



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:56 AM EDT

PDB ID : 2XA9 / pdb_00002xa9
Title : Crystal structure of trehalose synthase TreT mutant E326A from *P. horikoshii* in complex with UDPG
Authors : Song, H.-N.; Jung, T.-Y.; Yoon, S.-M.; Lee, S.-B.; Lim, M.-Y.; Woo, E.-J.
Deposited on : 2010-03-30
Resolution : 2.50 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

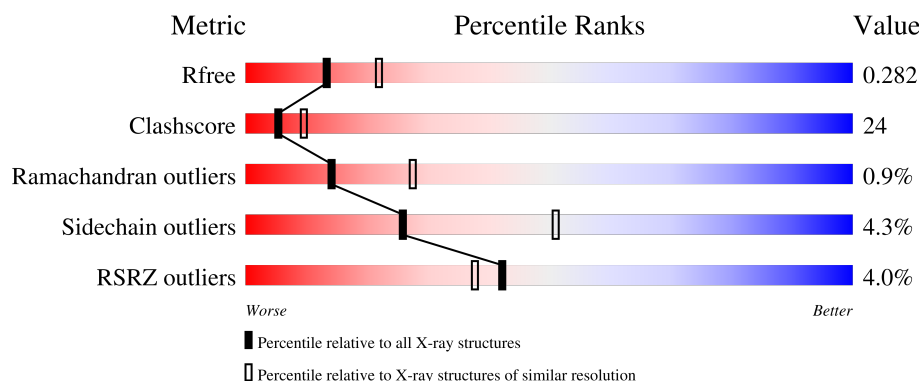
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	416	4% 54% 40% 5%
1	B	416	4% 53% 41%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6954 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.

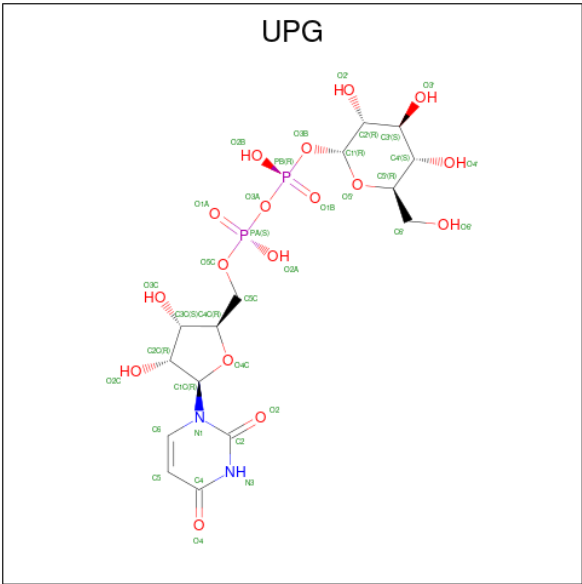
- Molecule 1 is a protein called TREHALOSE-SYNTHASE TRET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	1
			3374	2181	572	612	9			
1	B	413	Total	C	N	O	S	0	0	1
			3374	2181	572	612	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	ALA	GLU	engineered mutation	UNP O58762
A	372	VAL	LYS	conflict	UNP O58762
B	326	ALA	GLU	engineered mutation	UNP O58762
B	372	VAL	LYS	conflict	UNP O58762

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula: C₁₅H₂₄N₂O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total	O	0	0
			72	72		
3	B	62	Total	O	0	0
			62	62		

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.

Chain A:

4% 54% 40% 5%

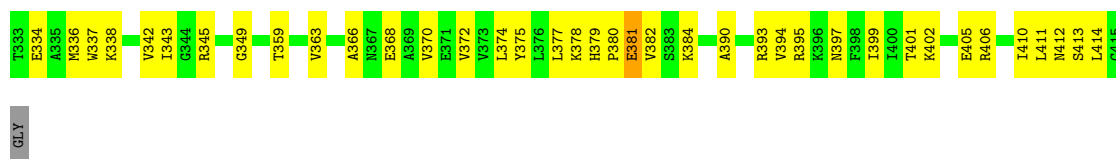
Amino Acid	Category
T331	Green
T332	Green
V353	Green
E334	Green
A335	Green
M336	Green
K337	Green
K338	Green
V342	Green
I343	Green
G344	Green
R345	Green
G349	Green
T359	Green
V363	Green
A366	Green
E368	Green
A369	Green
V370	Green
E371	Green
V372	Green
V373	Green
L374	Green
V375	Green
L376	Green
L377	Green
K378	Green
H379	Green
P380	Green
E381	Green
K384	Green
A390	Green
R393	Green
V394	Green
R395	Green
N397	Green
F398	Green
I399	Green
I400	Green
T401	Green
R406	Green
I410	Green
L411	Green
L414	Green
G415	Green
GLY	Green
S159	Red
I246	Green
F247	Green
I250	Green
E251	Green
I252	Green
V256	Green
V263	Green
Q264	Green
G269	Green
V270	Green
D274	Green
D275	Green
P276	Green
E277	Green
G278	Green
E283	Green
R287	Green
K288	Green
I289	Green
I290	Green
L291	Green
D292	Green
Y293	Green
D294	Green
V295	Green
K296	Green
V297	Green
L298	Green
L301	Green
I302	Green
G303	Green
V304	Green
H305	Green
A306	Green
R307	Green
E308	Green
F312	Green
Q313	Green
R314	Green
L320	Green
Q321	Green
M322	Green
S323	Green
S324	Green
R325	Green
A326	Green
G327	Green
F328	Green
G329	Green
L330	Green
F84	Green
F85	Green
R86	Green
Y87	Green
T88	Green
K89	Green
Q96	Green
G97	Green
L103	Green
T104	Green
M107	Green
L110	Green
Y111	Green
L112	Green
N113	Green
N114	Green
N115	Green
R116	Green
F121	Green
I122	Green
D123	Green
L124	Green
S125	Green
S126	Green
P127	Green
D128	Green
Y129	Green
V130	Green
L131	Green
V132	Green
H133	Green
D134	Green
P135	Green
Q136	Green
P137	Green
A138	Green
A139	Green
L140	Green
I141	Green
E142	Green
F143	Green
Y144	Green
E145	Green
K146	Green
F147	Green
S148	Green
L151	Green
V152	Green
R153	Green
C154	Green
H155	Green
I156	Green
D157	Green
L158	Green
E159	Green
R163	Green
F164	Green
F165	Green
L169	Green
R170	Green
F172	Green
V173	Green
E174	Green
K175	Green
Y179	Green
F181	Green
H182	Green
E185	Green
V186	Green
Y187	Green
Q188	Green
P189	Green
E190	Green
L191	Green
D192	Green
R193	Green
N194	Green
K195	Green
A196	Green
V197	Green
I198	Green
M199	Green
P200	Green
P201	Green
K209	Green
E212	Green
T216	Green
E217	Green
R220	Green
R224	Green
F225	Green
D226	Green
V227	Green
D228	Green
P232	Green
F240	Green
D241	Green
I242	Green
E243	Green
E244	Green
E245	Green
E246	Green
E247	Green
E248	Green
E249	Green
E250	Green
E251	Green
E252	Green
E253	Green
E254	Green
E255	Green
E256	Green
E257	Green
E258	Green
E259	Green
E260	Green
E261	Green
E262	Green
E263	Green
E264	Green
E265	Green
E266	Green
E267	Green
E268	

Chain B:

4%

53%

41%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.84Å 63.14Å 91.52Å 90.00° 98.83° 90.00°	Depositor
Resolution (Å)	29.81 – 2.50 29.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.81-2.50) 97.1 (29.81-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.227 , 0.286 0.223 , 0.282	Depositor DCC
R_{free} test set	1534 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6954	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.42	1/3451 (0.0%)	1.01	17/4658 (0.4%)
1	B	0.43	1/3451 (0.0%)	0.99	19/4658 (0.4%)
All	All	0.43	2/6902 (0.0%)	1.00	36/9316 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	414	LEU	C-N	-5.61	1.25	1.33
1	A	414	LEU	C-N	-5.54	1.25	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	ILE	N-CA-C	-8.82	104.23	111.81
1	B	324	ILE	N-CA-C	-8.71	104.32	111.81
1	A	67	ARG	NE-CZ-NH2	8.53	126.87	119.20
1	A	170	ARG	NE-CZ-NH2	8.17	126.55	119.20
1	A	67	ARG	NE-CZ-NH1	-8.14	113.36	121.50
1	B	116	ARG	NE-CZ-NH2	7.96	126.37	119.20
1	A	294	ASP	N-CA-C	-7.88	103.38	113.16
1	A	135	PRO	N-CA-C	7.83	125.41	113.75
1	A	170	ARG	NE-CZ-NH1	-7.79	113.71	121.50
1	B	294	ASP	N-CA-C	-7.72	103.59	113.16
1	B	116	ARG	NE-CZ-NH1	-7.44	114.06	121.50
1	B	67	ARG	CD-NE-CZ	6.33	133.27	124.40
1	B	67	ARG	NE-CZ-NH2	-6.30	113.53	119.20
1	B	194	ASN	N-CA-C	-6.04	106.04	113.41
1	B	170	ARG	NE-CZ-NH2	-5.98	113.82	119.20
1	B	162	ASN	N-CA-C	-5.93	101.41	110.30
1	A	194	ASN	N-CA-C	-5.89	106.22	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ARG	CD-NE-CZ	5.89	132.64	124.40
1	A	170	ARG	CD-NE-CZ	5.78	132.49	124.40
1	A	241	ASP	CA-C-N	5.77	127.05	119.84
1	A	241	ASP	C-N-CA	5.77	127.05	119.84
1	B	147	LYS	N-CA-C	-5.71	105.23	114.09
1	B	170	ARG	CD-NE-CZ	5.70	132.38	124.40
1	A	116	ARG	NE-CZ-NH2	-5.67	114.09	119.20
1	A	326	ALA	N-CA-C	5.67	117.79	109.24
1	B	116	ARG	CD-NE-CZ	5.59	132.23	124.40
1	B	412	ASN	N-CA-C	-5.59	105.72	112.54
1	B	241	ASP	CA-C-N	5.58	126.82	119.84
1	B	241	ASP	C-N-CA	5.58	126.82	119.84
1	B	326	ALA	N-CA-C	5.58	117.87	109.23
1	A	147	LYS	N-CA-C	-5.38	105.39	113.89
1	B	67	ARG	NE-CZ-NH1	5.37	126.87	121.50
1	A	116	ARG	CD-NE-CZ	5.24	131.73	124.40
1	B	382	VAL	N-CA-C	-5.17	105.35	110.62
1	A	89	LYS	N-CA-C	-5.10	105.80	111.36
1	B	89	LYS	N-CA-C	-5.01	105.90	111.36

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	3374	0	3412	159	0
1	B	3374	0	3412	170	0
2	A	36	0	22	10	0
2	B	36	0	22	16	0
3	A	72	0	0	3	0
3	B	62	0	0	3	0
All	All	6954	0	6868	329	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 24.

All (329) 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:B:209:LYS:HE2	2:B:1415:UPG:O2C	1.33	1.25
1:A:209:LYS:NZ	2:A:1415:UPG:O2C	1.72	1.19
1:B:209:LYS:CE	2:B:1415:UPG:O2C	1.95	1.13
1:B:209:LYS:CE	2:B:1415:UPG:HO2C	1.72	0.98
1:B:269:GLY:HA2	2:B:1415:UPG:O4	1.66	0.95
1:A:305:HIS:H	1:A:308:GLU:HG2	1.28	0.95
1:B:305:HIS:H	1:B:308:GLU:HG2	1.27	0.95
1:B:209:LYS:HE2	2:B:1415:UPG:HO2C	0.81	0.93
1:B:305:HIS:H	1:B:308:GLU:CG	1.86	0.88
1:B:343:ILE:HD13	1:B:372:VAL:HG23	1.54	0.86
1:A:343:ILE:HD13	1:A:372:VAL:HG23	1.54	0.86
1:B:334:GLU:OE2	2:B:1415:UPG:O3C	1.93	0.86
1:A:305:HIS:H	1:A:308:GLU:CG	1.88	0.85
1:A:334:GLU:OE2	2:A:1415:UPG:O3C	1.92	0.84
1:A:269:GLY:HA2	2:A:1415:UPG:O4	1.78	0.83
1:B:304:VAL:HA	1:B:308:GLU:HG3	1.62	0.82
1:B:270:VAL:H	2:B:1415:UPG:C4	1.93	0.81
1:B:25:GLU:HA	1:B:28:VAL:HG12	1.62	0.81
1:A:157:ASP:HA	1:A:186:TYR:CD2	2.15	0.81
1:A:304:VAL:HA	1:A:308:GLU:HG3	1.61	0.81
1:B:157:ASP:HA	1:B:186:TYR:CD2	2.15	0.80
1:A:25:GLU:HA	1:A:28:VAL:HG12	1.64	0.80
1:B:167:GLU:HG2	1:B:170:ARG:HH22	1.47	0.79
1:B:42:SER:HB2	1:B:128:ASP:H	1.48	0.78
1:B:410:ILE:O	1:B:413:SER:HB3	1.84	0.77
1:A:42:SER:HB2	1:A:128:ASP:H	1.50	0.77
1:B:121:PHE:C	1:B:122:ILE:HD12	2.10	0.76
1:A:330:LEU:O	1:A:334:GLU:HG3	1.84	0.76
1:B:330:LEU:O	1:B:334:GLU:HG3	1.85	0.76
1:A:121:PHE:C	1:A:122:ILE:HD12	2.10	0.76
1:B:270:VAL:N	2:B:1415:UPG:O4	2.21	0.74
1:A:384:LYS:NZ	1:A:384:LYS:HB3	2.04	0.73
1:B:151:LEU:HD22	1:B:178:ARG:HB2	1.71	0.72
1:B:384:LYS:HB3	1:B:384:LYS:NZ	2.04	0.72
1:A:320:LEU:HD22	1:A:343:ILE:HB	1.72	0.72
1:A:212:GLU:OE2	1:B:216:THR:HG23	1.88	0.72
1:B:269:GLY:CA	2:B:1415:UPG:O4	2.38	0.72
1:A:5:GLU:OE2	1:A:74:ARG:HD2	1.91	0.71
1:A:123:ASP:OD2	1:A:126:SER:HB3	1.91	0.71
1:A:151:LEU:HD22	1:A:178:ARG:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ASP:OD2	1:B:126:SER:HB3	1.91	0.69
1:B:330:LEU:HB2	2:B:1415:UPG:H5C2	1.75	0.69
1:B:158:LEU:HD12	1:B:181:PHE:HE2	1.57	0.69
1:A:132:VAL:CG1	1:A:137:PRO:HG2	2.22	0.69
1:B:132:VAL:CG1	1:B:137:PRO:HG2	2.23	0.69
1:B:115:ASN:ND2	1:B:139:ALA:HB3	2.08	0.68
1:A:115:ASN:ND2	1:A:139:ALA:HB3	2.08	0.68
1:B:320:LEU:HD22	1:B:343:ILE:HB	1.75	0.68
1:B:325:ARG:HB3	1:B:325:ARG:NH1	2.09	0.68
1:A:63:VAL:HB	1:A:64:PRO:HD3	1.76	0.67
1:A:85:PHE:O	1:A:89:LYS:HG3	1.94	0.67
1:A:158:LEU:HD12	1:A:181:PHE:HE2	1.57	0.67
1:B:33:GLU:O	1:B:36:GLU:HG2	1.94	0.67
1:A:33:GLU:O	1:A:36:GLU:HG2	1.94	0.67
1:B:331:THR:HG23	2:B:1415:UPG:H5C1	1.77	0.67
1:B:393:ARG:HG3	1:B:393:ARG:HH11	1.59	0.67
1:B:85:PHE:O	1:B:89:LYS:HG3	1.95	0.67
1:B:14:ARG:HD2	1:B:19:TYR:OH	1.94	0.66
1:B:63:VAL:HB	1:B:64:PRO:HD3	1.76	0.66
1:A:325:ARG:HB3	1:A:325:ARG:NH1	2.10	0.65
1:B:167:GLU:HG2	1:B:170:ARG:NH2	2.10	0.65
1:B:209:LYS:NZ	2:B:1415:UPG:O2C	2.27	0.65
1:A:393:ARG:HG3	1:A:393:ARG:HH11	1.61	0.64
2:B:1415:UPG:O6'	3:B:2062:HOH:O	2.13	0.64
1:B:216:THR:O	1:B:220:ARG:HG3	1.97	0.64
1:B:9:PHE:CD1	1:B:64:PRO:HG3	2.32	0.64
1:B:305:HIS:N	1:B:308:GLU:HG2	2.08	0.64
1:A:54:GLY:O	1:A:58:ILE:HG12	1.98	0.63
1:A:216:THR:O	1:A:220:ARG:HG3	1.99	0.63
1:B:274:ASP:C	1:B:276:PRO:HD3	2.24	0.63
1:A:199:MET:HE2	1:A:406:ARG:HB3	1.79	0.63
1:B:5:GLU:OE1	1:B:74:ARG:HD2	1.98	0.63
1:A:274:ASP:C	1:A:276:PRO:HD3	2.23	0.63
1:A:228:ASP:H	1:A:264:GLN:HE22	1.46	0.63
1:B:228:ASP:H	1:B:264:GLN:HE22	1.47	0.62
1:A:179:TYR:CE1	1:A:195:LYS:HG3	2.34	0.62
1:B:179:TYR:CE1	1:B:195:LYS:HG3	2.34	0.62
1:B:5:GLU:CD	1:B:74:ARG:HD2	2.24	0.62
1:B:54:GLY:O	1:B:58:ILE:HG12	2.00	0.62
1:B:192:ASP:HB3	1:B:195:LYS:HG2	1.81	0.62
1:A:197:VAL:HG11	1:A:410:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PHE:HA	1:A:88:THR:OG1	2.01	0.61
1:B:125:SER:HB3	1:B:144:TYR:HB3	1.82	0.61
1:A:125:SER:HB3	1:A:144:TYR:HB3	1.82	0.61
1:A:6:VAL:HG13	1:A:7:LYS:N	2.16	0.61
1:B:199:MET:HE2	1:B:406:ARG:HB3	1.83	0.61
1:A:192:ASP:HB3	1:A:195:LYS:HG2	1.81	0.60
1:A:74:ARG:HH21	1:A:127:PHE:HE2	1.50	0.60
1:B:157:ASP:HA	1:B:186:TYR:HD2	1.66	0.60
1:A:83:GLU:O	1:A:87:VAL:HG23	2.02	0.60
1:B:74:ARG:HH21	1:B:127:PHE:HE2	1.50	0.60
1:A:302:ILE:HG23	1:A:302:ILE:O	2.02	0.59
1:B:85:PHE:HA	1:B:88:THR:OG1	2.02	0.59
1:A:136:GLN:HB2	1:A:137:PRO:HD3	1.84	0.59
1:B:25:GLU:HA	1:B:28:VAL:CG1	2.31	0.59
1:A:157:ASP:HA	1:A:186:TYR:HD2	1.66	0.59
1:A:25:GLU:HA	1:A:28:VAL:CG1	2.33	0.59
1:A:324:ILE:HD12	1:A:345:ARG:HD2	1.85	0.59
1:B:83:GLU:O	1:B:87:VAL:HG23	2.03	0.58
1:A:374:LEU:O	1:A:378:LYS:HB2	2.03	0.58
1:A:133:HIS:HD2	1:A:155:HIS:NE2	2.01	0.58
1:B:112:LEU:HD21	1:B:172:PHE:CZ	2.38	0.58
1:A:112:LEU:HD21	1:A:172:PHE:CZ	2.39	0.58
1:B:374:LEU:O	1:B:378:LYS:HB2	2.03	0.58
1:B:324:ILE:HD12	1:B:345:ARG:HD2	1.86	0.58
1:A:183:LEU:HB2	1:A:186:TYR:CE1	2.39	0.58
1:A:116:ARG:HG3	1:A:143:PHE:HE2	1.69	0.57
1:B:133:HIS:HD2	1:B:155:HIS:NE2	2.02	0.57
1:B:136:GLN:HB2	1:B:137:PRO:HD3	1.84	0.57
1:B:132:VAL:HG13	1:B:137:PRO:HG2	1.86	0.57
1:A:320:LEU:CD2	1:A:343:ILE:HB	2.33	0.57
1:B:183:LEU:HB2	1:B:186:TYR:CE1	2.39	0.57
1:A:6:VAL:HG22	1:A:8:GLU:O	2.05	0.57
1:A:46:VAL:HA	1:A:76:PHE:O	2.05	0.57
1:A:283:GLU:O	1:A:287:ARG:HG3	2.04	0.57
1:B:283:GLU:O	1:B:287:ARG:HG3	2.04	0.57
1:A:334:GLU:OE2	2:A:1415:UPG:C3C	2.52	0.57
1:B:302:ILE:HG23	1:B:302:ILE:O	2.03	0.57
1:B:325:ARG:HB3	1:B:325:ARG:HH11	1.69	0.57
1:B:199:MET:HE1	1:B:410:ILE:HD12	1.87	0.56
1:B:320:LEU:CD2	1:B:343:ILE:HB	2.35	0.56
1:B:25:GLU:CA	1:B:28:VAL:HG12	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:THR:HG23	2:A:1415:UPG:H5C1	1.87	0.55
1:B:359:THR:HB	1:B:390:ALA:HB2	1.88	0.55
1:B:46:VAL:HA	1:B:76:PHE:O	2.06	0.55
1:A:325:ARG:HB3	1:A:325:ARG:HH11	1.70	0.55
1:B:289:ILE:HD13	1:B:295:VAL:HG11	1.87	0.55
1:A:132:VAL:HG13	1:A:137:PRO:HG2	1.86	0.55
1:A:134:ASP:HB3	1:A:135:PRO:HD2	1.89	0.55
1:A:328:PHE:O	1:A:349:GLY:HA3	2.07	0.55
1:B:104:THR:OG1	1:B:107:MET:HG3	2.07	0.55
1:B:328:PHE:O	1:B:349:GLY:HA3	2.07	0.54
1:B:366:ALA:O	1:B:370:VAL:HG23	2.07	0.54
1:B:384:LYS:HB3	1:B:384:LYS:HZ3	1.73	0.54
1:A:217:GLU:OE1	1:A:307:ARG:HD3	2.08	0.54
1:B:134:ASP:HB3	1:B:135:PRO:CD	2.38	0.54
1:B:325:ARG:HH11	1:B:325:ARG:CB	2.20	0.54
1:B:110:LEU:O	1:B:114:VAL:HG23	2.08	0.54
1:A:134:ASP:HB3	1:A:135:PRO:CD	2.37	0.54
1:A:25:GLU:CA	1:A:28:VAL:HG12	2.37	0.54
1:B:14:ARG:HB3	1:B:65:LEU:HD13	1.89	0.54
1:A:129:TYR:CD2	1:A:411:LEU:HD22	2.43	0.54
1:A:224:ARG:NE	3:A:2019:HOH:O	2.40	0.54
1:B:217:GLU:OE1	1:B:307:ARG:HD3	2.07	0.54
1:A:359:THR:HB	1:A:390:ALA:HB2	1.90	0.53
1:A:104:THR:OG1	1:A:107:MET:HG3	2.08	0.53
1:A:325:ARG:HH11	1:A:325:ARG:CB	2.21	0.53
1:B:134:ASP:HB3	1:B:135:PRO:HD2	1.90	0.53
1:B:131:LEU:HD21	1:B:153:ARG:HB2	1.91	0.53
1:B:393:ARG:HG3	1:B:393:ARG:NH1	2.24	0.53
1:A:289:ILE:HD13	1:A:295:VAL:HG11	1.91	0.53
1:B:313:GLN:OE1	1:B:338:LYS:HE2	2.08	0.53
1:A:110:LEU:O	1:A:114:VAL:HG23	2.08	0.53
1:A:27:GLU:OE2	1:A:30:LYS:HD3	2.09	0.52
1:A:216:THR:HG23	1:B:212:GLU:OE2	2.09	0.52
1:A:384:LYS:HB3	1:A:384:LYS:HZ3	1.73	0.52
1:A:336:MET:HE1	1:A:393:ARG:HD3	1.91	0.52
1:B:336:MET:HE1	1:B:393:ARG:HD3	1.92	0.52
1:A:366:ALA:O	1:A:370:VAL:HG23	2.10	0.52
1:B:402:LYS:HD2	1:B:405:GLU:OE2	2.09	0.52
1:A:393:ARG:HG3	1:A:393:ARG:NH1	2.25	0.52
1:B:158:LEU:O	1:B:188:GLN:HG2	2.10	0.52
1:B:188:GLN:HA	1:B:188:GLN:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:GLU:HA	1:A:314:ARG:NH2	2.24	0.52
1:A:158:LEU:O	1:A:188:GLN:HG2	2.10	0.52
1:A:313:GLN:OE1	1:A:338:LYS:HE2	2.09	0.52
1:B:224:ARG:NE	3:B:2017:HOH:O	2.38	0.52
1:A:131:LEU:HD21	1:A:153:ARG:HB2	1.91	0.51
1:B:201:PRO:HD2	1:B:328:PHE:CD2	2.46	0.51
1:B:27:GLU:OE2	1:B:30:LYS:HD3	2.10	0.51
1:A:188:GLN:OE1	1:A:188:GLN:HA	2.09	0.51
1:A:9:PHE:CD2	1:A:64:PRO:HG3	2.47	0.50
1:A:170:ARG:HD3	1:A:174:GLU:OE1	2.11	0.50
1:A:159:SER:HB3	1:A:185:GLU:O	2.11	0.50
1:A:4:TYR:CG	1:A:5:GLU:N	2.78	0.50
1:A:16:LEU:HG	1:A:28:VAL:HG23	1.93	0.50
1:A:116:ARG:HG3	1:A:143:PHE:CE2	2.46	0.50
1:B:343:ILE:HD13	1:B:372:VAL:CG2	2.34	0.50
1:B:16:LEU:HG	1:B:28:VAL:HG23	1.92	0.50
1:A:25:GLU:O	1:A:28:VAL:HG12	2.11	0.50
1:B:36:GLU:HG3	1:B:37:LYS:N	2.26	0.49
1:A:141:ILE:HG23	1:A:175:LYS:HD2	1.94	0.49
1:A:145:GLU:O	1:A:147:LYS:HG3	2.12	0.49
1:A:343:ILE:HD13	1:A:372:VAL:CG2	2.33	0.49
1:B:25:GLU:O	1:B:28:VAL:HG12	2.12	0.49
1:A:14:ARG:HD2	1:A:19:TYR:OH	2.12	0.49
1:B:145:GLU:O	1:B:147:LYS:HG3	2.12	0.49
1:A:36:GLU:HG3	1:A:37:LYS:N	2.27	0.49
1:A:192:ASP:HB3	1:A:195:LYS:CG	2.43	0.49
1:A:379:HIS:HB3	1:A:381:GLU:OE1	2.13	0.49
1:A:42:SER:HB2	1:A:128:ASP:N	2.25	0.48
1:A:305:HIS:N	1:A:308:GLU:HG2	2.10	0.48
1:A:399:ILE:HG22	1:A:401:THR:H	1.79	0.48
1:B:399:ILE:HG22	1:B:401:THR:H	1.78	0.48
1:B:129:TYR:CD2	1:B:411:LEU:HD22	2.49	0.48
1:B:289:ILE:HD13	1:B:295:VAL:CG1	2.44	0.48
1:A:232:PRO:HG2	1:A:263:VAL:HA	1.96	0.48
1:B:44:VAL:HG12	1:B:74:ARG:HB3	1.96	0.48
1:A:314:ARG:HG3	1:A:338:LYS:HD3	1.96	0.48
1:B:192:ASP:HB3	1:B:195:LYS:CG	2.43	0.48
1:A:134:ASP:C	1:A:152:TRP:CH2	2.92	0.47
1:A:270:VAL:N	2:A:1415:UPG:O4	2.41	0.47
1:B:379:HIS:HB3	1:B:381:GLU:OE1	2.14	0.47
1:B:112:LEU:HD21	1:B:172:PHE:HZ	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:VAL:HG12	1:A:74:ARG:HB3	1.97	0.47
1:B:232:PRO:HG2	1:B:263:VAL:HA	1.96	0.47
1:B:302:ILE:O	1:B:302:ILE:CG2	2.63	0.47
1:B:159:SER:HB3	1:B:185:GLU:O	2.14	0.47
1:A:302:ILE:O	1:A:302:ILE:CG2	2.62	0.46
1:B:77:VAL:HG12	1:B:78:ILE:N	2.30	0.46
1:B:212:GLU:HA	1:B:314:ARG:NH2	2.30	0.46
1:B:314:ARG:HG3	1:B:338:LYS:HD3	1.97	0.46
1:B:134:ASP:C	1:B:152:TRP:CH2	2.93	0.46
1:B:25:GLU:C	1:B:28:VAL:HG12	2.40	0.46
1:B:189:PRO:C	1:B:191:LEU:H	2.23	0.46
1:B:141:ILE:HG23	1:B:175:LYS:HD2	1.97	0.46
1:A:189:PRO:C	1:A:191:LEU:H	2.23	0.46
1:A:25:GLU:C	1:A:28:VAL:HG12	2.41	0.46
1:A:163:ARG:O	1:A:164:GLU:C	2.59	0.46
1:B:298:LEU:HD13	1:B:312:PHE:CZ	2.50	0.46
1:A:77:VAL:HG12	1:A:78:ILE:N	2.31	0.46
1:A:199:MET:HE2	1:A:406:ARG:CB	2.45	0.46
1:A:42:SER:HB3	1:A:127:PHE:HD2	1.81	0.46
1:A:298:LEU:HD13	1:A:312:PHE:CZ	2.51	0.45
1:B:10:SER:C	1:B:12:GLY:H	2.24	0.45
1:B:252:ILE:O	1:B:256:VAL:HG23	2.15	0.45
1:B:380:PRO:O	1:B:384:LYS:HG3	2.16	0.45
1:A:112:LEU:HD21	1:A:172:PHE:HZ	1.79	0.45
1:B:42:SER:HB2	1:B:128:ASP:N	2.24	0.45
1:B:197:VAL:HG11	1:B:410:ILE:HD11	1.98	0.45
1:A:6:VAL:HG13	1:A:7:LYS:H	1.82	0.45
1:A:134:ASP:O	1:A:152:TRP:HZ3	1.99	0.45
1:B:42:SER:HB3	1:B:127:PHE:HD2	1.82	0.45
1:B:332:VAL:HG13	1:B:342:VAL:HG11	1.99	0.45
1:A:201:PRO:HG2	1:A:328:PHE:CD2	2.52	0.45
1:A:270:VAL:H	2:A:1415:UPG:C4	2.28	0.45
1:A:375:TYR:CE1	1:A:379:HIS:CD2	3.05	0.45
1:B:289:ILE:CD1	1:B:295:VAL:HG11	2.47	0.45
1:B:96:GLN:HE22	2:B:1415:UPG:H6'1	1.82	0.45
1:B:186:TYR:OH	1:B:327:GLY:HA2	2.17	0.45
1:B:375:TYR:CE1	1:B:379:HIS:CD2	3.05	0.44
1:B:199:MET:HE2	1:B:406:ARG:CB	2.46	0.44
1:B:334:GLU:OE2	2:B:1415:UPG:C3C	2.65	0.44
1:A:375:TYR:CD1	1:A:379:HIS:HD2	2.35	0.44
2:A:1415:UPG:H1'	3:A:2072:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLN:HG2	3:B:2023:HOH:O	2.17	0.44
1:B:11:SER:O	1:B:12:GLY:C	2.59	0.44
1:A:287:ARG:HD2	3:A:2040:HOH:O	2.16	0.44
1:B:243:TRP:HB2	1:B:325:ARG:HH12	1.82	0.44
1:B:247:PHE:CD2	1:B:288:LYS:HE3	2.53	0.44
1:B:375:TYR:CD1	1:B:379:HIS:HD2	2.36	0.44
1:A:3:MET:HE1	1:A:124:LEU:HD11	2.00	0.44
1:A:380:PRO:O	1:A:384:LYS:HG3	2.18	0.44
1:B:128:ASP:O	1:B:148:SER:HB2	2.18	0.44
1:A:252:ILE:O	1:A:256:VAL:HG23	2.18	0.44
1:A:289:ILE:HD13	1:A:295:VAL:CG1	2.47	0.44
1:B:45:HIS:ND1	1:B:133:HIS:HE1	2.16	0.44
1:B:116:ARG:HG3	1:B:143:PHE:CE2	2.52	0.44
1:B:199:MET:CE	1:B:410:ILE:HD12	2.47	0.44
1:A:9:PHE:CG	1:A:64:PRO:HG3	2.53	0.43
1:A:189:PRO:C	1:A:191:LEU:N	2.76	0.43
1:A:180:ILE:CG2	1:A:199:MET:HB3	2.49	0.43
1:A:226:ASP:O	1:A:296:LYS:NZ	2.48	0.43
1:B:384:LYS:HB3	1:B:384:LYS:HZ2	1.81	0.43
1:A:134:ASP:O	1:A:152:TRP:CZ3	2.71	0.43
1:A:243:TRP:HB2	1:A:325:ARG:HH12	1.84	0.43
1:A:330:LEU:HB2	2:A:1415:UPG:H5C2	2.01	0.43
1:B:305:HIS:O	1:B:308:GLU:HG2	2.19	0.43
1:B:3:MET:HA	1:B:77:VAL:O	2.19	0.43
1:A:76:PHE:CE2	1:A:122:ILE:HG12	2.54	0.43
1:A:6:VAL:CG1	1:A:7:LYS:N	2.81	0.43
1:A:289:ILE:CD1	1:A:295:VAL:HG11	2.49	0.43
1:B:180:ILE:CG2	1:B:199:MET:HB3	2.49	0.43
1:B:305:HIS:H	1:B:308:GLU:HG3	1.78	0.43
1:A:45:HIS:ND1	1:A:133:HIS:HE1	2.16	0.42
1:A:188:GLN:HA	1:A:189:PRO:HD3	1.94	0.42
1:A:247:PHE:CD2	1:A:288:LYS:HE3	2.54	0.42
1:B:78:ILE:HG13	1:B:137:PRO:HB3	2.01	0.42
1:B:134:ASP:O	1:B:152:TRP:HZ3	2.02	0.42
1:B:270:VAL:H	2:B:1415:UPG:HN3	1.66	0.42
1:A:78:ILE:HG13	1:A:137:PRO:HB3	2.01	0.42
1:B:134:ASP:O	1:B:137:PRO:HD2	2.19	0.42
1:B:179:TYR:HB2	1:B:181:PHE:HE1	1.85	0.42
1:B:76:PHE:CE2	1:B:122:ILE:HG12	2.54	0.42
1:B:113:ASN:O	1:B:116:ARG:N	2.49	0.42
1:A:128:ASP:O	1:A:148:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ASN:O	1:A:116:ARG:N	2.49	0.42
1:A:199:MET:HA	1:A:200:PRO:HD2	1.93	0.42
1:B:134:ASP:CB	1:B:135:PRO:CD	2.98	0.42
1:A:134:ASP:CB	1:A:135:PRO:CD	2.97	0.42
1:A:322:MET:HE1	1:A:363:VAL:CG2	2.50	0.42
1:B:41:ARG:HD2	1:B:129:TYR:HE1	1.85	0.42
1:B:247:PHE:CE2	1:B:288:LYS:HE3	2.55	0.42
1:B:336:MET:HE3	1:B:390:ALA:HB1	2.02	0.42
1:A:334:GLU:OE2	2:A:1415:UPG:O2C	2.37	0.41
1:A:363:VAL:HB	1:A:368:GLU:HB3	2.01	0.41
1:A:240:PHE:O	1:A:278:GLY:HA2	2.20	0.41
1:A:305:HIS:O	1:A:308:GLU:HG2	2.19	0.41
1:A:41:ARG:HD2	1:A:129:TYR:HE1	1.85	0.41
1:A:65:LEU:O	1:A:69:ILE:HG23	2.20	0.41
1:A:246:ILE:O	1:A:250:ILE:HG13	2.21	0.41
1:B:3:MET:HE1	1:B:124:LEU:HD11	2.01	0.41
1:B:286:LEU:HD23	1:B:297:VAL:HG21	2.02	0.41
1:A:96:GLN:OE1	1:A:156:ILE:HB	2.20	0.41
1:B:192:ASP:C	1:B:194:ASN:H	2.29	0.41
1:B:240:PHE:O	1:B:278:GLY:HA2	2.20	0.41
1:B:337:TRP:HB2	1:B:394:VAL:HG11	2.02	0.41
1:B:393:ARG:O	1:B:397:ASN:HB2	2.21	0.41
1:B:65:LEU:O	1:B:69:ILE:HG23	2.21	0.41
1:A:179:TYR:HB2	1:A:181:PHE:HE1	1.86	0.41
1:A:181:PHE:CD1	1:A:187:VAL:HG22	2.56	0.41
1:A:199:MET:HE1	1:A:410:ILE:HD12	2.03	0.41
1:A:292:ASP:OD1	1:A:292:ASP:C	2.63	0.41
1:A:395:ARG:HA	1:A:399:ILE:CG1	2.51	0.41
1:B:122:ILE:HD12	1:B:122:ILE:N	2.35	0.41
1:B:189:PRO:C	1:B:191:LEU:N	2.76	0.41
1:B:296:LYS:HB3	1:B:298:LEU:HD21	2.03	0.41
1:B:363:VAL:HB	1:B:368:GLU:HB3	2.03	0.41
1:A:179:TYR:HE1	1:A:195:LYS:HG3	1.84	0.40
1:B:44:VAL:HA	1:B:74:ARG:O	2.22	0.40
1:B:103:LEU:HB2	1:B:165:PHE:CE1	2.56	0.40
1:A:384:LYS:HB3	1:A:384:LYS:HZ2	1.80	0.40
1:B:153:ARG:NH1	1:B:180:ILE:HG22	2.36	0.40
1:B:322:MET:HE1	1:B:363:VAL:CG2	2.51	0.40
1:B:395:ARG:HA	1:B:399:ILE:CG1	2.51	0.40
1:A:103:LEU:HB2	1:A:165:PHE:CE1	2.56	0.40
1:A:332:VAL:HG13	1:A:342:VAL:HG11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ARG:O	1:A:397:ASN:HB2	2.22	0.40
1:B:14:ARG:NE	1:B:206:LEU:HD12	2.36	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	411/416 (99%)	379 (92%)	29 (7%)	3 (1%)	18	34
1	B	411/416 (99%)	380 (92%)	27 (7%)	4 (1%)	12	24
All	All	822/832 (99%)	759 (92%)	56 (7%)	7 (1%)	14	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ARG
1	B	193	ARG
1	A	134	ASP
1	B	134	ASP
1	B	136	GLN
1	A	137	PRO
1	B	137	PRO

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/372 (100%)	355 (96%)	15 (4%)	27	53
1	B	370/372 (100%)	353 (95%)	17 (5%)	24	48
All	All	740/744 (100%)	708 (96%)	32 (4%)	26	51

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	14	ARG
1	A	65	LEU
1	A	103	LEU
1	A	131	LEU
1	A	163	ARG
1	A	179	TYR
1	A	194	ASN
1	A	301	LEU
1	A	302	ILE
1	A	308	GLU
1	A	324	ILE
1	A	331	THR
1	A	377	LEU
1	A	381	GLU
1	B	14	ARG
1	B	65	LEU
1	B	67	ARG
1	B	103	LEU
1	B	117	GLU
1	B	131	LEU
1	B	163	ARG
1	B	179	TYR
1	B	194	ASN
1	B	209	LYS
1	B	301	LEU
1	B	302	ILE
1	B	308	GLU
1	B	324	ILE
1	B	331	THR
1	B	377	LEU
1	B	381	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	60	HIS
1	A	92	HIS
1	A	113	ASN
1	A	115	ASN
1	A	133	HIS
1	A	182	HIS
1	A	215	GLN
1	A	264	GLN
1	A	379	HIS
1	A	403	HIS
1	B	32	GLN
1	B	98	ASN
1	B	113	ASN
1	B	133	HIS
1	B	182	HIS
1	B	215	GLN
1	B	264	GLN
1	B	305	HIS
1	B	379	HIS
1	B	403	HIS

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 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
2	UPG	A	1415	-	37,38,38	1.10	3 (8%)	55,58,58	2.03	12 (21%)
2	UPG	B	1415	-	37,38,38	0.93	1 (2%)	55,58,58	3.20	17 (30%)

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	UPG	A	1415	-	-	2/23/59/59	0/3/3/3
2	UPG	B	1415	-	-	3/23/59/59	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1415	UPG	PA-O3A	2.93	1.62	1.59
2	A	1415	UPG	PB-O3A	2.34	1.62	1.59
2	A	1415	UPG	O4C-C1C	2.09	1.46	1.42
2	B	1415	UPG	O5'-C1'	2.05	1.47	1.41

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1415	UPG	O3A-PB-O1B	-10.82	78.16	110.70
2	B	1415	UPG	O2B-PB-O3A	-10.20	79.70	107.27
2	B	1415	UPG	O3B-PB-O1B	-9.67	78.91	109.81
2	B	1415	UPG	O2B-PB-O3B	-6.38	80.72	106.70
2	A	1415	UPG	O5C-PA-O1A	-5.94	85.41	108.94
2	B	1415	UPG	O5C-PA-O1A	-5.52	87.05	108.94
2	A	1415	UPG	O2A-PA-O5C	-5.03	84.75	107.57
2	B	1415	UPG	O2A-PA-O5C	-4.75	86.06	107.57
2	B	1415	UPG	C4-N3-C2	-4.67	120.82	126.61
2	A	1415	UPG	C4-N3-C2	-4.53	120.99	126.61
2	A	1415	UPG	O5'-C1'-O3B	-4.50	105.48	111.36
2	B	1415	UPG	O2B-PB-O1B	4.20	132.00	112.44
2	A	1415	UPG	O3B-C1'-C2'	4.15	115.98	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1415	UPG	C5-C4-N3	3.90	120.26	114.80
2	A	1415	UPG	C5-C4-N3	3.80	120.12	114.80
2	A	1415	UPG	N3-C2-N1	3.69	119.70	114.89
2	B	1415	UPG	O2A-PA-O3A	3.69	117.25	107.27
2	B	1415	UPG	N3-C2-N1	3.46	119.39	114.89
2	B	1415	UPG	O4-C4-C5	-3.43	119.25	125.16
2	A	1415	UPG	O2A-PA-O3A	3.37	116.38	107.27
2	B	1415	UPG	O5'-C1'-O3B	-3.23	107.14	111.36
2	A	1415	UPG	O4-C4-C5	-3.22	119.61	125.16
2	A	1415	UPG	O2A-PA-O1A	2.66	124.81	112.44
2	A	1415	UPG	C3C-C2C-C1C	2.48	106.15	101.46
2	B	1415	UPG	O2A-PA-O1A	2.36	123.41	112.44
2	B	1415	UPG	O4C-C4C-C3C	2.34	109.80	105.15
2	B	1415	UPG	C1C-N1-C2	2.32	121.76	117.59
2	A	1415	UPG	O4C-C4C-C3C	2.18	109.49	105.15
2	B	1415	UPG	PB-O3B-C1'	-2.08	112.75	121.21

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1415	UPG	C2'-C1'-O3B-PB
2	A	1415	UPG	O5'-C1'-O3B-PB
2	B	1415	UPG	O5'-C1'-O3B-PB
2	B	1415	UPG	C1'-O3B-PB-O2B
2	B	1415	UPG	PA-O3A-PB-O1B

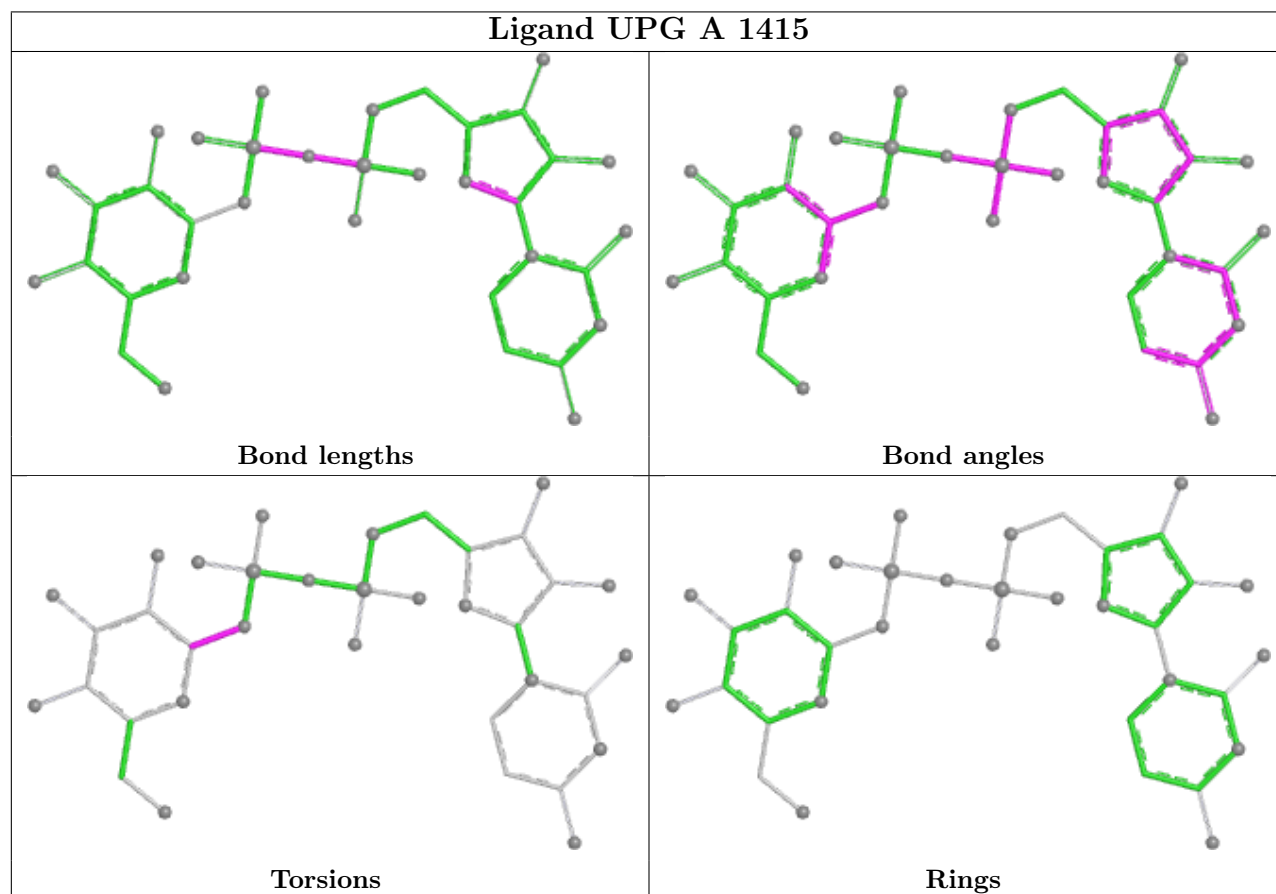
There are no ring outliers.

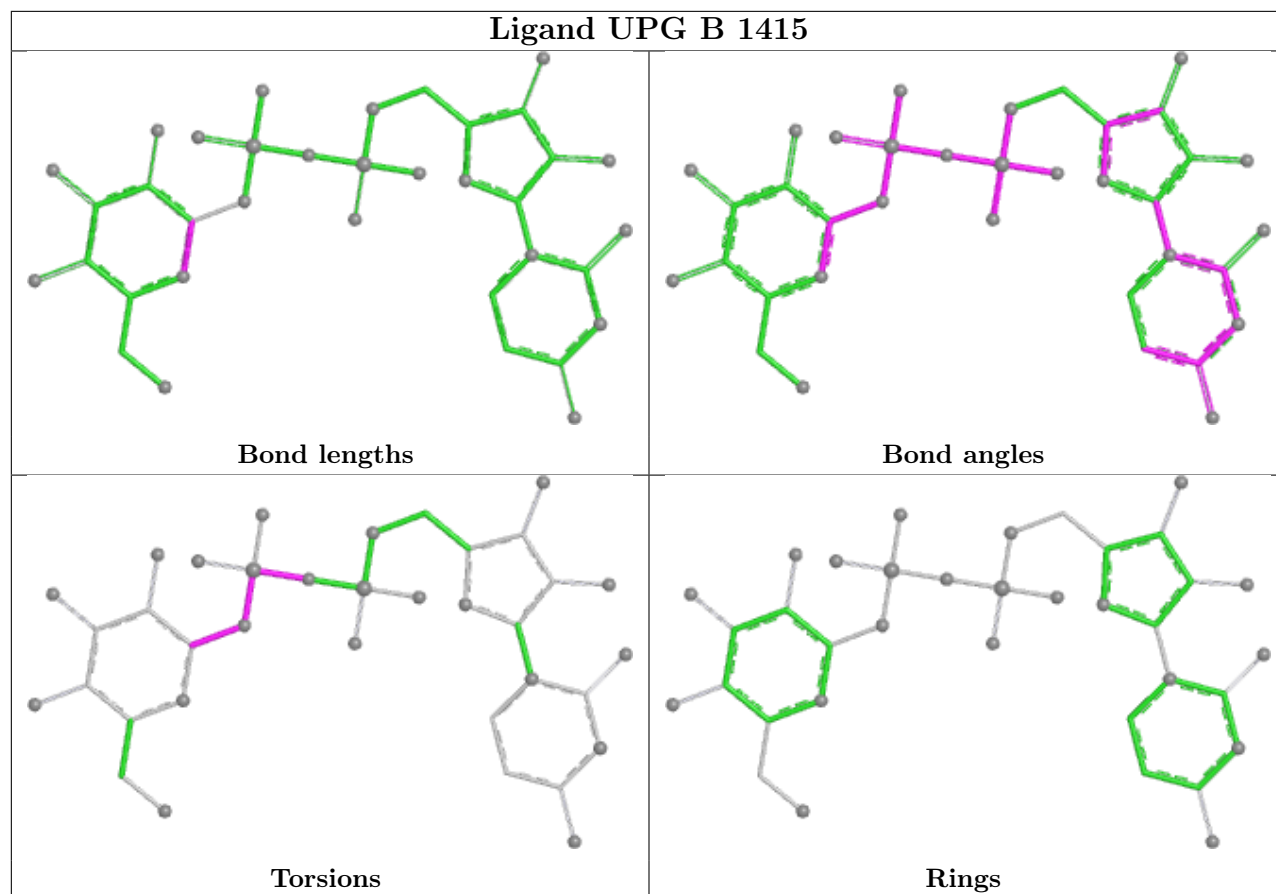
2 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1415	UPG	10	0
2	B	1415	UPG	16	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	413/416 (99%)	0.23	18 (4%) 39 34	6, 37, 81, 100	0
1	B	413/416 (99%)	0.11	15 (3%) 46 41	4, 35, 73, 102	0
All	All	826/832 (99%)	0.17	33 (3%) 42 38	4, 36, 79, 102	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	PHE	4.8
1	A	6	VAL	4.1
1	A	4	TYR	3.9
1	B	121	PHE	3.7
1	A	52	GLY	3.6
1	A	186	TYR	3.4
1	B	70	GLY	3.3
1	B	52	GLY	2.9
1	B	186	TYR	2.9
1	A	159	SER	2.8
1	B	53	GLY	2.8
1	A	12	GLY	2.7
1	A	53	GLY	2.7
1	A	152	TRP	2.6
1	A	72	GLU	2.5
1	A	190	GLU	2.4
1	A	69	ILE	2.4
1	A	97	GLY	2.4
1	B	159	SER	2.4
1	A	54	GLY	2.3
1	A	188	GLN	2.3
1	B	160	SER	2.3
1	B	69	ILE	2.3
1	B	189	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	11	SER	2.3
1	B	12	GLY	2.2
1	A	189	PRO	2.2
1	B	54	GLY	2.2
1	A	187	VAL	2.1
1	A	169	LEU	2.1
1	B	220	ARG	2.1
1	B	78	ILE	2.1
1	B	190	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

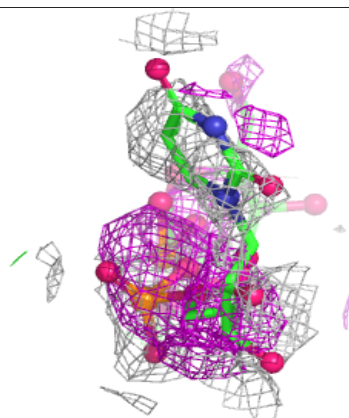
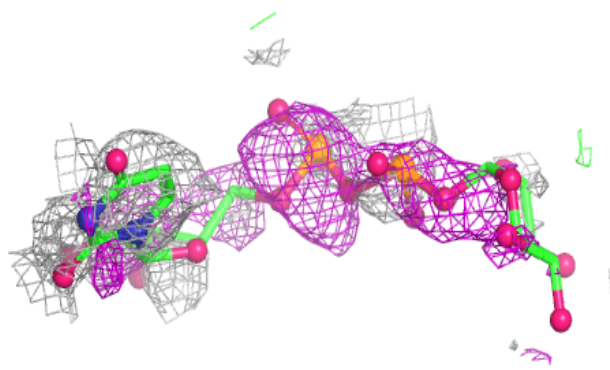
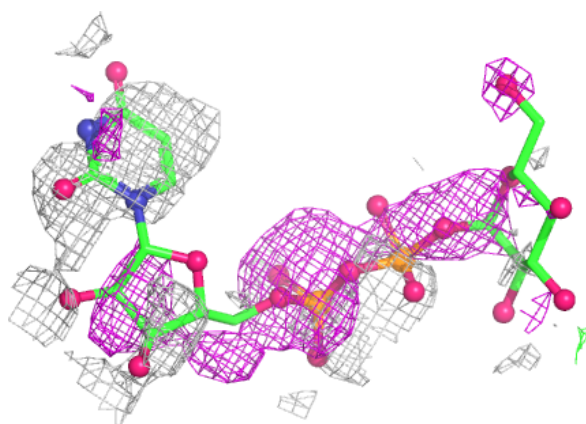
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	UPG	B	1415	36/36	0.44	0.23	67,86,114,119	0
2	UPG	A	1415	36/36	0.53	0.21	59,96,110,112	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.

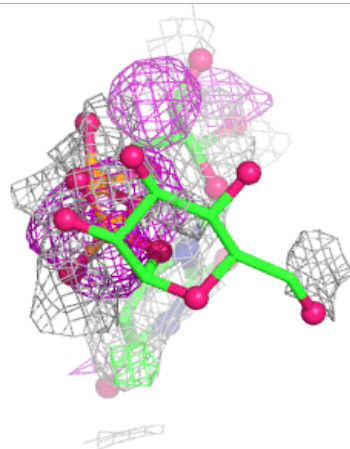
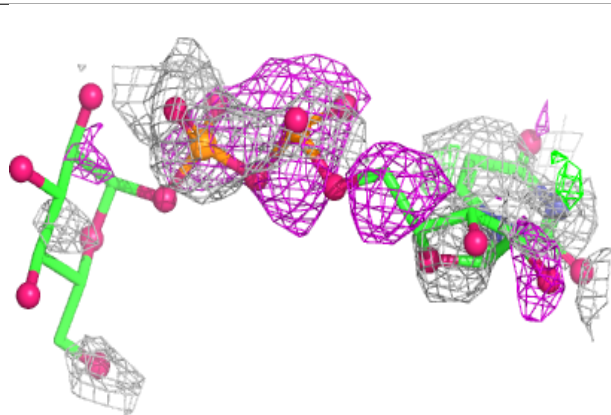
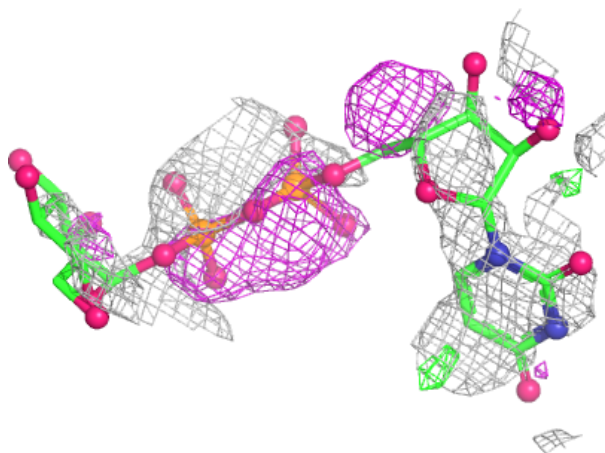
Electron density around UPG B 1415:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UPG A 1415:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.