



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:46 AM UTC

PDB ID : 1RT7 / pdb_00001rt7
Title : HIV-1 REVERSE TRANSCRIPTASE COMPLEXED WITH UC84
Authors : Ren, J.; Stammers, D.K.; Stuart, D.I.
Deposited on : 1998-07-29
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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

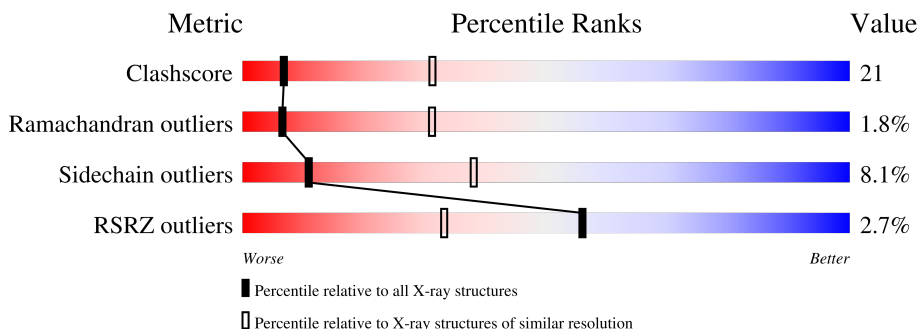
1 Overall quality at a glance

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))
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	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
4	UC4	A	999	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7850 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	536	4389	2839	731	811	8	0	0	0

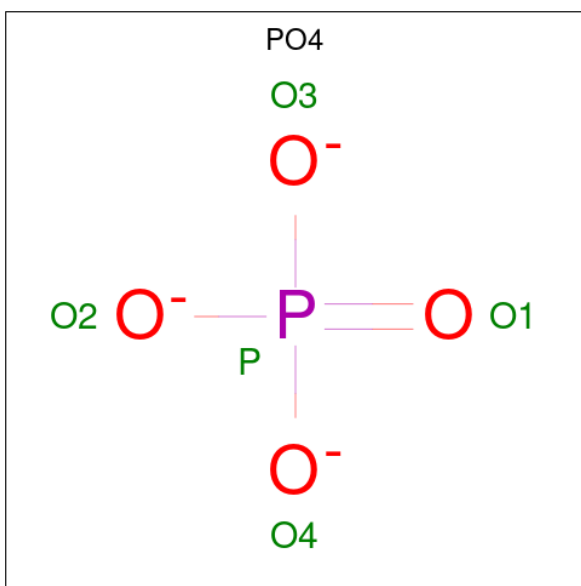
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	modified residue	UNP P04585

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

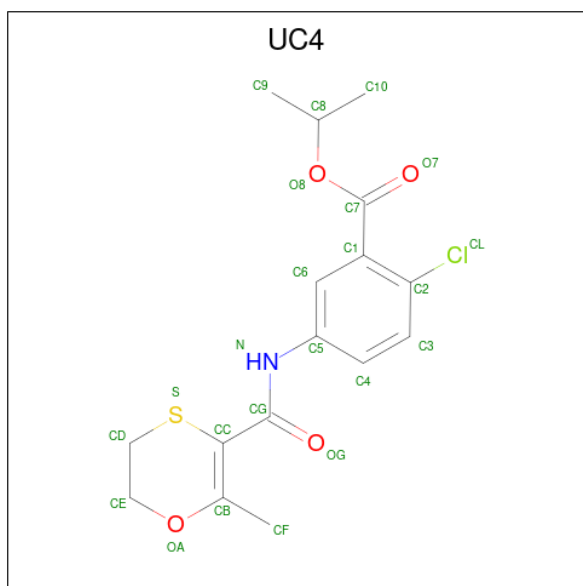
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	415	3428	2230	568	623	7	0	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is 1-METHYL ETHYL 1-CHLORO-5-[[[(5,6DIHYDRO-2-METHYL-1,4-OXATHIIN-3-YL)CARBONYL]AMINO]BENZOATE (CCD ID: UC4) (formula: C₁₆H₁₈ClNO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	Cl	N	O	S	0	0
			23	16	1	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		

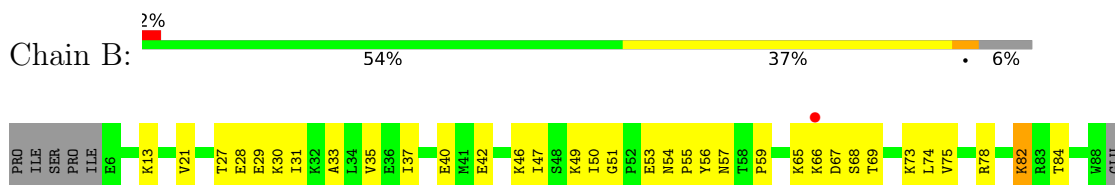
3 Residue-property plots

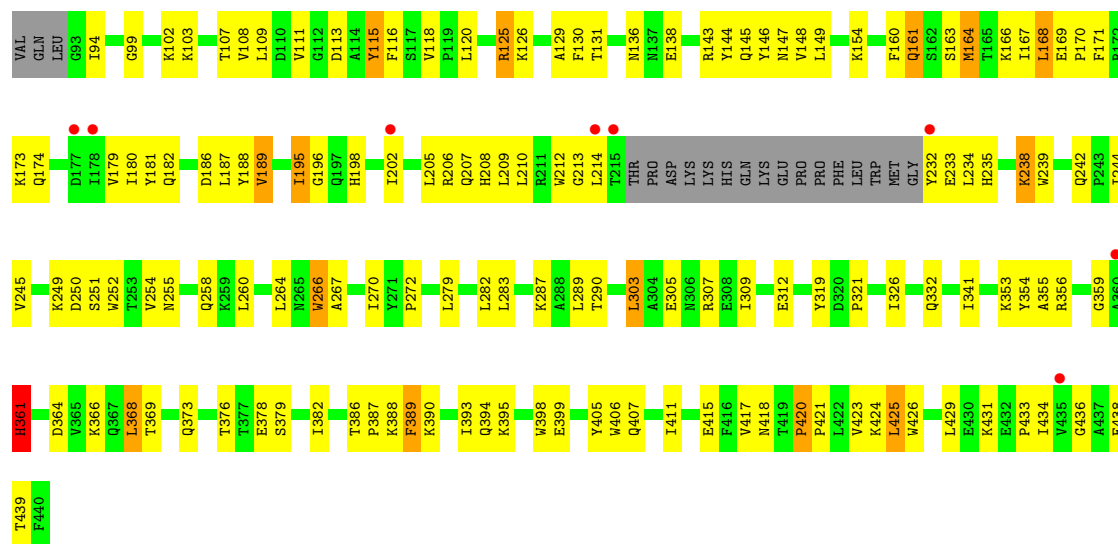
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: HIV-1 REVERSE TRANSCRIPTASE



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.60Å 109.50Å 72.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.3 (30.00-3.00) 87.3 (30.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 3.00Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.258 , 0.335 0.267 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtrriage
Anisotropy	0.266	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 88.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7850	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: CSD, UC4, PO4

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	0.52	0/4497	1.09	27/6112 (0.4%)
2	B	0.53	0/3524	1.05	24/4786 (0.5%)
All	All	0.53	0/8021	1.07	51/10898 (0.5%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	LYS	CA-C-N	10.23	151.56	127.00
1	A	13	LYS	C-N-CA	10.23	151.56	127.00
1	A	13	LYS	C-N-CD	-9.81	99.03	120.60
1	A	13	LYS	N-CA-C	8.03	127.56	109.81
1	A	217	PRO	N-CA-C	7.80	128.53	112.47
1	A	245	VAL	N-CA-C	7.68	118.92	108.17
1	A	503	LEU	N-CA-C	-7.42	103.19	111.28
2	B	168	LEU	N-CA-C	7.08	118.78	111.14
2	B	312	GLU	CA-C-N	7.00	126.97	119.76
2	B	312	GLU	C-N-CA	7.00	126.97	119.76
2	B	250	ASP	N-CA-C	-6.84	103.75	111.14
1	A	388	LYS	N-CA-C	-6.74	101.00	110.50
2	B	420	PRO	CA-C-N	6.70	128.21	119.84
2	B	420	PRO	C-N-CA	6.70	128.21	119.84
2	B	389	PHE	N-CA-C	6.62	121.08	109.96
2	B	417	VAL	N-CA-C	6.36	116.58	108.82
1	A	235	HIS	N-CA-C	-6.32	100.78	110.32
1	A	51	GLY	CA-C-N	6.21	126.33	119.87
1	A	51	GLY	C-N-CA	6.21	126.33	119.87
1	A	316	GLY	N-CA-C	6.05	119.94	111.10
1	A	216	THR	CA-C-N	6.02	127.36	119.84
1	A	216	THR	C-N-CA	6.02	127.36	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	382	ILE	N-CA-C	5.98	117.01	111.45
2	B	131	THR	N-CA-C	5.89	119.07	109.06
1	A	14	PRO	N-CA-C	5.82	127.23	112.10
1	A	184	MET	CB-CA-C	-5.70	110.01	116.63
2	B	186	ASP	N-CA-C	5.70	119.26	110.42
1	A	218	ASP	N-CA-C	-5.69	99.91	109.07
1	A	382	ILE	N-CA-C	5.67	115.86	110.53
2	B	125	ARG	N-CA-C	5.60	118.11	111.33
2	B	242	GLN	CA-C-N	5.53	126.75	119.84
2	B	242	GLN	C-N-CA	5.53	126.75	119.84
2	B	69	THR	N-CA-C	-5.52	106.04	112.89
2	B	266	TRP	N-CA-C	-5.49	105.21	111.14
1	A	343	GLN	N-CA-C	-5.47	106.28	113.12
1	A	90	VAL	N-CA-C	-5.44	104.06	110.21
2	B	434	ILE	N-CA-C	-5.43	105.32	110.42
1	A	233	GLU	N-CA-C	-5.29	99.89	108.52
1	A	368	LEU	N-CA-C	-5.27	105.43	111.07
1	A	216	THR	CB-CA-C	5.24	117.10	109.08
2	B	51	GLY	CA-C-N	5.22	125.68	120.04
2	B	51	GLY	C-N-CA	5.22	125.68	120.04
2	B	147	ASN	N-CA-C	-5.18	107.34	113.97
1	A	118	VAL	N-CA-C	5.16	113.07	108.63
2	B	361	HIS	N-CA-C	5.16	121.79	110.80
1	A	397	THR	N-CA-C	-5.15	105.56	111.07
1	A	115	TYR	N-CA-C	-5.12	105.59	111.07
2	B	115	TYR	N-CA-C	5.06	117.46	111.33
1	A	371	ALA	N-CA-C	-5.03	105.70	111.14
2	B	390	LYS	N-CA-C	-5.03	99.09	107.99
2	B	42	GLU	N-CA-C	-5.02	105.71	111.14

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	4389	0	4429	224	0
2	B	3428	0	3455	118	0
3	A	5	0	0	0	0
4	A	23	0	18	14	0
5	A	5	0	0	1	0
All	All	7850	0	7902	337	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 (337) 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:103:LYS:HG3	4:A:999:UC4:CF	1.90	1.00
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.45	0.97
1:A:103:LYS:HG3	4:A:999:UC4:HF1	1.48	0.95
1:A:114:ALA:HB3	1:A:160:PHE:HE2	1.34	0.92
1:A:9:PRO:HG2	2:B:53:GLU:HG3	1.52	0.90
1:A:188:TYR:O	4:A:999:UC4:HE2	1.74	0.87
1:A:216:THR:HG23	1:A:217:PRO:HD2	1.57	0.87
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.13	0.83
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.62	0.80
1:A:103:LYS:HG3	4:A:999:UC4:HF3	1.64	0.78
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.64	0.78
1:A:50:ILE:HG12	1:A:51:GLY:H	1.47	0.76
1:A:114:ALA:HB3	1:A:160:PHE:CE2	2.20	0.76
1:A:241:VAL:HB	1:A:314:VAL:HG23	1.68	0.76
1:A:448:ARG:HE	1:A:474:ASN:H	1.35	0.75
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.69	0.74
1:A:106:VAL:HG22	4:A:999:UC4:HF2	1.71	0.73
2:B:84:THR:HB	2:B:154:LYS:HE2	1.71	0.73
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.24	0.72
1:A:257:ILE:O	1:A:261:VAL:HG23	1.89	0.71
2:B:353:LYS:NZ	2:B:355:ALA:HB2	2.05	0.71
1:A:340:GLN:CB	1:A:351:THR:HG22	2.21	0.70
2:B:56:TYR:HE2	2:B:126:LYS:HE2	1.56	0.70
1:A:326:ILE:HG12	1:A:388:LYS:HE2	1.74	0.69
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.28	0.69
2:B:74:LEU:HD12	2:B:75:VAL:N	2.07	0.69
1:A:238:LYS:HB2	1:A:316:GLY:O	1.93	0.69
2:B:74:LEU:HD12	2:B:75:VAL:H	1.57	0.69
1:A:65:LYS:HG2	1:A:66:LYS:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:HD13	1:A:94:ILE:H	1.59	0.68
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.76	0.67
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.76	0.67
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.75	0.67
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.77	0.67
1:A:41:MET:HE2	1:A:46:LYS:HZ1	1.61	0.66
1:A:103:LYS:CG	4:A:999:UC4:HF1	2.24	0.66
1:A:448:ARG:HH21	1:A:475:GLN:H	1.44	0.65
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.77	0.65
1:A:433:PRO:HG3	1:A:532:TYR:CE2	2.32	0.64
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.78	0.64
1:A:216:THR:CG2	1:A:217:PRO:HD2	2.26	0.64
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.32	0.64
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.80	0.64
1:A:479:LEU:HA	1:A:482:ILE:HD12	1.78	0.64
1:A:135:ILE:O	1:A:138:GLU:HG3	1.97	0.63
1:A:330:GLN:HB2	1:A:338:THR:OG1	1.99	0.63
1:A:522:ILE:HA	1:A:525:LEU:HD12	1.81	0.63
1:A:332:GLN:O	1:A:336:GLN:HB2	1.98	0.63
1:A:227:PHE:HD2	4:A:999:UC4:CL	2.19	0.63
1:A:253:THR:O	1:A:257:ILE:HG13	1.98	0.63
2:B:279:LEU:HA	2:B:282:LEU:HD12	1.81	0.63
1:A:129:ALA:HB1	1:A:143:ARG:HH12	1.63	0.62
2:B:202:ILE:O	2:B:205:LEU:HB3	2.00	0.62
1:A:190:GLY:HA3	4:A:999:UC4:HF3	1.82	0.62
2:B:163:SER:O	2:B:167:ILE:HG23	1.99	0.62
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.33	0.61
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.81	0.61
2:B:118:VAL:HB	2:B:149:LEU:HG	1.82	0.61
1:A:431:LYS:HA	1:A:431:LYS:HE3	1.83	0.60
2:B:305:GLU:O	2:B:309:ILE:HG13	2.01	0.60
1:A:522:ILE:O	1:A:526:ILE:HG13	2.01	0.60
1:A:181:TYR:HB3	1:A:188:TYR:HB2	1.83	0.60
1:A:206:ARG:HG2	1:A:216:THR:HG21	1.84	0.60
2:B:107:THR:HA	2:B:232:TYR:O	2.02	0.59
1:A:41:MET:HE2	1:A:46:LYS:NZ	2.18	0.59
2:B:27:THR:O	2:B:31:ILE:HG13	2.01	0.59
1:A:378:GLU:O	1:A:382:ILE:HG12	2.03	0.59
2:B:426:TRP:O	2:B:429:LEU:HB2	2.01	0.59
1:A:244:ILE:HD11	1:A:263:LYS:HB3	1.85	0.58
1:A:516:GLU:O	1:A:519:ASN:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:SER:CB	2:B:387:PRO:HD3	2.33	0.58
1:A:34:LEU:HD21	1:A:73:LYS:HB2	1.85	0.58
1:A:169:GLU:O	1:A:173:LYS:HD3	2.03	0.58
1:A:169:GLU:HG2	1:A:173:LYS:CD	2.34	0.58
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.03	0.58
1:A:448:ARG:NE	1:A:474:ASN:H	1.99	0.58
1:A:515:SER:OG	1:A:518:VAL:HG23	2.04	0.58
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.39	0.58
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.39	0.57
1:A:278:GLN:O	1:A:282:LEU:HD13	2.03	0.57
1:A:182:GLN:HG2	1:A:187:LEU:CD2	2.34	0.57
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.86	0.57
1:A:280:CSD:HA	1:A:283:LEU:HD22	1.85	0.57
2:B:56:TYR:CE2	2:B:126:LYS:HE2	2.37	0.57
2:B:245:VAL:HG13	2:B:431:LYS:HB2	1.87	0.56
1:A:328:GLU:O	1:A:339:TYR:HA	2.05	0.56
1:A:90:VAL:HG12	1:A:158:ALA:HB2	1.87	0.56
1:A:108:VAL:HG11	1:A:223:LYS:HB2	1.87	0.56
2:B:353:LYS:HZ2	2:B:355:ALA:HB2	1.69	0.56
2:B:319:TYR:CE2	2:B:321:PRO:HG3	2.41	0.56
1:A:380:ILE:HD11	1:A:386:THR:CG2	2.29	0.56
1:A:448:ARG:NH2	1:A:475:GLN:H	2.04	0.56
1:A:175:ASN:HB2	1:A:178:ILE:HD13	1.88	0.55
1:A:241:VAL:HG11	1:A:270:ILE:HD13	1.87	0.55
1:A:177:ASP:O	1:A:178:ILE:HD12	2.06	0.55
1:A:366:LYS:O	1:A:369:THR:HB	2.06	0.55
1:A:65:LYS:O	1:A:69:THR:HA	2.06	0.55
1:A:188:TYR:CD2	4:A:999:UC4:H102	2.41	0.55
2:B:366:LYS:HG3	2:B:405:TYR:CD1	2.42	0.54
1:A:50:ILE:HG12	1:A:51:GLY:N	2.20	0.54
1:A:106:VAL:HG22	4:A:999:UC4:CF	2.37	0.54
2:B:235:HIS:O	2:B:238:LYS:HG2	2.07	0.54
1:A:491:LEU:HG	1:A:529:GLU:HG3	1.89	0.54
2:B:353:LYS:HZ1	2:B:355:ALA:HB2	1.73	0.54
1:A:254:VAL:O	1:A:258:GLN:HG3	2.08	0.54
2:B:376:THR:CG2	2:B:386:THR:HG22	2.38	0.54
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.43	0.54
1:A:410:TRP:CZ2	1:A:412:PRO:HA	2.42	0.54
1:A:420:PRO:HA	1:A:421:PRO:C	2.31	0.53
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.22	0.53
1:A:205:LEU:O	1:A:208:HIS:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ASP:C	1:A:178:ILE:HD12	2.33	0.53
1:A:114:ALA:HA	1:A:117:SER:OG	2.09	0.53
1:A:116:PHE:CE2	1:A:146:TYR:HE2	2.26	0.53
2:B:113:ASP:HB2	2:B:214:LEU:HD23	1.90	0.53
1:A:149:LEU:HD21	1:A:159:ILE:HG22	1.90	0.53
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.09	0.53
1:A:178:ILE:HD11	1:A:193:LEU:HD11	1.90	0.53
1:A:206:ARG:O	1:A:210:LEU:HD23	2.08	0.53
1:A:335:GLY:HA3	1:A:356:ARG:HD2	1.90	0.53
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.91	0.53
1:A:241:VAL:HB	1:A:314:VAL:CG2	2.37	0.53
1:A:106:VAL:CG2	4:A:999:UC4:HF2	2.38	0.53
1:A:507:GLN:OE1	2:B:421:PRO:HG3	2.08	0.53
2:B:379:SER:OG	2:B:387:PRO:HD3	2.08	0.53
1:A:208:HIS:O	1:A:211:ARG:HB2	2.09	0.52
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.89	0.52
2:B:29:GLU:CG	2:B:30:LYS:N	2.72	0.52
2:B:234:LEU:HD12	2:B:234:LEU:H	1.73	0.52
2:B:332:GLN:NE2	2:B:424:LYS:HE2	2.23	0.52
1:A:64:LYS:H	1:A:64:LYS:HD2	1.74	0.52
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.44	0.52
1:A:240:THR:HG22	1:A:315:HIS:CG	2.44	0.52
2:B:78:ARG:O	2:B:82:LYS:HG3	2.09	0.52
1:A:331:LYS:CE	1:A:334:GLN:HA	2.39	0.52
1:A:502:ALA:O	1:A:506:ILE:HG13	2.09	0.52
1:A:108:VAL:CG1	1:A:223:LYS:HB2	2.40	0.52
1:A:122:GLU:H	1:A:122:GLU:CD	2.17	0.52
1:A:268:SER:HB3	1:A:353:LYS:HE2	1.92	0.52
1:A:22:LYS:H	1:A:22:LYS:HD3	1.75	0.51
1:A:454:LYS:HA	1:A:467:VAL:O	2.11	0.51
1:A:149:LEU:HD21	1:A:159:ILE:CG2	2.41	0.51
1:A:149:LEU:HG	1:A:156:SER:HA	1.93	0.51
2:B:13:LYS:HE3	2:B:84:THR:O	2.10	0.51
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.92	0.51
1:A:139:THR:HB	1:A:140:PRO:HD2	1.92	0.51
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.46	0.51
2:B:33:ALA:O	2:B:37:ILE:HG13	2.11	0.51
1:A:233:GLU:HG3	1:A:242:GLN:HG2	1.93	0.50
1:A:8:VAL:O	1:A:121:ASP:HB2	2.11	0.50
1:A:340:GLN:HB2	1:A:351:THR:HG22	1.91	0.50
1:A:134:SER:OG	1:A:138:GLU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HD22	1:A:83:ARG:O	2.12	0.50
1:A:14:PRO:O	1:A:16:MET:HG3	2.10	0.50
1:A:68:SER:C	1:A:70:LYS:N	2.69	0.50
1:A:475:GLN:HA	1:A:478:GLU:OE2	2.11	0.50
2:B:244:ILE:HG23	2:B:429:LEU:HB3	1.94	0.50
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.93	0.50
1:A:517:LEU:O	1:A:521:ILE:HG13	2.12	0.50
1:A:518:VAL:O	1:A:522:ILE:HG13	2.12	0.50
2:B:31:ILE:O	2:B:35:VAL:HG23	2.12	0.49
1:A:68:SER:C	1:A:70:LYS:H	2.18	0.49
1:A:302:GLU:HA	1:A:305:GLU:OE1	2.12	0.49
1:A:46:LYS:HE2	1:A:116:PHE:HB3	1.94	0.49
1:A:169:GLU:HG2	1:A:173:LYS:HD3	1.94	0.49
1:A:518:VAL:HA	1:A:521:ILE:HD12	1.94	0.49
2:B:369:THR:O	2:B:373:GLN:HG3	2.13	0.49
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.94	0.49
1:A:100:LEU:HD11	4:A:999:UC4:H93	1.95	0.49
1:A:442:VAL:HG22	1:A:496:VAL:O	2.13	0.49
1:A:475:GLN:HG3	1:A:476:LYS:N	2.28	0.49
1:A:521:ILE:O	1:A:525:LEU:HG	2.13	0.49
2:B:205:LEU:O	2:B:208:HIS:HB3	2.11	0.49
2:B:433:PRO:HB2	2:B:436:GLY:HA2	1.94	0.49
1:A:109:LEU:HG	1:A:216:THR:HG23	1.92	0.49
1:A:79:GLU:HA	1:A:82:LYS:HG2	1.94	0.49
1:A:206:ARG:HE	1:A:216:THR:CG2	2.26	0.49
2:B:50:ILE:HG21	2:B:145:GLN:HB3	1.95	0.48
1:A:65:LYS:HB2	1:A:72:ARG:HD2	1.95	0.48
1:A:427:TYR:O	1:A:428:GLN:HG3	2.13	0.48
2:B:395:LYS:O	2:B:399:GLU:HG3	2.13	0.48
1:A:325:LEU:HD11	1:A:383:TRP:CE3	2.48	0.48
1:A:207:GLN:O	1:A:210:LEU:HB2	2.14	0.48
1:A:11:LYS:O	1:A:85:GLN:HB3	2.14	0.48
2:B:254:VAL:O	2:B:258:GLN:HG3	2.13	0.48
1:A:228:LEU:HD22	1:A:242:GLN:CD	2.39	0.48
1:A:293:ILE:N	1:A:293:ILE:HD12	2.29	0.48
1:A:118:VAL:HB	1:A:149:LEU:HD22	1.95	0.48
1:A:325:LEU:HD11	1:A:383:TRP:CD2	2.49	0.48
2:B:205:LEU:HD13	2:B:205:LEU:C	2.39	0.48
2:B:29:GLU:HG3	2:B:30:LYS:N	2.30	0.47
1:A:486:LEU:O	1:A:528:LYS:NZ	2.46	0.47
2:B:130:PHE:CE1	2:B:144:TYR:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASN:HA	1:A:129:ALA:O	2.15	0.47
1:A:475:GLN:HG3	1:A:476:LYS:H	1.78	0.47
2:B:120:LEU:HB2	2:B:148:VAL:O	2.14	0.47
1:A:65:LYS:HD3	1:A:67:ASP:OD2	2.14	0.47
1:A:426:TRP:O	1:A:526:ILE:HG23	2.14	0.47
1:A:519:ASN:O	1:A:522:ILE:HB	2.14	0.47
2:B:160:PHE:O	2:B:164:MET:HB2	2.15	0.47
1:A:34:LEU:CD2	1:A:73:LYS:HB2	2.44	0.47
1:A:362:THR:HB	1:A:363:ASN:H	1.55	0.47
1:A:532:TYR:HE2	1:A:534:ALA:HB2	1.80	0.47
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.95	0.47
1:A:498:ASP:HA	1:A:536:VAL:O	2.15	0.47
1:A:31:ILE:HG12	1:A:133:PRO:HG2	1.97	0.47
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.97	0.47
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.45	0.46
2:B:303:LEU:O	2:B:307:ARG:HG3	2.15	0.46
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.50	0.46
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.97	0.46
1:A:216:THR:HG23	1:A:217:PRO:CD	2.38	0.46
2:B:368:LEU:HD13	2:B:398:TRP:CZ3	2.49	0.46
1:A:253:THR:HA	1:A:291:GLU:O	2.15	0.46
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.51	0.46
1:A:198:HIS:O	1:A:202:ILE:HD13	2.15	0.46
2:B:107:THR:O	2:B:188:TYR:HA	2.16	0.46
2:B:195:ILE:HG23	2:B:196:GLY:N	2.30	0.46
1:A:329:ILE:HA	1:A:338:THR:O	2.16	0.46
1:A:500:GLN:O	1:A:503:LEU:HB3	2.16	0.46
2:B:393:ILE:HG12	2:B:394:GLN:N	2.31	0.46
1:A:216:THR:CG2	1:A:217:PRO:CD	2.94	0.45
2:B:249:LYS:HB3	2:B:251:SER:O	2.16	0.45
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.34	0.45
2:B:169:GLU:O	2:B:173:LYS:HD3	2.15	0.45
2:B:255:ASN:O	2:B:258:GLN:HB2	2.15	0.45
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.98	0.45
1:A:43:LYS:HA	1:A:43:LYS:HD3	1.47	0.45
1:A:274:ILE:O	1:A:275:LYS:HG3	2.17	0.45
2:B:56:TYR:HE2	2:B:126:LYS:CE	2.28	0.45
1:A:197:GLN:O	1:A:200:THR:HB	2.16	0.45
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.52	0.45
1:A:225:PRO:HA	1:A:226:PRO:C	2.41	0.45
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:VAL:HA	2:B:187:LEU:O	2.17	0.45
1:A:22:LYS:H	1:A:22:LYS:CD	2.28	0.45
1:A:517:LEU:O	1:A:520:GLN:HB2	2.16	0.45
2:B:169:GLU:HB2	2:B:170:PRO:CD	2.44	0.45
2:B:232:TYR:HD1	2:B:233:GLU:H	1.65	0.45
1:A:12:LEU:HD23	1:A:12:LEU:HA	1.80	0.44
1:A:14:PRO:O	1:A:16:MET:N	2.51	0.44
1:A:46:LYS:HE2	1:A:116:PHE:CB	2.47	0.44
1:A:110:ASP:HB2	5:A:1002:HOH:O	2.16	0.44
2:B:210:LEU:C	2:B:212:TRP:H	2.24	0.44
4:A:999:UC4:CC	4:A:999:UC4:H6	2.48	0.44
2:B:356:ARG:HH12	2:B:359:GLY:H	1.65	0.44
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.52	0.44
1:A:326:ILE:O	1:A:341:ILE:HA	2.17	0.44
1:A:342:TYR:HA	1:A:349:LEU:HD12	2.00	0.44
1:A:96:HIS:HD2	1:A:98:ALA:HB3	1.82	0.44
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.41	0.44
2:B:53:GLU:O	2:B:55:PRO:HD3	2.18	0.44
2:B:353:LYS:HD2	2:B:354:TYR:N	2.32	0.44
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.53	0.43
2:B:195:ILE:O	2:B:198:HIS:HB3	2.18	0.43
1:A:23:GLN:OE1	1:A:59:PRO:HA	2.19	0.43
1:A:379:SER:CB	1:A:387:PRO:HD3	2.48	0.43
1:A:112:GLY:C	1:A:114:ALA:H	2.27	0.43
1:A:115:TYR:O	1:A:149:LEU:HB2	2.18	0.43
1:A:241:VAL:CB	1:A:314:VAL:HG23	2.44	0.43
2:B:108:VAL:HG22	2:B:188:TYR:HD2	1.83	0.43
2:B:406:TRP:O	2:B:407:GLN:HG3	2.19	0.43
1:A:340:GLN:HA	1:A:351:THR:HA	2.00	0.43
1:A:188:TYR:HB3	4:A:999:UC4:O7	2.19	0.43
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.54	0.43
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.19	0.43
1:A:39:THR:O	1:A:42:GLU:HB3	2.19	0.43
1:A:312:GLU:HG2	1:A:313:PRO:HD2	2.00	0.43
1:A:335:GLY:O	1:A:356:ARG:HA	2.18	0.43
2:B:108:VAL:O	2:B:109:LEU:HD23	2.19	0.43
1:A:19:PRO:HG3	1:A:80:LEU:HB2	2.01	0.43
2:B:168:LEU:O	2:B:169:GLU:C	2.62	0.43
1:A:478:GLU:O	1:A:481:ALA:HB3	2.19	0.42
2:B:54:ASN:O	2:B:143:ARG:NH2	2.51	0.42
2:B:161:GLN:HE22	2:B:182:GLN:HE22	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:LEU:HD12	2:B:234:LEU:N	2.33	0.42
2:B:373:GLN:HG2	2:B:406:TRP:CZ3	2.54	0.42
1:A:244:ILE:HG23	1:A:310:LEU:HD13	2.01	0.42
1:A:380:ILE:O	1:A:384:GLY:HA2	2.20	0.42
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.53	0.42
1:A:77:PHE:O	1:A:78:ARG:C	2.61	0.42
1:A:256:ASP:O	1:A:260:LEU:HB2	2.19	0.42
1:A:484:LEU:HD23	1:A:487:GLN:OE1	2.18	0.42
2:B:266:TRP:CZ2	2:B:423:VAL:HG22	2.54	0.42
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.82	0.42
1:A:175:ASN:HA	1:A:176:PRO:HD2	1.86	0.42
1:A:516:GLU:O	1:A:520:GLN:HG3	2.20	0.42
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.54	0.42
1:A:409:THR:O	2:B:364:ASP:HB2	2.20	0.42
2:B:388:LYS:HE2	2:B:415:GLU:HB3	2.01	0.42
2:B:206:ARG:O	2:B:207:GLN:C	2.63	0.41
2:B:254:VAL:HB	2:B:289:LEU:HA	2.01	0.41
1:A:184:MET:HB3	1:A:185:ASP:H	1.53	0.41
2:B:46:LYS:HE2	2:B:116:PHE:CD2	2.55	0.41
2:B:195:ILE:HG23	2:B:196:GLY:H	1.85	0.41
1:A:376:THR:O	1:A:380:ILE:HG12	2.20	0.41
2:B:136:ASN:HB3	2:B:138:GLU:HG3	2.03	0.41
2:B:376:THR:HG23	2:B:386:THR:HG22	2.02	0.41
1:A:342:TYR:CD1	1:A:342:TYR:N	2.89	0.41
2:B:57:ASN:HA	2:B:129:ALA:O	2.20	0.41
1:A:8:VAL:HG13	1:A:9:PRO:HD2	2.02	0.41
1:A:129:ALA:HB1	1:A:143:ARG:NH1	2.35	0.41
2:B:425:LEU:HD12	2:B:425:LEU:HA	1.93	0.41
2:B:206:ARG:HH11	2:B:206:ARG:HB2	1.86	0.41
2:B:264:LEU:HA	2:B:267:ALA:HB3	2.02	0.41
2:B:270:ILE:O	2:B:272:PRO:HD3	2.21	0.41
2:B:356:ARG:CZ	2:B:361:HIS:HB3	2.51	0.41
1:A:134:SER:HG	1:A:138:GLU:HB2	1.86	0.41
1:A:283:LEU:O	1:A:286:THR:HG23	2.21	0.41
1:A:433:PRO:HA	1:A:532:TYR:CG	2.56	0.41
1:A:507:GLN:CD	2:B:421:PRO:HG3	2.46	0.41
2:B:94:ILE:HD11	2:B:181:TYR:CD1	2.56	0.41
2:B:326:ILE:O	2:B:341:ILE:HA	2.21	0.41
2:B:433:PRO:CB	2:B:436:GLY:HA2	2.51	0.41
1:A:329:ILE:HG22	1:A:330:GLN:N	2.36	0.41
1:A:436:GLY:O	1:A:461:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLN:HE21	1:A:475:GLN:HB2	1.56	0.41
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.85	0.40
2:B:27:THR:HG22	2:B:28:GLU:N	2.36	0.40
1:A:22:LYS:HD3	1:A:22:LYS:N	2.35	0.40
1:A:33:ALA:HB1	1:A:71:TRP:HB3	2.03	0.40
1:A:254:VAL:HG22	1:A:293:ILE:HD13	2.03	0.40
2:B:47:ILE:HG22	2:B:146:TYR:HA	2.03	0.40
2:B:49:LYS:HA	2:B:143:ARG:O	2.20	0.40
1:A:28:GLU:HG3	1:A:29:GLU:N	2.36	0.40
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.94	0.40
1:A:438:GLU:OE2	1:A:461:ARG:HB2	2.22	0.40
1:A:448:ARG:HH21	1:A:475:GLN:N	2.15	0.40
1:A:523:GLU:O	1:A:527:LYS:HG3	2.21	0.40
2:B:53:GLU:CD	2:B:53:GLU:H	2.30	0.40
2:B:78:ARG:HD3	2:B:411:ILE:O	2.21	0.40
2:B:166:LYS:HE3	2:B:166:LYS:HB3	1.98	0.40
1:A:32:LYS:HA	1:A:32:LYS:HD3	1.81	0.40
2:B:99:GLY:HA2	2:B:102:LYS:HE3	2.02	0.40
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.79	0.40
1:A:418:ASN:OD1	1:A:420:PRO:HD3	2.22	0.40
2:B:66:LYS:O	2:B:67:ASP: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	533/560 (95%)	465 (87%)	54 (10%)	14 (3%)	4 23
2	B	409/440 (93%)	375 (92%)	31 (8%)	3 (1%)	18 53
All	All	942/1000 (94%)	840 (89%)	85 (9%)	17 (2%)	6 31

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	14	PRO
1	A	15	GLY
1	A	412	PRO
1	A	112	GLY
1	A	122	GLU
1	A	217	PRO
1	A	230	MET
2	B	195	ILE
2	B	438	GLU
1	A	219	LYS
1	A	361	HIS
1	A	140	PRO
1	A	356	ARG
2	B	213	GLY
1	A	67	ASP
1	A	111	VAL

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	480/499 (96%)	429 (89%)	51 (11%)	6	27
2	B	376/400 (94%)	358 (95%)	18 (5%)	23	57
All	All	856/899 (95%)	787 (92%)	69 (8%)	11	38

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	21	VAL
1	A	22	LYS
1	A	32	LYS
1	A	43	LYS
1	A	48	SER

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Mol	Chain	Res	Type
1	A	73	LYS
1	A	89	GLU
1	A	92	LEU
1	A	94	ILE
1	A	97	PRO
1	A	104	LYS
1	A	111	VAL
1	A	120	LEU
1	A	122	GLU
1	A	139	THR
1	A	140	PRO
1	A	175	ASN
1	A	182	GLN
1	A	184	MET
1	A	205	LEU
1	A	215	THR
1	A	237	ASP
1	A	238	LYS
1	A	250	ASP
1	A	283	LEU
1	A	325	LEU
1	A	338	THR
1	A	340	GLN
1	A	345	PRO
1	A	362	THR
1	A	365	VAL
1	A	368	LEU
1	A	369	THR
1	A	373	GLN
1	A	393	ILE
1	A	396	GLU
1	A	402	TRP
1	A	403	THR
1	A	404	GLU
1	A	423	VAL
1	A	431	LYS
1	A	452	LEU
1	A	474	ASN
1	A	475	GLN
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL

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Mol	Chain	Res	Type
1	A	500	GLN
1	A	515	SER
1	A	517	LEU
2	B	40	GLU
2	B	65	LYS
2	B	68	SER
2	B	73	LYS
2	B	82	LYS
2	B	161	GLN
2	B	164	MET
2	B	174	GLN
2	B	189	VAL
2	B	209	LEU
2	B	238	LYS
2	B	283	LEU
2	B	287	LYS
2	B	303	LEU
2	B	361	HIS
2	B	368	LEU
2	B	425	LEU
2	B	439	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	96	HIS
1	A	242	GLN
1	A	278	GLN
1	A	330	GLN
1	A	340	GLN
1	A	361	HIS
1	A	475	GLN
1	A	500	GLN
1	A	512	GLN
2	B	147	ASN
2	B	161	GLN
2	B	182	GLN
2	B	197	GLN
2	B	235	HIS
2	B	278	GLN
2	B	332	GLN

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Mol	Chain	Res	Type
2	B	334	GLN
2	B	428	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	4,7,8	1.39	1 (25%)	1,8,10	4.16	1 (100%)

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	-	2/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	OD1-SG	2.22	1.49	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	4.16	113.26	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
4	UC4	A	999	-	23,24,24	1.26	3 (13%)	28,33,33	1.06	3 (10%)
3	PO4	A	1000	-	4,4,4	1.80	2 (50%)	6,6,6	0.45	0

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	UC4	A	999	-	-	6/14/27/27	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	UC4	CG-CC	2.78	1.54	1.49
3	A	1000	PO4	P-O4	-2.26	1.48	1.54
4	A	999	UC4	CG-N	2.14	1.40	1.35
4	A	999	UC4	C1-C2	2.14	1.42	1.39
3	A	1000	PO4	P-O2	-2.09	1.48	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	UC4	C1-C2-CL	2.21	124.27	121.01
4	A	999	UC4	C6-C1-C7	-2.15	114.15	118.41
4	A	999	UC4	C5-N-CG	2.05	131.09	127.45

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	999	UC4	C1-C7-O8-C8
4	A	999	UC4	O7-C7-O8-C8
4	A	999	UC4	OG-CG-N-C5
4	A	999	UC4	CC-CG-N-C5
4	A	999	UC4	CB-CC-CG-OG
4	A	999	UC4	CB-CC-CG-N

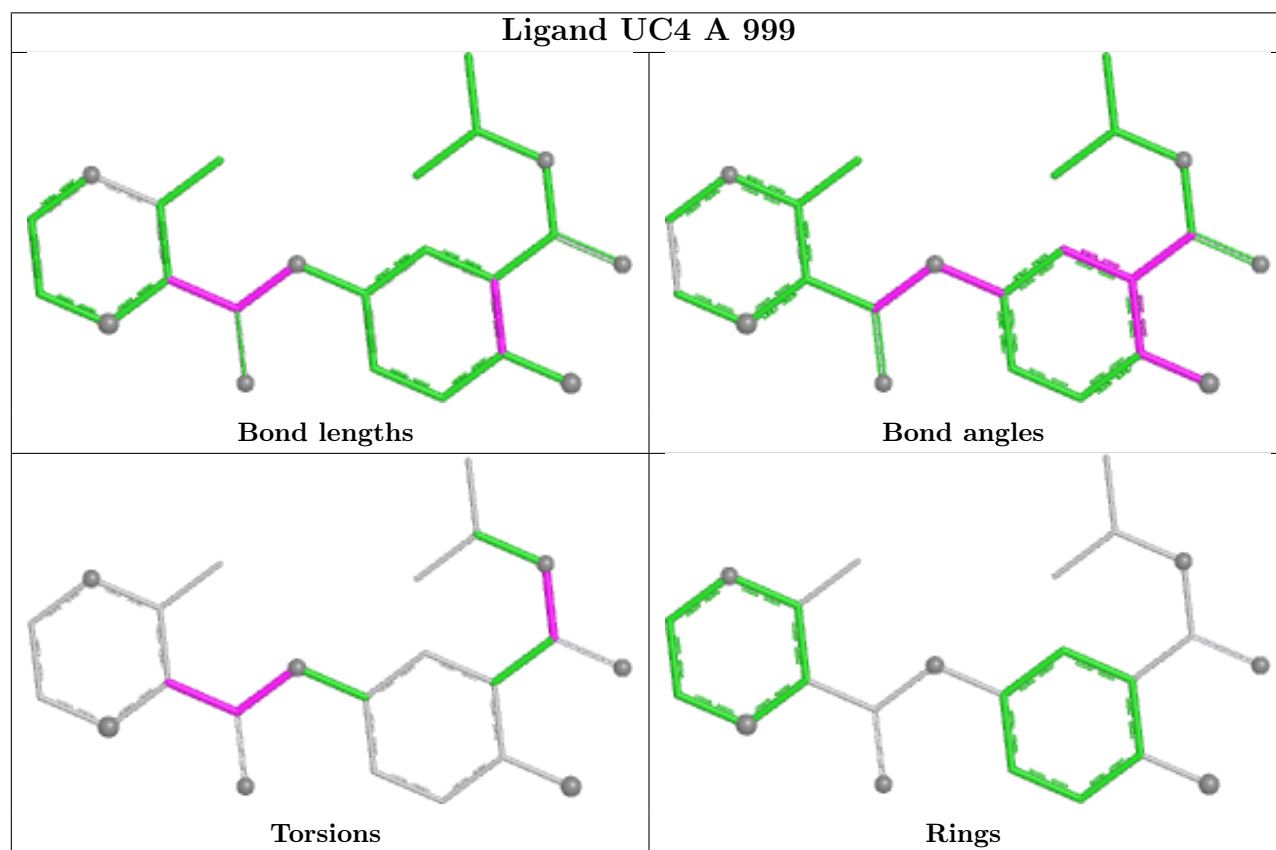
There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	UC4	14	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	535/560 (95%)	0.33	17 (3%) 50 29	3, 49, 115, 151	0
2	B	415/440 (94%)	0.25	9 (2%) 62 39	5, 44, 111, 152	0
All	All	950/1000 (95%)	0.30	26 (2%) 56 33	3, 46, 114, 152	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	435	VAL	4.1
2	B	215	THR	4.0
2	B	232	TYR	3.8
1	A	136	ASN	3.5
2	B	214	LEU	3.1
1	A	244	ILE	3.1
2	B	360	ALA	2.9
1	A	219	LYS	2.8
1	A	357	MET	2.7
1	A	62	ALA	2.6
1	A	245	VAL	2.5
1	A	130	PHE	2.5
1	A	4	PRO	2.5
1	A	68	SER	2.4
2	B	202	ILE	2.3
2	B	178	ILE	2.3
1	A	91	GLN	2.2
1	A	217	PRO	2.2
1	A	469	LEU	2.2
1	A	67	ASP	2.2
2	B	66	LYS	2.1
2	B	177	ASP	2.1
1	A	402	TRP	2.0
1	A	139	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	69	THR	2.0
1	A	214	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	A	280	8/9	0.91	0.09	30,35,42,51	0

6.3 Carbohydrates [i](#)

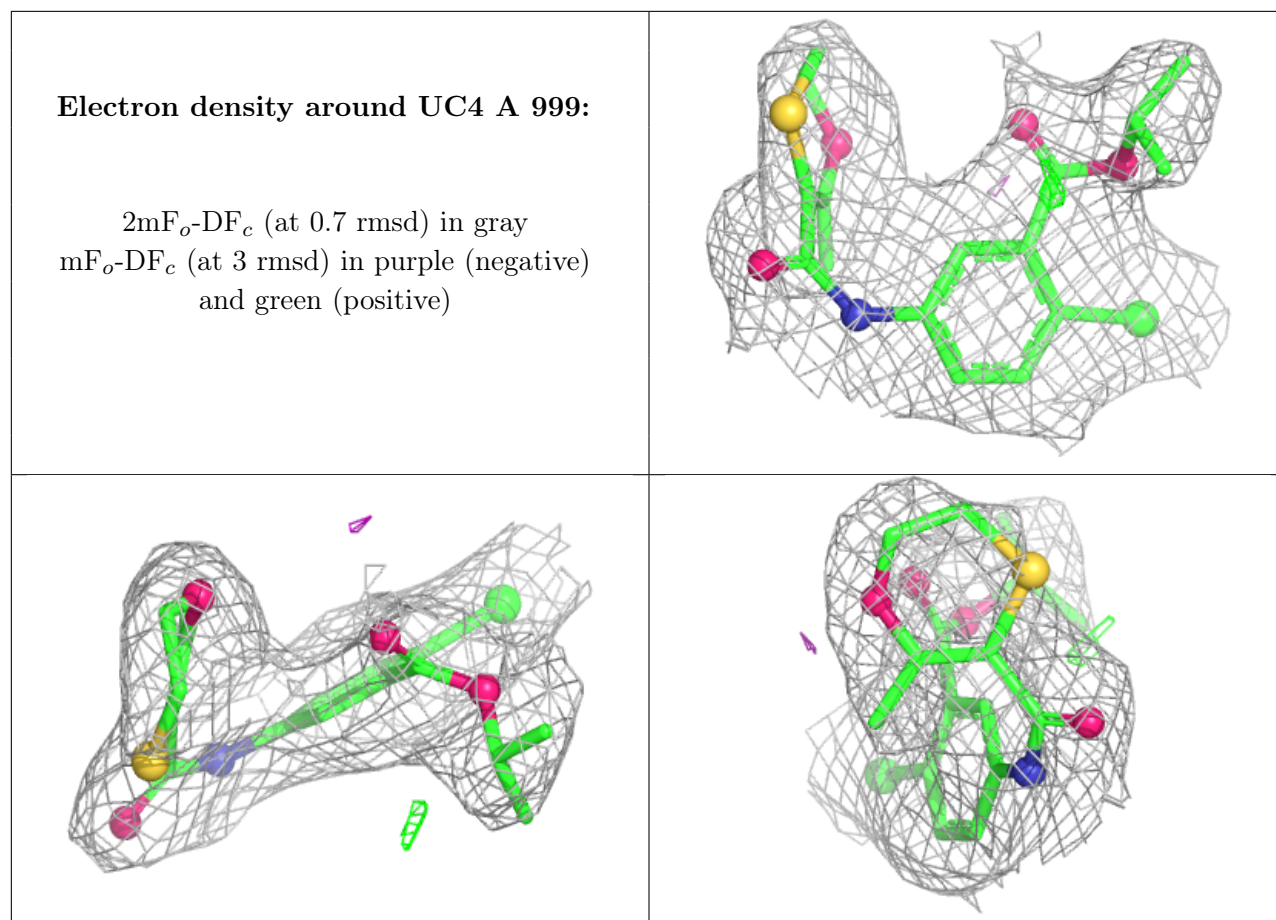
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
3	PO4	A	1000	5/5	0.72	0.25	119,121,125,127	0
4	UC4	A	999	23/23	0.91	0.11	14,26,53,58	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.