WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:32 AM GMT

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PDB ID	:	2XGS
Title	:	XCOGT IN COMPLEX WITH C-UDP
Authors	:	Dorfmueller, H.C.; Borodkin, V.S.; Blair, D.E.; Pathak, S.; Navratilova, I.; Van Aalten, D.M.
Deposited on	:	2010-06-07
Resolution	:	2.39 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
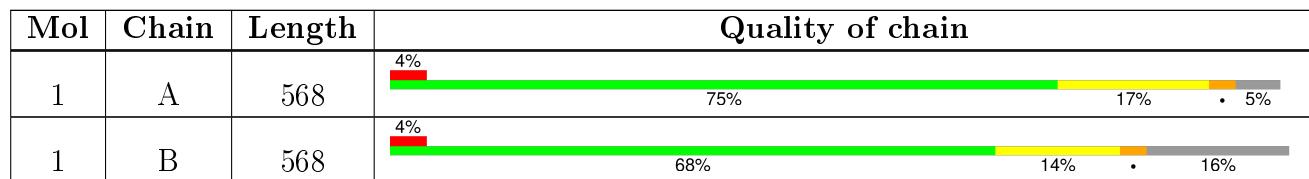
The reported resolution of this entry is 2.39 Å.

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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 <=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	568	4% ... 75% ... 17% · 5%
1	B	568	4% ... 68% ... 14% · 16%

2 Entry composition (i)
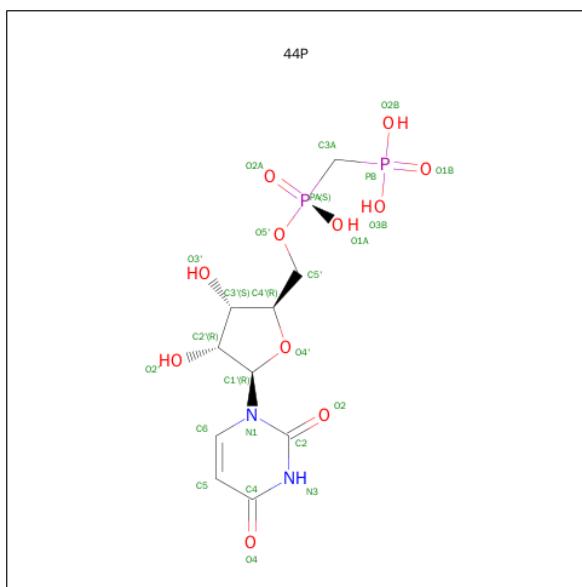
There are 3 unique types of molecules in this entry. The entry contains 7901 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 XCOGT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	542	Total	C	N	O	S	0	0	0
			4117	2598	763	740	16			
1	B	479	Total	C	N	O	S	0	0	0
			3651	2313	673	652	13			

- Molecule 2 is 5'-O-[(S)-HYDROXY(PHOSPHONOMETHYL)PHOSPHORYL]URIDINE (three-letter code: 44P) (formula: $C_{10}H_{16}N_2O_{11}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
2	B	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
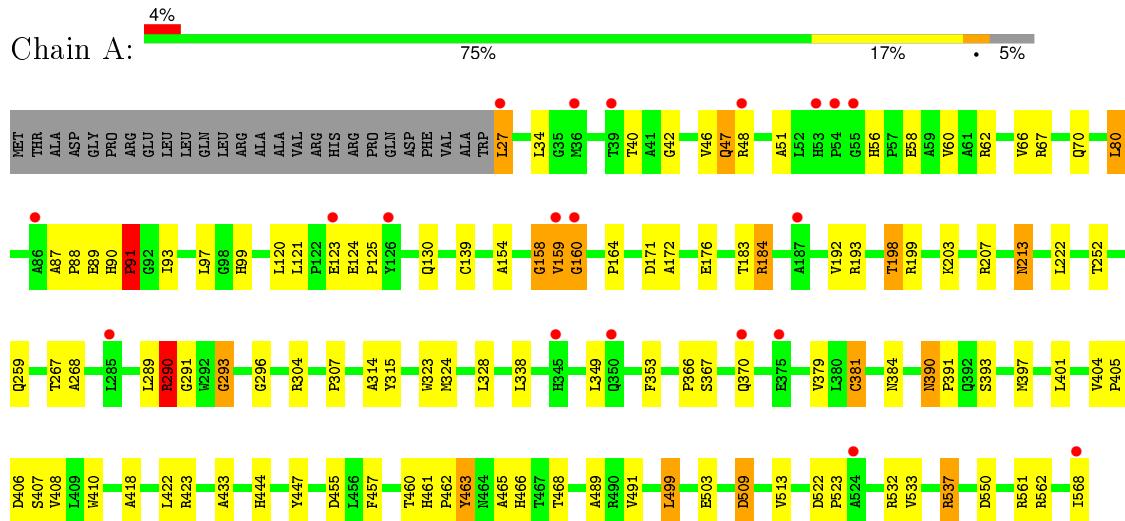
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total 50	O 50	0	0
3	B	33	Total 33	O 33	0	0
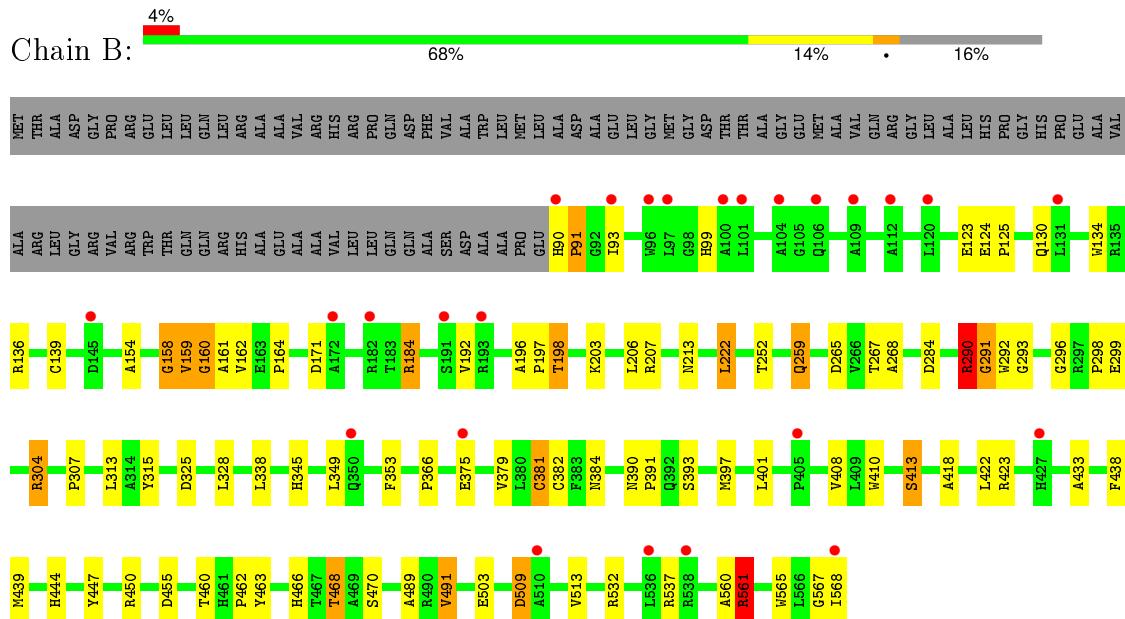
3 Residue-property plots ⓘ

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: XCOGT

Chain A:

- Molecule 1: XCOGT

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.29Å 94.98Å 157.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 2.39 19.86 – 2.39	Depositor EDS
% Data completeness (in resolution range)	92.8 (19.87-2.39) 92.8 (19.86-2.39)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.257 , 0.316 0.255 , 0.310	Depositor DCC
R_{free} test set	965 reflections (2.09%)	DCC
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 26.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Outliers	0 of 47186 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7901	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 44P

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	0.76	0/4223	0.86	10/5761 (0.2%)
1	B	0.81	2/3749 (0.1%)	0.85	9/5117 (0.2%)
All	All	0.78	2/7972 (0.0%)	0.86	19/10878 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	GLY	C-O	-5.79	1.14	1.23
1	B	491	VAL	CB-CG2	-5.59	1.41	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	ASP	CB-CG-OD2	7.77	125.29	118.30
1	A	499	LEU	CA-CB-CG	7.74	133.10	115.30
1	A	293	GLY	N-CA-C	7.55	131.99	113.10
1	B	491	VAL	CG1-CB-CG2	-6.90	99.86	110.90
1	B	561	ARG	NE-CZ-NH2	6.27	123.44	120.30
1	A	509	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	67	ARG	NE-CZ-NH2	6.04	123.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	296	GLY	N-CA-C	5.71	127.36	113.10
1	B	290	ARG	NE-CZ-NH2	5.65	123.13	120.30
1	A	293	GLY	CA-C-N	5.52	127.24	116.20
1	A	290	ARG	N-CA-C	5.39	125.54	111.00
1	A	91	PRO	N-CA-C	5.27	125.80	112.10
1	B	561	ARG	CG-CD-NE	5.22	122.77	111.80
1	B	401	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	401	LEU	CA-CB-CG	5.15	127.15	115.30
1	B	561	ARG	CA-CB-CG	5.14	124.71	113.40
1	B	296	GLY	N-CA-C	5.14	125.94	113.10
1	B	291	GLY	N-CA-C	-5.12	100.29	113.10
1	B	455	ASP	CB-CG-OD2	5.08	122.88	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	VAL	Peptide
1	A	160	GLY	Peptide
1	A	290	ARG	Peptide
1	A	91	PRO	Peptide
1	B	159	VAL	Peptide
1	B	160	GLY	Peptide
1	B	290	ARG	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4117	0	4048	85	3
1	B	3651	0	3589	75	3
2	A	25	0	13	0	0
2	B	25	0	13	1	0
3	A	50	0	0	3	0
3	B	33	0	0	6	0
All	All	7901	0	7663	159	3

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 10.

All (159) 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:562:ARG:NH2	3:A:2048:HOH:O	1.82	1.10
1:A:468:THR:HG22	3:A:2049:HOH:O	1.70	0.90
1:A:164:PRO:HD3	1:A:184:ARG:HD3	1.53	0.90
1:B:164:PRO:HD3	1:B:184:ARG:HD3	1.53	0.87
1:A:125:PRO:C	3:A:2003:HOH:O	2.18	0.82
1:A:561:ARG:HH21	1:A:561:ARG:HG2	1.44	0.80
1:A:465:ALA:HB1	1:A:468:THR:HG23	1.64	0.80
1:B:468:THR:HG23	3:B:2033:HOH:O	1.82	0.80
1:A:466:HIS:CD2	1:A:491:VAL:HG21	2.15	0.79
1:B:468:THR:CG2	3:B:2033:HOH:O	2.33	0.75
1:A:159:VAL:O	1:A:159:VAL:HG12	1.87	0.74
1:B:164:PRO:CD	1:B:184:ARG:HD3	2.17	0.74
1:A:328:LEU:HD11	1:A:349:LEU:HD12	1.69	0.73
1:B:422:LEU:N	1:B:422:LEU:HD12	2.03	0.73
1:A:466:HIS:NE2	1:A:491:VAL:HG21	2.04	0.72
2:B:1569:44P:O3B	3:B:2033:HOH:O	2.07	0.72
1:B:160:GLY:HA2	1:B:162:VAL:H	1.56	0.70
1:B:267:THR:O	1:B:268:ALA:HB3	1.90	0.70
1:B:99:HIS:HE1	1:B:130:GLN:NE2	1.89	0.69
1:B:353:PHE:CE2	1:B:491:VAL:HG12	2.29	0.68
1:A:252:THR:HG22	1:B:252:THR:HA	1.75	0.67
1:A:164:PRO:CD	1:A:184:ARG:HD3	2.25	0.65
1:A:423:ARG:HG2	1:A:433:ALA:HB1	1.78	0.65
1:B:154:ALA:O	1:B:158:GLY:N	2.28	0.65
1:A:42:GLY:O	1:A:46:VAL:HG23	1.96	0.64
1:B:298:PRO:HD2	1:B:299:GLU:OE1	1.97	0.64
1:A:390:ASN:ND2	1:A:393:SER:H	1.95	0.64
1:A:252:THR:HA	1:B:252:THR:HG22	1.79	0.64
1:B:413:SER:HB2	1:B:438:PHE:HB3	1.79	0.64
1:A:154:ALA:O	1:A:158:GLY:CA	2.46	0.63
1:A:213:ASN:ND2	1:A:290:ARG:HD3	2.13	0.63
1:A:561:ARG:NH2	1:A:561:ARG:HG2	2.14	0.63
1:A:154:ALA:O	1:A:158:GLY:N	2.31	0.63
1:A:99:HIS:HE1	1:A:130:GLN:HE21	1.47	0.62
1:A:267:THR:O	1:A:268:ALA:HB3	2.00	0.62
1:B:290:ARG:HB3	1:B:290:ARG:NH2	2.16	0.61
1:B:154:ALA:O	1:B:158:GLY:CA	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ALA:O	1:A:158:GLY:HA2	2.01	0.60
1:B:99:HIS:HE1	1:B:130:GLN:HE21	1.47	0.60
1:A:503:GLU:OE2	1:A:532:ARG:NH1	2.35	0.60
1:A:159:VAL:CG1	1:A:159:VAL:O	2.50	0.59
1:A:90:HIS:HD2	1:A:93:ILE:HG13	1.67	0.59
1:A:393:SER:O	1:A:397:MET:HG3	2.03	0.58
1:A:422:LEU:HD12	1:A:422:LEU:N	2.18	0.58
1:B:328:LEU:HD11	1:B:349:LEU:HD12	1.85	0.58
1:B:466:HIS:CE1	1:B:491:VAL:HG21	2.38	0.58
1:A:353:PHE:CE2	1:A:491:VAL:HG13	2.39	0.57
1:B:158:GLY:HA2	1:B:159:VAL:C	2.25	0.56
1:B:304:ARG:NH2	1:B:325:ASP:OD2	2.35	0.56
1:A:466:HIS:CD2	1:A:491:VAL:CG2	2.86	0.56
1:A:158:GLY:HA2	1:A:159:VAL:C	2.25	0.55
1:A:90:HIS:HD2	1:A:93:ILE:CG1	2.19	0.55
1:A:160:GLY:HA2	1:A:183:THR:HG21	1.88	0.55
1:B:423:ARG:HG2	1:B:433:ALA:HB1	1.88	0.55
1:B:160:GLY:CA	1:B:162:VAL:H	2.19	0.54
1:A:463:TYR:HE2	1:A:466:HIS:CE1	2.26	0.54
1:B:90:HIS:HD2	1:B:93:ILE:CG1	2.20	0.53
1:B:203:LYS:HZ2	1:B:203:LYS:HB3	1.74	0.53
1:A:56:HIS:O	1:A:60:VAL:HG23	2.09	0.53
1:B:466:HIS:CD2	1:B:491:VAL:HG21	2.44	0.52
1:B:222:LEU:HD21	1:B:444:HIS:CE1	2.44	0.52
1:B:136:ARG:O	3:B:2001:HOH:O	2.19	0.52
1:A:47:GLN:HE21	1:A:47:GLN:HA	1.73	0.52
1:A:323:TRP:CD1	1:A:324:MET:HE2	2.43	0.52
1:B:567:GLY:O	1:B:568:ILE:HB	2.09	0.52
1:B:381:CYS:HB2	1:B:410:TRP:HB3	1.92	0.51
1:B:561:ARG:HH21	1:B:561:ARG:HG3	1.74	0.51
1:B:423:ARG:NH2	3:B:2021:HOH:O	2.33	0.51
1:B:90:HIS:HD2	1:B:93:ILE:HG13	1.74	0.51
1:B:328:LEU:HD21	1:B:349:LEU:CD1	2.41	0.51
1:B:462:PRO:O	1:B:489:ALA:HB2	2.12	0.50
1:A:291:GLY:H	1:A:315:TYR:HB2	1.75	0.50
1:A:47:GLN:HE21	1:A:47:GLN:CA	2.24	0.50
1:B:561:ARG:HB2	1:B:565:TRP:O	2.12	0.50
1:A:381:CYS:HB2	1:A:410:TRP:HB3	1.93	0.50
1:A:99:HIS:HE1	1:A:130:GLN:NE2	2.09	0.50
1:B:345:HIS:ND1	3:B:2014:HOH:O	2.35	0.49
1:B:198:THR:HG22	1:B:307:PRO:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:HIS:CG	1:B:491:VAL:HG21	2.48	0.49
1:A:90:HIS:CD2	1:A:93:ILE:HG13	2.47	0.49
1:A:353:PHE:HE2	1:A:491:VAL:HG13	1.78	0.48
1:B:154:ALA:O	1:B:158:GLY:HA2	2.12	0.48
1:A:198:THR:HG22	1:A:307:PRO:HG3	1.95	0.48
1:A:87:ALA:C	1:A:89:GLU:H	2.17	0.48
1:B:291:GLY:H	1:B:315:TYR:HB2	1.78	0.48
1:B:503:GLU:OE2	1:B:532:ARG:NH1	2.47	0.48
1:B:353:PHE:HE2	1:B:491:VAL:HG12	1.76	0.48
1:A:561:ARG:NH2	1:A:561:ARG:CG	2.74	0.48
1:B:203:LYS:NZ	1:B:203:LYS:HB3	2.28	0.48
1:B:206:LEU:HD21	1:B:560:ALA:HB2	1.95	0.48
1:A:466:HIS:NE2	1:A:491:VAL:CG2	2.76	0.48
1:B:290:ARG:CB	1:B:290:ARG:HH21	2.26	0.48
1:B:159:VAL:HG23	1:B:159:VAL:O	2.14	0.48
1:A:384:ASN:ND2	1:A:460:THR:OG1	2.48	0.47
1:A:139:CYS:CB	1:A:422:LEU:HD11	2.45	0.47
1:A:533:VAL:O	1:A:537:ARG:HB2	2.15	0.47
1:A:367:SER:OG	1:A:370:GLN:HG3	2.15	0.47
1:A:62:ARG:O	1:A:66:VAL:HG23	2.15	0.46
1:A:418:ALA:O	1:A:422:LEU:HD13	2.15	0.46
1:A:509:ASP:O	1:A:513:VAL:HG23	2.16	0.46
1:A:289:LEU:O	1:A:314:ALA:HB3	2.16	0.46
1:B:382:CYS:HB2	1:B:397:MET:HE2	1.97	0.46
1:A:463:TYR:CE2	1:A:466:HIS:CE1	3.03	0.46
1:B:422:LEU:N	1:B:422:LEU:CD1	2.76	0.46
1:A:198:THR:CG2	1:A:307:PRO:HG3	2.46	0.45
1:A:47:GLN:NE2	1:A:47:GLN:HA	2.31	0.45
1:B:267:THR:O	1:B:268:ALA:CB	2.55	0.45
1:B:90:HIS:CD2	1:B:93:ILE:HG13	2.52	0.45
1:B:509:ASP:O	1:B:513:VAL:HG23	2.17	0.45
1:A:172:ALA:HB1	1:A:176:GLU:HB2	1.99	0.45
1:B:466:HIS:CE1	1:B:491:VAL:CG2	3.00	0.45
1:B:124:GLU:OE1	1:B:125:PRO:HD2	2.17	0.45
1:A:222:LEU:HD21	1:A:444:HIS:CE1	2.52	0.45
1:A:124:GLU:OE1	1:A:125:PRO:HD2	2.16	0.44
1:A:27:LEU:HD23	1:A:62:ARG:HH11	1.83	0.44
1:B:291:GLY:N	1:B:315:TYR:HB2	2.32	0.44
1:B:284:ASP:O	1:B:307:PRO:HD2	2.17	0.44
1:A:27:LEU:HG	1:A:62:ARG:HE	1.83	0.44
1:B:90:HIS:CD2	1:B:93:ILE:H	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ARG:CB	1:B:290:ARG:NH2	2.81	0.43
1:B:328:LEU:HD21	1:B:349:LEU:HD11	2.00	0.43
1:A:203:LYS:HZ1	1:A:568:ILE:HG21	1.83	0.43
1:B:90:HIS:HA	1:B:91:PRO:HD3	1.77	0.43
1:A:87:ALA:O	1:A:89:GLU:N	2.51	0.43
1:B:390:ASN:HB2	1:B:391:PRO:CD	2.48	0.43
1:B:418:ALA:O	1:B:422:LEU:HD13	2.18	0.43
1:B:139:CYS:CB	1:B:422:LEU:HD11	2.48	0.43
1:B:134:TRP:HA	1:B:134:TRP:CE3	2.53	0.43
1:A:390:ASN:HB2	1:A:391:PRO:CD	2.49	0.43
1:A:90:HIS:CD2	1:A:93:ILE:H	2.36	0.42
1:B:338:LEU:HA	1:B:338:LEU:HD12	1.83	0.42
1:A:291:GLY:N	1:A:315:TYR:HB2	2.34	0.42
1:A:48:ARG:O	1:A:51:ALA:HB3	2.19	0.42
1:A:462:PRO:O	1:A:489:ALA:HB2	2.19	0.42
1:A:338:LEU:HD12	1:A:338:LEU:HA	1.90	0.42
1:B:328:LEU:HD11	1:B:349:LEU:CD1	2.50	0.42
1:A:461:HIS:CG	1:A:462:PRO:HA	2.54	0.42
1:A:404:VAL:HA	1:A:405:PRO:HD3	1.86	0.42
1:A:390:ASN:HB2	1:A:391:PRO:HD2	2.02	0.42
1:A:323:TRP:HD1	1:A:324:MET:HE2	1.83	0.42
1:B:384:ASN:ND2	1:B:460:THR:OG1	2.52	0.42
1:A:353:PHE:CZ	1:A:491:VAL:HG13	2.55	0.42
1:A:466:HIS:CD2	1:A:491:VAL:CB	3.02	0.41
1:B:90:HIS:HD2	1:B:93:ILE:CB	2.33	0.41
1:A:58:GLU:O	1:A:62:ARG:HG3	2.20	0.41
1:A:80:LEU:HB3	1:A:97:LEU:HD13	2.01	0.41
1:A:522:ASP:HA	1:A:523:PRO:HD2	1.92	0.41
1:A:328:LEU:HD21	1:A:349:LEU:HD11	2.02	0.41
1:A:381:CYS:O	1:A:457:PHE:HA	2.21	0.41
1:B:353:PHE:CZ	1:B:491:VAL:HG12	2.56	0.41
1:B:390:ASN:HB2	1:B:391:PRO:HD2	2.02	0.41
1:B:439:MET:SD	1:B:450:ARG:HG3	2.61	0.41
1:B:292:TRP:HB2	1:B:315:TYR:CE1	2.56	0.40
1:B:99:HIS:CE1	1:B:130:GLN:HE21	2.33	0.40
1:A:90:HIS:HA	1:A:91:PRO:HD3	1.82	0.40
1:A:328:LEU:HD21	1:A:349:LEU:CD1	2.51	0.40
1:A:390:ASN:HD22	1:A:390:ASN:C	2.24	0.40
1:B:393:SER:O	1:B:397:MET:HG3	2.22	0.40
1:B:196:ALA:HA	1:B:197:PRO:HD2	1.93	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:NH2	1:B:265:ASP:O[4_455]	1.91	0.29
1:A:193:ARG:NH2	1:B:259:GLN:O[4_455]	2.02	0.18
1:A:550:ASP:OD2	1:B:375:GLU:OE1[4_555]	2.11	0.09

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	540/568 (95%)	515 (95%)	19 (4%)	6 (1%)	17	25
1	B	477/568 (84%)	458 (96%)	14 (3%)	5 (1%)	19	28
All	All	1017/1136 (90%)	973 (96%)	33 (3%)	11 (1%)	17	25

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	GLY
1	A	293	GLY
1	B	158	GLY
1	B	161	ALA
1	A	70	GLN
1	A	91	PRO
1	B	91	PRO
1	B	313	LEU
1	A	88	PRO
1	A	366	PRO
1	B	366	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

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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	408/429 (95%)	381 (93%)	27 (7%)	21	32
1	B	364/429 (85%)	342 (94%)	22 (6%)	24	37
All	All	772/858 (90%)	723 (94%)	49 (6%)	22	35

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	34	LEU
1	A	40	THR
1	A	47	GLN
1	A	80	LEU
1	A	120	LEU
1	A	121	LEU
1	A	123	GLU
1	A	171	ASP
1	A	184	ARG
1	A	192	VAL
1	A	198	THR
1	A	207	ARG
1	A	213	ASN
1	A	259	GLN
1	A	290	ARG
1	A	304	ARG
1	A	379	VAL
1	A	381	CYS
1	A	390	ASN
1	A	406	ASP
1	A	407	SER
1	A	408	VAL
1	A	447	TYR
1	A	463	TYR
1	A	499	LEU
1	A	537	ARG
1	B	123	GLU
1	B	171	ASP
1	B	184	ARG
1	B	192	VAL

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Mol	Chain	Res	Type
1	B	198	THR
1	B	207	ARG
1	B	213	ASN
1	B	222	LEU
1	B	259	GLN
1	B	290	ARG
1	B	304	ARG
1	B	379	VAL
1	B	381	CYS
1	B	408	VAL
1	B	413	SER
1	B	447	TYR
1	B	463	TYR
1	B	468	THR
1	B	470	SER
1	B	509	ASP
1	B	537	ARG
1	B	561	ARG

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

Mol	Chain	Res	Type
1	A	47	GLN
1	A	90	HIS
1	A	99	HIS
1	A	130	GLN
1	A	177	GLN
1	A	213	ASN
1	A	370	GLN
1	A	376	GLN
1	A	390	ASN
1	A	392	GLN
1	B	90	HIS
1	B	99	HIS
1	B	130	GLN
1	B	177	GLN
1	B	213	ASN
1	B	370	GLN
1	B	376	GLN
1	B	392	GLN
1	B	464	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	#$|Z| > 2$
2	44P	A	1569	-	18,26,26	3.30	8 (44%)	26,40,40	2.42	8 (30%)
2	44P	B	1569	-	18,26,26	2.84	7 (38%)	26,40,40	1.85	7 (26%)

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
2	44P	A	1569	-	-	0/12/32/32	0/2/2/2
2	44P	B	1569	-	-	0/12/32/32	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1569	44P	PA-O1A	-3.99	1.46	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1569	44P	PB-O3B	-3.10	1.47	1.54
2	A	1569	44P	PA-O1A	-2.96	1.49	1.56
2	A	1569	44P	PB-O3B	-2.65	1.48	1.54
2	A	1569	44P	PA-O5'	2.13	1.59	1.57
2	B	1569	44P	O4'-C1'	2.69	1.44	1.41
2	B	1569	44P	C6-N1	3.11	1.40	1.35
2	B	1569	44P	C4-N3	3.45	1.39	1.33
2	A	1569	44P	C4-N3	3.49	1.39	1.33
2	B	1569	44P	PA-O5'	3.73	1.61	1.57
2	A	1569	44P	PB-O2B	4.64	1.66	1.54
2	A	1569	44P	C6-N1	5.53	1.43	1.35
2	A	1569	44P	PB-O1B	6.89	1.65	1.50
2	A	1569	44P	O4'-C1'	7.57	1.50	1.41
2	B	1569	44P	PB-O1B	8.21	1.68	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1569	44P	O1B-PB-C3A	-3.92	102.19	111.13
2	B	1569	44P	O4'-C1'-N1	-3.46	100.80	108.08
2	A	1569	44P	O5'-PA-O2A	-3.19	105.49	113.98
2	A	1569	44P	C6-N1-C2	-3.11	116.25	121.28
2	B	1569	44P	O2B-PB-O1B	-3.00	104.72	112.40
2	B	1569	44P	C4'-O4'-C1'	-2.42	107.06	109.72
2	B	1569	44P	O5'-PA-O2A	-2.33	107.79	113.98
2	A	1569	44P	C4'-O4'-C1'	-2.06	107.46	109.72
2	B	1569	44P	O1A-PA-O2A	2.28	117.28	110.12
2	A	1569	44P	C6-C5-C4	2.32	121.62	117.28
2	A	1569	44P	O2B-PB-C3A	2.69	112.93	106.40
2	B	1569	44P	O2A-PA-C3A	3.00	116.56	109.02
2	A	1569	44P	O1A-PA-O2A	3.13	119.96	110.12
2	B	1569	44P	C4-N3-C2	5.51	119.60	114.14
2	A	1569	44P	C4-N3-C2	8.26	122.32	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1569	44P	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	542/568 (95%)	0.18	20 (3%)	45 46	25, 37, 57, 70	0
1	B	479/568 (84%)	0.22	25 (5%)	31 31	25, 36, 53, 65	0
All	All	1021/1136 (89%)	0.20	45 (4%)	38 39	25, 36, 55, 70	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	93	ILE	6.1
1	B	96	TRP	5.3
1	B	104	ALA	5.1
1	B	568	ILE	5.1
1	B	97	LEU	4.1
1	A	123	GLU	3.7
1	B	191	SER	3.5
1	A	524	ALA	3.2
1	B	109	ALA	3.2
1	A	126	TYR	3.2
1	A	375	GLU	3.1
1	B	193	ARG	3.1
1	A	160	GLY	2.9
1	B	90	HIS	2.9
1	B	538	ARG	2.9
1	B	427	HIS	2.8
1	A	350	GLN	2.8
1	A	36	MET	2.7
1	B	172	ALA	2.7
1	B	145	ASP	2.7
1	A	370	GLN	2.7
1	A	39	THR	2.7
1	A	55	GLY	2.6
1	A	568	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	510	ALA	2.5
1	A	345	HIS	2.5
1	A	48	ARG	2.5
1	A	285	LEU	2.5
1	B	536	LEU	2.4
1	A	86	ALA	2.4
1	B	182	ARG	2.4
1	B	405	PRO	2.3
1	A	187	ALA	2.3
1	B	101	LEU	2.3
1	A	53	HIS	2.3
1	B	375	GLU	2.3
1	A	54	PRO	2.2
1	B	120	LEU	2.2
1	B	106	GLN	2.1
1	A	27	LEU	2.1
1	A	159	VAL	2.1
1	B	131	LEU	2.1
1	B	112	ALA	2.0
1	B	100	ALA	2.0
1	B	350	GLN	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, 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
2	44P	A	1569	25/25	0.95	0.15	0.42	20,24,31,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	44P	B	1569	25/25	0.97	0.10	-0.70	30,35,40,42	0

6.5 Other polymers (i)

There are no such residues in this entry.