.43	0.53
1:A:503:LEU:HA	1:A:506:ILE:HD12	1.89	0.53
2:B:356:ARG:NH2	2:B:361:HIS:HB3	2.24	0.53
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.44	0.53
1:A:282:LEU:HB3	1:A:293:ILE:HG21	1.90	0.53
1:A:21:VAL:HG22	1:A:22:LYS:HD3	1.91	0.52
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.91	0.52
1:A:31:ILE:O	1:A:35:VAL:HG23	2.09	0.52
1:A:216:THR:HG23	1:A:217:PRO:HD2	1.92	0.51
4:A:999:UC1:H2	4:A:999:UC1:HD	1.92	0.51
2:B:365:VAL:O	2:B:369:THR:HG23	2.11	0.51
4:A:999:UC1:H2	4:A:999:UC1:C9	2.41	0.51
1:A:37:ILE:O	1:A:40:GLU:HB3	2.11	0.50
1:A:142:ILE:N	1:A:142:ILE:HD12	2.26	0.50
1:A:358:ARG:HH11	1:A:358:ARG:HB3	1.76	0.50
1:A:542:ILE:HD12	1:A:542:ILE:H	1.77	0.50
1:A:344:GLU:HB2	1:A:347:LYS:HD3	1.94	0.50
1:A:454:LYS:HA	1:A:467:VAL:O	2.11	0.50
1:A:489:SER:HB2	1:A:493:VAL:CG2	2.41	0.49
1:A:94:ILE:HG23	1:A:229:TRP:HZ2	1.76	0.49
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.93	0.49
1:A:57:ASN:HB2	1:A:143:ARG:HH22	1.77	0.49
2:B:95:PRO:O	2:B:181:TYR:HE1	1.95	0.49
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.11	0.49
4:A:999:UC1:H2	4:A:999:UC1:CD	2.43	0.49
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.48	0.49
2:B:103:LYS:O	2:B:236:PRO:HD2	2.12	0.49
1:A:362:THR:HG22	1:A:363:ASN:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:VAL:HG13	1:A:283:LEU:HD12	1.95	0.49
1:A:17:ASP:O	1:A:83:ARG:HD3	2.13	0.49
1:A:9:PRO:HA	1:A:121:ASP:OD2	2.13	0.48
1:A:432:GLU:HB2	1:A:433:PRO:HD2	1.96	0.48
2:B:361:HIS:HD2	2:B:362:THR:HG23	1.78	0.48
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.94	0.48
1:A:13:LYS:HE3	1:A:84:THR:O	2.13	0.48
4:A:999:UC1:C10	4:A:999:UC1:C2	2.92	0.48
2:B:5:ILE:HG22	2:B:6:GLU:H	1.78	0.48
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.43	0.47
4:A:999:UC1:H2	4:A:999:UC1:C10	2.44	0.47
1:A:57:ASN:HA	1:A:129:ALA:O	2.15	0.47
1:A:72:ARG:HH21	1:A:74:LEU:HD11	1.79	0.47
1:A:19:PRO:HG2	1:A:80:LEU:HB2	1.96	0.47
2:B:120:LEU:HD12	2:B:150:PRO:HD3	1.97	0.47
1:A:497:THR:O	1:A:535:TRP:HA	2.14	0.47
2:B:98:ALA:O	2:B:101:LYS:HD3	2.15	0.46
2:B:379:SER:CB	2:B:387:PRO:HD3	2.44	0.46
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.50	0.46
1:A:283:LEU:O	1:A:286:THR:HG23	2.16	0.46
2:B:175:ASN:N	2:B:176:PRO:HD3	2.31	0.46
1:A:7:THR:HG22	1:A:119:PRO:O	2.16	0.46
2:B:81:ASN:OD1	2:B:153:TRP:HD1	1.99	0.45
2:B:31:ILE:O	2:B:35:VAL:HG23	2.17	0.45
2:B:356:ARG:HB2	2:B:367:GLN:HG2	1.98	0.45
1:A:234:LEU:HB3	4:A:999:UC1:CL	2.54	0.45
2:B:206:ARG:HH22	2:B:210:LEU:HD21	1.81	0.45
2:B:170:PRO:HB2	2:B:208:HIS:HE1	1.81	0.45
1:A:197:GLN:NE2	1:A:197:GLN:HA	2.31	0.45
2:B:66:LYS:HG3	2:B:67:ASP:OD1	2.17	0.45
1:A:13:LYS:HG2	1:A:83:ARG:O	2.17	0.45
1:A:40:GLU:O	1:A:43:LYS:HG2	2.17	0.44
2:B:66:LYS:O	2:B:67:ASP:HB2	2.16	0.44
1:A:125:ARG:NH1	1:A:147:ASN:HB3	2.33	0.44
1:A:419:THR:O	1:A:419:THR:HG23	2.17	0.44
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.83	0.44
2:B:244:ILE:HG21	2:B:426:TRP:CH2	2.52	0.44
1:A:542:ILE:HG12	2:B:283:LEU:HD23	1.99	0.44
1:A:111:VAL:HG22	1:A:185:ASP:O	2.17	0.44
2:B:366:LYS:HG2	2:B:405:TYR:CD1	2.52	0.44
2:B:65:LYS:O	2:B:68:SER:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ILE:HD13	2:B:72:ARG:O	2.17	0.44
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.99	0.44
1:A:218:ASP:O	1:A:222:GLN:HG3	2.17	0.44
1:A:116:PHE:O	1:A:148:VAL:HG21	2.17	0.44
1:A:122:GLU:HA	1:A:125:ARG:NE	2.33	0.44
1:A:228:LEU:HD11	1:A:242:GLN:HE22	1.84	0.43
1:A:260:LEU:O	1:A:264:LEU:HD23	2.18	0.43
1:A:216:THR:CG2	1:A:217:PRO:HD2	2.48	0.43
1:A:356:ARG:HB2	1:A:367:GLN:NE2	2.34	0.43
4:A:999:UC1:S	4:A:999:UC1:HA1	2.58	0.43
2:B:64:LYS:HD2	2:B:71:TRP:CE2	2.54	0.43
1:A:69:THR:HG22	1:A:70:LYS:N	2.33	0.43
1:A:393:ILE:HB	1:A:423:VAL:HG22	2.01	0.43
2:B:157:PRO:CG	2:B:184:MET:HA	2.47	0.43
1:A:356:ARG:HE	1:A:374:LYS:HZ3	1.65	0.43
2:B:30:LYS:HE2	2:B:30:LYS:HB3	1.80	0.43
1:A:442:VAL:HG11	1:A:485:ALA:HB2	2.00	0.43
2:B:171:PHE:O	2:B:175:ASN:HB2	2.19	0.42
1:A:257:ILE:O	1:A:261:VAL:HG23	2.18	0.42
1:A:26:LEU:HB3	1:A:30:LYS:HB2	2.00	0.42
2:B:72:ARG:NH2	2:B:151:GLN:NE2	2.67	0.42
2:B:65:LYS:HZ1	2:B:72:ARG:HE	1.66	0.42
2:B:105:SER:HA	2:B:234:LEU:O	2.18	0.42
1:A:273:GLY:O	1:A:275:LYS:HG3	2.19	0.42
1:A:401:TRP:CZ3	1:A:409:THR:HG21	2.55	0.42
1:A:287:LYS:HG2	1:A:291:GLU:OE2	2.19	0.42
1:A:293:ILE:HD12	1:A:293:ILE:N	2.35	0.42
2:B:206:ARG:NH2	2:B:210:LEU:HD21	2.33	0.42
1:A:11:LYS:HE2	1:A:11:LYS:HB2	1.92	0.42
1:A:439:THR:HG21	2:B:289:LEU:HD13	2.01	0.42
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.55	0.42
1:A:452:LEU:HD22	1:A:470:THR:HA	2.01	0.42
2:B:363:ASN:HD21	2:B:366:LYS:HB2	1.84	0.42
1:A:438:GLU:HG3	1:A:461:ARG:HD2	2.02	0.42
2:B:432:GLU:HB3	2:B:433:PRO:HD2	2.01	0.42
2:B:328:GLU:O	2:B:339:TYR:HA	2.20	0.41
1:A:366:LYS:O	1:A:369:THR:HB	2.20	0.41
1:A:475:GLN:HB2	1:A:475:GLN:HE21	1.72	0.41
2:B:93:GLY:O	2:B:94:ILE:HG13	2.20	0.41
1:A:248:GLU:HA	1:A:307:ARG:NH2	2.36	0.41
1:A:135:ILE:HD13	1:A:135:ILE:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLN:HG3	1:A:349:LEU:HD11	2.02	0.41
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.55	0.41
1:A:73:LYS:O	1:A:74:LEU:HD12	2.19	0.41
2:B:10:VAL:HG11	2:B:153:TRP:CH2	2.56	0.41
1:A:439:THR:O	1:A:459:THR:HA	2.21	0.41
1:A:254:VAL:HG22	1:A:293:ILE:HD11	2.02	0.41
1:A:115:TYR:O	1:A:149:LEU:HB2	2.20	0.41
1:A:201:LYS:HD3	1:A:201:LYS:HA	1.91	0.41
2:B:345:PRO:O	2:B:346:PHE:HB2	2.21	0.41
1:A:2:ILE:HG22	1:A:3:SER:N	2.36	0.41
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.56	0.41
2:B:206:ARG:HB3	2:B:206:ARG:NH1	2.35	0.41
2:B:376:THR:O	2:B:380:ILE:HG13	2.21	0.41
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.56	0.40
1:A:438:GLU:CG	1:A:461:ARG:HD2	2.51	0.40
1:A:356:ARG:HE	1:A:374:LYS:NZ	2.18	0.40
2:B:78:ARG:O	2:B:82:LYS:HG3	2.21	0.40
1:A:56:TYR:O	1:A:143:ARG:NH2	2.54	0.40
2:B:115:TYR:HB3	2:B:149:LEU:HB2	2.04	0.40
2:B:288:ALA:O	2:B:291:GLU:HB3	2.21	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	532/560 (95%)	499 (94%)	27 (5%)	6 (1%)	17	51
2	B	398/440 (90%)	378 (95%)	19 (5%)	1 (0%)	46	79
All	All	930/1000 (93%)	877 (94%)	46 (5%)	7 (1%)	24	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLY
1	A	66	LYS
1	A	92	LEU
1	A	67	ASP
1	A	358	ARG
2	B	361	HIS
1	A	111	VAL

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	481/499 (96%)	441 (92%)	40 (8%)	14	38
2	B	368/400 (92%)	343 (93%)	25 (7%)	20	49
All	All	849/899 (94%)	784 (92%)	65 (8%)	16	42

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	53	GLU
1	A	67	ASP
1	A	68	SER
1	A	135	ILE
1	A	197	GLN
1	A	205	LEU
1	A	208	HIS
1	A	211	ARG
1	A	228	LEU
1	A	230	MET
1	A	248	GLU
1	A	251	SER
1	A	263	LYS
1	A	277	ARG
1	A	295	LEU
1	A	296	THR

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Mol	Chain	Res	Type
1	A	297	GLU
1	A	301	LEU
1	A	303	LEU
1	A	311	LYS
1	A	315	HIS
1	A	340	GLN
1	A	347	LYS
1	A	358	ARG
1	A	361	HIS
1	A	362	THR
1	A	368	LEU
1	A	404	GLU
1	A	424	LYS
1	A	431	LYS
1	A	452	LEU
1	A	464	GLN
1	A	474	ASN
1	A	475	GLN
1	A	491	LEU
1	A	496	VAL
1	A	517	LEU
1	A	540	LYS
1	A	542	ILE
2	B	6	GLU
2	B	8	VAL
2	B	24	TRP
2	B	63	ILE
2	B	65	LYS
2	B	69	THR
2	B	72	ARG
2	B	87	PHE
2	B	95	PRO
2	B	101	LYS
2	B	109	LEU
2	B	123	ASP
2	B	139	THR
2	B	186	ASP
2	B	194	GLU
2	B	242	GLN
2	B	263	LYS
2	B	283	LEU
2	B	289	LEU

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Mol	Chain	Res	Type
2	B	357	MET
2	B	358	ARG
2	B	363	ASN
2	B	368	LEU
2	B	424	LYS
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	91	GLN
1	A	96	HIS
1	A	136	ASN
1	A	174	GLN
1	A	197	GLN
1	A	242	GLN
1	A	332	GLN
1	A	336	GLN
1	A	394	GLN
1	A	474	ASN
2	B	57	ASN
2	B	85	GLN
2	B	151	GLN
2	B	242	GLN
2	B	361	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSD	A	280	1	3,7,8	0.76	0	3,8,10	2.30	1 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	280	1	-	1/2/6/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	280	CSD	OD1-SG-CB	3.60	111.41	105.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	A	1003	-	4,4,4	1.22	0	6,6,6	0.27	0
4	UC1	A	999	-	19,23,23	1.18	2 (10%)	21,31,31	1.47	2 (9%)

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	PO4	A	1003	-	-	0/0/0/0	0/0/0/0
4	UC1	A	999	-	-	1/10/14/14	0/1/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	UC1	C10-C9	2.02	1.51	1.42
4	A	999	UC1	CA-C8	3.05	1.53	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	UC1	OB-C3-C4	2.88	120.13	116.36
4	A	999	UC1	C9-C-N	4.93	120.30	114.12

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	999	UC1	S-C-N-C1

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	UC1	7	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	536/560 (95%)	0.03	41 (7%)	17 11	10, 57, 126, 182	0
2	B	404/440 (91%)	-0.16	12 (2%)	54 47	11, 50, 112, 155	0
All	All	940/1000 (94%)	-0.05	53 (5%)	28 21	10, 53, 119, 182	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	ASN	6.2
1	A	135	ILE	4.9
2	B	5	ILE	4.8
1	A	29	GLU	4.8
1	A	134	SER	4.6
1	A	28	GLU	4.6
1	A	52	PRO	4.4
1	A	1	PRO	4.1
1	A	67	ASP	4.0
1	A	90	VAL	4.0
1	A	63	ILE	3.8
1	A	91	GLN	3.8
1	A	30	LYS	3.7
1	A	68	SER	3.5
1	A	472	THR	3.4
1	A	55	PRO	3.4
1	A	132	ILE	3.4
1	A	33	ALA	3.4
2	B	433	PRO	3.4
1	A	542	ILE	3.3
2	B	67	ASP	3.3
1	A	245	VAL	3.3
2	B	432	GLU	3.2
1	A	27	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	3.2
2	B	6	GLU	3.0
1	A	450	THR	2.8
1	A	133	PRO	2.8
1	A	74	LEU	2.8
1	A	131	THR	2.8
2	B	198	HIS	2.7
1	A	473	THR	2.6
1	A	452	LEU	2.6
2	B	190	GLY	2.6
1	A	51	GLY	2.5
1	A	64	LYS	2.5
1	A	127	TYR	2.4
1	A	61	PHE	2.4
2	B	191	SER	2.4
2	B	242	GLN	2.4
1	A	65	LYS	2.4
1	A	21	VAL	2.3
1	A	62	ALA	2.3
1	A	69	THR	2.3
1	A	22	LYS	2.2
2	B	321	PRO	2.2
1	A	448	ARG	2.2
1	A	128	THR	2.1
1	A	25	PRO	2.1
2	B	66	LYS	2.0
2	B	184	MET	2.0
1	A	471	ASP	2.0
1	A	19	PRO	2.0

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

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, 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	LLDF	B-factors(Å ²)	Q<0.9
1	CSD	A	280	8/9	0.96	0.12	-	35,47,55,56	0

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	PO4	A	1003	5/5	0.92	0.27	4.60	122,122,126,131	0
4	UC1	A	999	22/22	0.98	0.12	-0.66	14,27,47,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.