Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:22 AM GMT

PDB ID	:	2WTX
Title	:	INSIGHT INTO THE MECHANISM OF ENZYMATIC GLYCOSYLTRANSFER WITH RETENTION THROUGH THE SYNTHESIS AND ANALYSIS OF BISUBSTRATE GLYCOMIMETICS OF TREHALOSE-6-PHOSPHATE SYNTHASE
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Deposited on	:	2009-09-25
Resolution	:	2.20 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

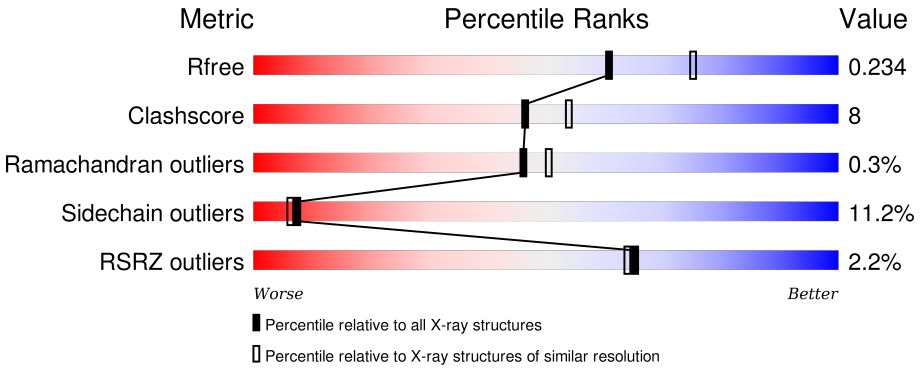
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	474	% 77% 15%
1	B	474	% 78% 16%
1	C	474	5% 70% 19% 7%
1	D	474	% 79% 13%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	1457	-	-	-	X
2	EDO	A	1458	-	-	X	X
2	EDO	A	1459	-	-	X	X
2	EDO	B	1459	-	-	X	X
2	EDO	B	1460	-	-	-	X

2 Entry composition

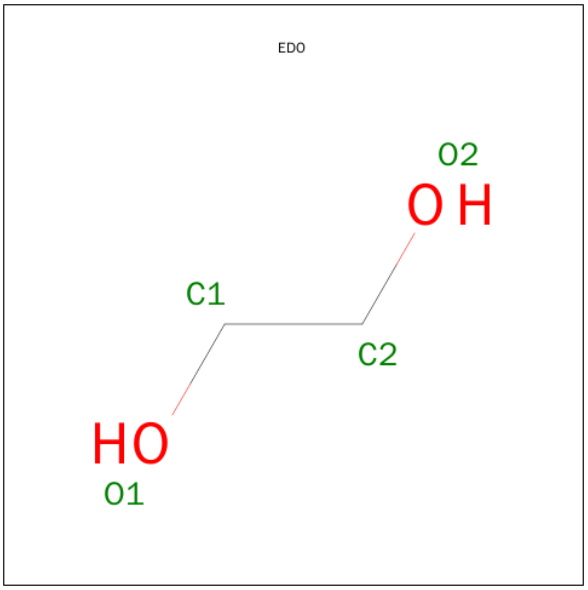
There are 5 unique types of molecules in this entry. The entry contains 15336 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALPHA, ALPHA-TREHALOSE-PHOSPHATE SYNTHASE [UDP-FORMING].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	3	0
			3674	2359	643	665	7			
1	B	454	Total	C	N	O	S	0	1	0
			3644	2343	633	661	7			
1	C	440	Total	C	N	O	S	0	1	0
			3545	2279	619	640	7			
1	D	457	Total	C	N	O	S	0	0	0
			3660	2349	638	666	7			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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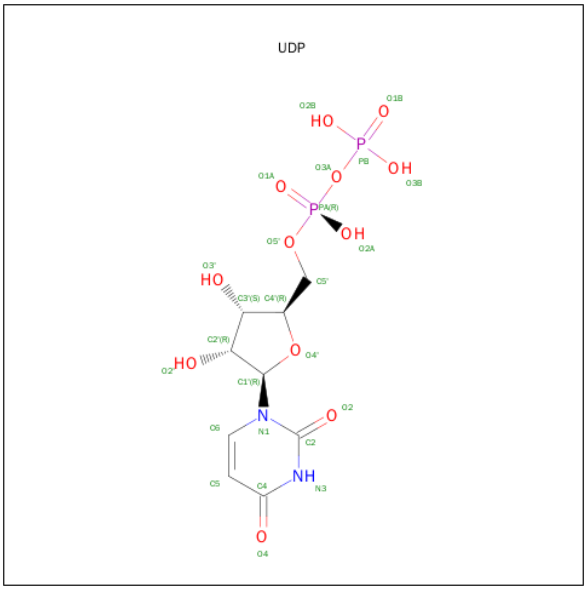
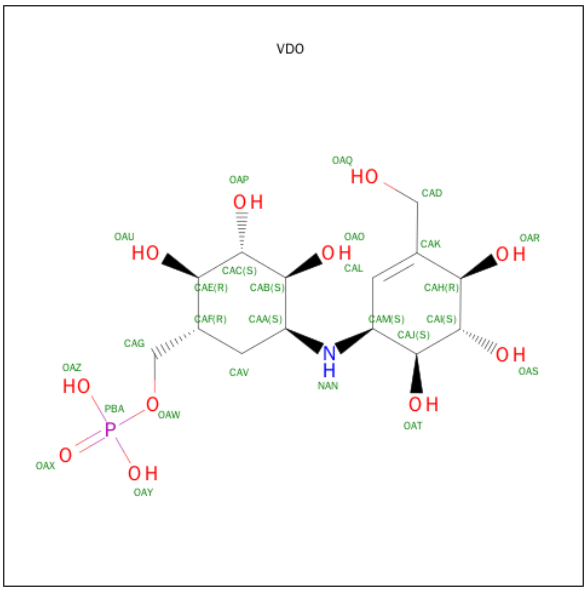
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 25 9 2 12 2	0	0
3	B	1	Total C N O P 25 9 2 12 2	0	0
3	C	1	Total C N O P 25 9 2 12 2	0	0
3	D	1	Total C N O P 25 9 2 12 2	0	0

- Molecule 4 is [(1R,2R,3S,4S,5S)-2,3,4-TRIHYDROXY-5-{[(1S,4R,5S,6S)-4,5,6-TRIHYDROXY-3-(HYDROXYMETHYL)CYCLOHEX-2-EN-1-YL]AMINO}CYCLOHEXYL]METHYL DIHYDROGEN PHOSPHATE (three-letter code: VDO) (formula: $C_{14}H_{26}NO_{11}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	14	1	11	1		
4	B	1	Total	C	N	O	P	0	0
			27	14	1	11	1		
4	C	1	Total	C	N	O	P	0	0
			27	14	1	11	1		
4	D	1	Total	C	N	O	P	0	0
			27	14	1	11	1		

- Molecule 5 is water.

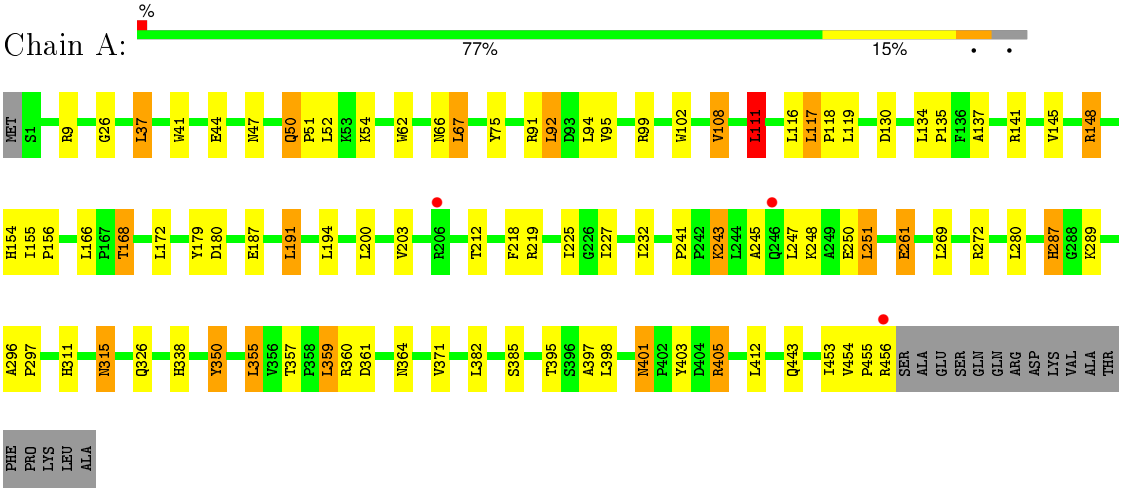
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	202	Total	O	0	0
			202	202		
5	B	152	Total	O	0	0
			152	152		
5	C	76	Total	O	0	0
			76	76		
5	D	155	Total	O	0	0
			155	155		

3 Residue-property plots (i)

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.

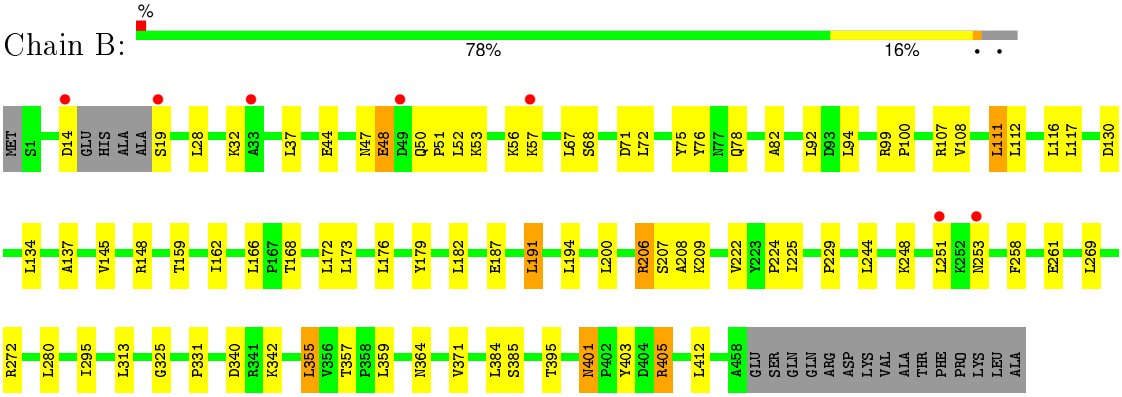
• Molecule 1: ALPHA, ALPHA-TREHALOSE-PHOSPHATE SYNTHASE [UDP-FORMING]

Chain A:



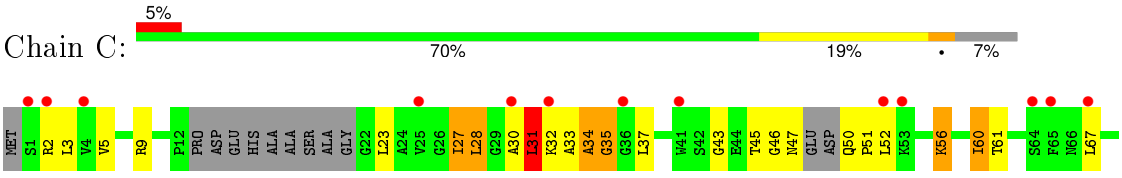
• Molecule 1: ALPHA, ALPHA-TREHALOSE-PHOSPHATE SYNTHASE [UDP-FORMING]

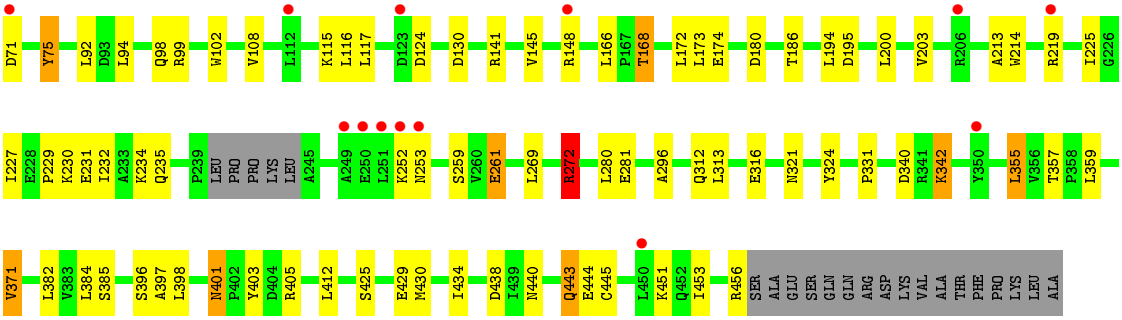
Chain B:



• Molecule 1: ALPHA, ALPHA-TREHALOSE-PHOSPHATE SYNTHASE [UDP-FORMING]

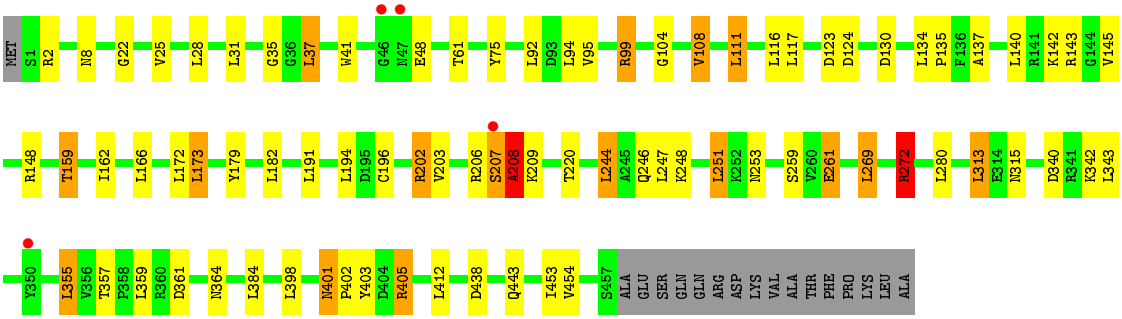
Chain C:





• Molecule 1: ALPHA, ALPHA-TREHALOSE-PHOSPHATE SYNTHASE [UDP-FORMING]

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.52Å 120.29Å 173.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.91 – 2.20 98.91 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (98.91-2.20) 99.9 (98.91-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.70 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.195 , 0.235 0.196 , 0.234	Depositor DCC
R_{free} test set	5583 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 111451 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15336	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, EDO, VDO

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	0.60	0/3777	0.72	3/5135 (0.1%)
1	B	0.62	5/3739 (0.1%)	0.76	5/5082 (0.1%)
1	C	0.60	6/3634 (0.2%)	0.67	4/4934 (0.1%)
1	D	0.65	3/3753 (0.1%)	0.77	10/5103 (0.2%)
All	All	0.62	14/14903 (0.1%)	0.73	22/20254 (0.1%)

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	B	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	208	ALA	N-CA	-8.89	1.28	1.46
1	C	34	ALA	CA-CB	-7.18	1.37	1.52
1	D	206	ARG	CZ-NH2	-6.93	1.24	1.33
1	B	209	LYS	CE-NZ	-6.56	1.32	1.49
1	C	33	ALA	CA-CB	-6.55	1.38	1.52
1	C	35	GLY	C-O	-6.23	1.13	1.23
1	C	31	LEU	N-CA	-6.21	1.33	1.46
1	B	209	LYS	C-O	-6.09	1.11	1.23
1	C	31	LEU	CA-CB	-6.00	1.40	1.53
1	D	206	ARG	N-CA	-5.88	1.34	1.46
1	C	31	LEU	CG-CD2	-5.40	1.31	1.51
1	B	206	ARG	CB-CG	-5.37	1.38	1.52
1	B	206	ARG	CZ-NH2	-5.20	1.26	1.33
1	B	209	LYS	CD-CE	-5.02	1.38	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	206	ARG	NE-CZ-NH1	13.53	127.06	120.30
1	B	206	ARG	NE-CZ-NH2	-13.00	113.80	120.30
1	C	31	LEU	CB-CG-CD2	-10.10	93.83	111.00
1	D	207	SER	CB-CA-C	9.69	128.51	110.10
1	A	111	LEU	CA-CB-CG	8.82	135.59	115.30
1	D	207	SER	CA-C-N	8.11	135.05	117.20
1	D	272	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	D	208	ALA	N-CA-CB	-7.00	100.29	110.10
1	B	207	SER	C-N-CA	-6.84	104.60	121.70
1	C	34	ALA	N-CA-C	-6.73	92.83	111.00
1	C	31	LEU	CB-CG-CD1	6.52	122.08	111.00
1	B	111	LEU	CA-CB-CG	6.07	129.25	115.30
1	A	37	LEU	CA-CB-CG	5.72	128.47	115.30
1	D	208	ALA	CA-C-N	-5.55	104.98	117.20
1	B	182	LEU	CA-CB-CG	5.54	128.04	115.30
1	C	272	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	D	206	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	119	LEU	CA-CB-CG	5.31	127.51	115.30
1	D	111	LEU	CA-CB-CG	5.29	127.47	115.30
1	D	272	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	182	LEU	CA-CB-CG	5.08	126.97	115.30
1	D	207	SER	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	208	ALA	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	3674	0	3650	58	0
1	B	3644	0	3619	34	0
1	C	3545	0	3523	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3660	0	3629	61	0
2	A	12	0	18	9	0
2	B	8	0	12	4	0
3	A	25	0	11	0	0
3	B	25	0	11	1	0
3	C	25	0	11	0	0
3	D	25	0	11	0	0
4	A	27	0	24	3	0
4	B	27	0	24	3	0
4	C	27	0	24	2	0
4	D	27	0	24	1	0
5	A	202	0	0	8	0
5	B	152	0	0	2	0
5	C	76	0	0	4	0
5	D	155	0	0	0	0
All	All	15336	0	14591	222	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 8.

All (222) 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:D:207:SER:CB	1:D:208:ALA:HB3	1.67	1.21
1:D:207:SER:HB2	1:D:208:ALA:HB3	1.27	1.15
1:D:207:SER:CB	1:D:208:ALA:CB	2.29	1.10
1:D:92:LEU:HD11	1:D:162:ILE:HG23	1.32	1.10
1:C:31:LEU:CD1	1:C:31:LEU:C	2.28	1.00
1:D:202:ARG:HG3	1:D:202:ARG:HH11	1.31	0.94
1:C:31:LEU:C	1:C:31:LEU:HD13	1.89	0.92
1:D:99:ARG:HH11	1:D:99:ARG:HG2	1.36	0.90
1:C:312[B]:GLN:HA	1:C:312[B]:GLN:HE21	1.37	0.88
1:D:207:SER:CA	1:D:208:ALA:CB	2.49	0.88
1:A:247:LEU:HD21	1:A:350:TYR:OH	1.75	0.87
1:D:207:SER:HB3	1:D:208:ALA:CB	2.05	0.86
1:D:244:LEU:HG	1:D:343:LEU:HD11	1.55	0.86
1:A:287[A]:HIS:CE1	1:A:326:GLN:NE2	2.45	0.84
1:C:30:ALA:HB2	1:C:443:GLN:CG	2.07	0.84
1:C:31:LEU:HD12	1:C:32:LYS:N	1.91	0.84
1:C:31:LEU:O	1:C:31:LEU:HD13	1.78	0.84
4:A:1461:VDO:OAO	4:A:1461:VDO:HAM	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:GLU:OE2	1:C:272:ARG:NH2	2.14	0.80
1:D:261:GLU:CD	1:D:272:ARG:HH22	1.87	0.78
1:C:31:LEU:CD1	1:C:32:LYS:N	2.46	0.77
1:C:9:ARG:HH21	1:C:43:GLY:HA3	1.50	0.77
1:D:261:GLU:OE2	1:D:272:ARG:NH2	2.18	0.77
1:C:2:ARG:HB2	1:C:124:ASP:OD1	1.85	0.76
1:D:75:TYR:CG	1:D:108:VAL:HG11	2.21	0.76
1:D:207:SER:CA	1:D:208:ALA:HB2	2.16	0.75
1:D:99:ARG:CG	1:D:99:ARG:HH11	1.98	0.75
1:C:272:ARG:HD2	1:C:357:THR:OG1	1.86	0.74
1:A:218:PHE:HA	2:A:1459:EDO:H21	1.69	0.74
1:A:287[A]:HIS:CE1	1:A:326:GLN:HE22	2.08	0.72
1:D:207:SER:CB	1:D:208:ALA:HB2	2.19	0.72
1:D:259:SER:HB3	1:D:272:ARG:HH21	1.54	0.71
1:C:31:LEU:O	1:C:35:GLY:HA2	1.89	0.71
1:A:453:ILE:CG2	2:A:1459:EDO:H11	2.20	0.71
1:C:56:LYS:HB3	1:C:61:THR:HG22	1.73	0.71
1:D:75:TYR:CB	1:D:108:VAL:HG11	2.22	0.69
1:C:340:ASP:OD1	1:C:342:LYS:HD3	1.91	0.69
1:C:261:GLU:CD	1:C:272:ARG:HH22	1.94	0.69
1:C:30:ALA:HB2	1:C:443:GLN:HG3	1.75	0.68
1:C:5:VAL:HG11	1:C:27:ILE:HG13	1.76	0.67
1:D:99:ARG:HG2	1:D:99:ARG:NH1	2.08	0.67
1:B:50:GLN:HG3	1:B:51:PRO:HD2	1.77	0.66
1:D:207:SER:HB3	1:D:208:ALA:HB2	1.78	0.66
1:C:60:ILE:HG13	1:C:61:THR:N	2.11	0.66
1:C:148:ARG:HD3	1:C:453:ILE:O	1.96	0.64
1:A:108:VAL:HA	1:A:111:LEU:HD13	1.78	0.64
1:B:107:ARG:NH1	5:B:2021:HOH:O	2.30	0.64
1:C:401:ASN:C	1:C:401:ASN:HD22	2.01	0.64
5:C:2011:HOH:O	1:D:405:ARG:HD2	1.97	0.63
1:C:148:ARG:HH21	1:C:451:LYS:HA	1.63	0.63
1:A:272:ARG:HD3	1:A:355:LEU:HD13	1.80	0.63
1:C:31:LEU:HD12	1:C:32:LYS:HG3	1.80	0.62
1:C:425:SER:O	1:C:429:GLU:HG3	1.99	0.62
1:D:75:TYR:HB2	1:D:108:VAL:HG11	1.81	0.62
1:C:219:ARG:HD3	1:C:453:ILE:HD11	1.81	0.62
1:C:401:ASN:ND2	1:C:403:TYR:H	1.98	0.62
1:A:359:LEU:HB3	2:A:1458:EDO:H11	1.81	0.61
1:C:46:GLY:O	1:C:47:ASN:C	2.38	0.61
1:D:202:ARG:HG3	1:D:202:ARG:NH1	2.02	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ILE:HG21	2:A:1459:EDO:H11	1.83	0.60
1:C:230:LYS:O	1:C:234:LYS:HG2	2.02	0.60
1:D:31:LEU:O	1:D:35:GLY:N	2.34	0.60
1:C:225:ILE:HG21	4:C:1458:VDO:OAQ	2.02	0.59
1:C:357:THR:HA	1:C:385:SER:HB2	1.82	0.59
1:A:47:ASN:O	1:A:50:GLN:HG2	2.02	0.59
1:A:50:GLN:HB2	1:A:51:PRO:HD2	1.84	0.59
1:D:37:LEU:HD23	1:D:61:THR:HB	1.83	0.59
1:C:259:SER:HB3	1:C:272:ARG:HH21	1.67	0.59
1:D:75:TYR:HB2	1:D:108:VAL:CG1	2.32	0.59
1:C:30:ALA:HB2	1:C:443:GLN:HG2	1.84	0.59
1:C:31:LEU:O	1:C:34:ALA:O	2.22	0.58
1:B:222:VAL:HG12	1:B:224:PRO:HD3	1.85	0.58
1:A:247:LEU:CD2	1:A:350:TYR:OH	2.50	0.57
1:B:71:ASP:OD2	1:B:107:ARG:NH2	2.36	0.57
1:B:78:GLN:O	1:B:82:ALA:HB3	2.05	0.57
4:B:1462:VDO:OAO	4:B:1462:VDO:HAM	2.04	0.57
1:A:355:LEU:HG	1:A:412:LEU:HD21	1.87	0.57
1:A:227:ILE:HD12	1:A:232:ILE:HD12	1.84	0.57
1:B:405:ARG:HB3	2:B:1459:EDO:H22	1.87	0.57
2:A:1458:EDO:H21	5:A:2036:HOH:O	2.06	0.56
1:B:401:ASN:HD22	1:B:401:ASN:C	2.09	0.56
1:D:401:ASN:HD22	1:D:401:ASN:C	2.09	0.56
1:B:162:ILE:HD12	1:B:162:ILE:N	2.21	0.56
1:B:272:ARG:HD3	1:B:355:LEU:HD13	1.87	0.56
1:D:207:SER:CA	1:D:208:ALA:HB3	2.08	0.56
1:D:355:LEU:HG	1:D:412:LEU:HD21	1.88	0.56
1:D:272:ARG:HD2	1:D:357:THR:OG1	2.05	0.56
1:A:180:ASP:O	2:A:1459:EDO:H22	2.05	0.55
1:B:187:GLU:HG3	1:B:191:LEU:HD22	1.88	0.54
4:C:1458:VDO:HAM	4:C:1458:VDO:OAO	2.06	0.54
1:A:245:ALA:HA	1:A:248:LYS:HE3	1.90	0.54
1:A:401:ASN:HD22	1:A:401:ASN:C	2.11	0.54
1:D:148:ARG:HD3	1:D:453:ILE:O	2.07	0.54
1:A:453:ILE:HG23	2:A:1459:EDO:H11	1.88	0.54
1:A:315:ASN:HD21	1:D:315:ASN:HB2	1.73	0.53
1:A:338:HIS:HE1	5:A:2199:HOH:O	1.91	0.53
1:D:401:ASN:HD21	1:D:403:TYR:HD1	1.57	0.52
1:A:315:ASN:ND2	1:D:315:ASN:HB2	2.24	0.52
1:A:187:GLU:HG3	1:A:191:LEU:HD22	1.89	0.52
1:C:28:LEU:O	1:C:31:LEU:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:ASN:O	1:D:41:TRP:HB3	2.09	0.52
1:C:396:SER:HB2	1:C:430:MET:HG3	1.92	0.52
1:A:117:LEU:HB3	1:A:118:PRO:HD3	1.90	0.52
1:A:289:LYS:HE3	5:A:2106:HOH:O	2.09	0.52
1:A:50:GLN:HG3	1:A:66:ASN:HD22	1.74	0.51
1:D:92:LEU:N	1:D:92:LEU:HD12	2.25	0.51
1:A:405:ARG:HD2	5:A:2162:HOH:O	2.11	0.51
1:D:269:LEU:HB3	1:D:313:LEU:HD11	1.93	0.50
1:C:355:LEU:HG	1:C:412:LEU:HD21	1.93	0.50
1:A:41:TRP:CD1	1:A:67:LEU:HD22	2.46	0.50
1:C:371:VAL:HG22	1:C:434:ILE:HD12	1.94	0.50
1:C:281:GLU:HG2	1:C:324:TYR:OH	2.11	0.50
1:A:154:HIS:ND1	4:A:1461:VDO:HAD1	2.27	0.50
1:A:401:ASN:ND2	1:A:403:TYR:H	2.09	0.50
1:B:401:ASN:HD22	1:B:403:TYR:H	1.60	0.50
1:D:104:GLY:O	1:D:108:VAL:HG12	2.12	0.50
1:A:357:THR:HA	1:A:385:SER:HB2	1.94	0.50
1:C:47:ASN:OD1	1:C:47:ASN:O	2.30	0.49
1:B:159:THR:HB	5:B:2036:HOH:O	2.12	0.49
1:B:28:LEU:O	1:B:32:LYS:HG3	2.13	0.49
1:C:401:ASN:HD22	1:C:403:TYR:H	1.59	0.49
1:A:134:LEU:N	1:A:135:PRO:CD	2.76	0.49
1:D:140:LEU:O	1:D:145:VAL:HG13	2.14	0.48
1:B:401:ASN:ND2	1:B:403:TYR:H	2.11	0.48
1:A:148:ARG:HD2	1:A:455:PRO:HD3	1.95	0.48
1:D:259:SER:HB3	1:D:272:ARG:NH2	2.26	0.48
1:B:134:LEU:HD22	1:B:176:LEU:HD21	1.96	0.48
1:A:261:GLU:O	1:A:296:ALA:HA	2.14	0.48
1:A:225:ILE:HG21	4:A:1461:VDO:HAD2	1.95	0.48
1:A:137:ALA:HB2	1:A:179:TYR:CE1	2.49	0.48
1:A:245:ALA:O	1:A:248:LYS:HG2	2.14	0.48
1:B:355:LEU:HG	1:B:412:LEU:HD21	1.95	0.47
1:C:312[B]:GLN:HA	1:C:312[B]:GLN:NE2	2.17	0.47
1:B:137:ALA:HB2	1:B:179:TYR:CE1	2.50	0.47
1:A:102:TRP:CZ3	1:A:168:THR:HG21	2.49	0.47
1:D:401:ASN:ND2	1:D:403:TYR:H	2.13	0.47
1:A:350:TYR:C	1:A:350:TYR:CD1	2.89	0.46
1:B:225:ILE:HG21	4:B:1462:VDO:HAD1	1.97	0.46
1:B:258[A]:PHE:HZ	1:B:295:ILE:HD12	1.80	0.46
1:A:241:PRO:HB3	1:A:243:LYS:HE2	1.98	0.46
1:C:23:LEU:O	1:C:27:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1461:UDP:O3B	4:B:1462:VDO:NAN	2.48	0.46
1:D:22:GLY:O	1:D:25:VAL:HG23	2.16	0.46
1:C:31:LEU:CD1	1:C:32:LYS:HG3	2.44	0.46
1:B:405:ARG:HB3	2:B:1459:EDO:C2	2.46	0.46
1:C:316:GLU:HG3	5:C:2030:HOH:O	2.15	0.46
1:A:251:LEU:HD21	1:A:350:TYR:CE1	2.51	0.46
1:B:72:LEU:O	1:B:76:TYR:HB3	2.16	0.46
1:B:75:TYR:CD2	1:B:108:VAL:HG22	2.51	0.45
1:B:313:LEU:HD12	1:B:313:LEU:HA	1.87	0.45
1:D:202:ARG:HH11	1:D:202:ARG:CG	2.15	0.45
1:A:102:TRP:CE3	1:A:168:THR:HG21	2.52	0.45
1:B:325:GLY:HA2	1:B:331:PRO:HD3	1.98	0.45
1:A:91:ARG:HD3	2:A:1458:EDO:H22	1.98	0.45
1:C:321:ASN:OD1	1:C:331:PRO:HD2	2.17	0.45
1:B:357:THR:HA	1:B:385:SER:HB2	1.99	0.45
1:D:340:ASP:OD2	1:D:342:LYS:HG2	2.17	0.45
1:A:155:ILE:HB	1:A:156:PRO:CD	2.48	0.44
1:C:102:TRP:CE3	1:C:168:THR:HG21	2.53	0.44
1:A:261:GLU:O	1:A:297:PRO:HD2	2.16	0.44
1:A:338:HIS:CE1	5:A:2199:HOH:O	2.69	0.44
1:D:75:TYR:CD2	1:D:108:VAL:HG13	2.52	0.44
1:B:405:ARG:HD2	2:B:1459:EDO:C1	2.48	0.44
1:B:253:ASN:N	1:B:253:ASN:OD1	2.46	0.44
1:D:75:TYR:CD2	1:D:108:VAL:CG1	3.01	0.44
1:A:134:LEU:N	1:A:135:PRO:HD3	2.33	0.44
1:C:227:ILE:O	1:C:229:PRO:HD3	2.18	0.44
5:C:2015:HOH:O	1:D:159:THR:HG21	2.18	0.44
1:D:92:LEU:HA	1:D:95:VAL:HG13	2.00	0.44
1:A:137:ALA:O	1:A:141:ARG:HG2	2.17	0.43
1:C:444:GLU:HG3	1:C:445:CYS:N	2.33	0.43
1:C:31:LEU:HD21	1:C:60:ILE:HD12	2.00	0.43
1:D:209:LYS:HB3	1:D:220:THR:O	2.18	0.43
1:C:180:ASP:HB3	1:C:453:ILE:HG21	2.00	0.43
1:C:9:ARG:NH2	1:C:43:GLY:HA3	2.27	0.43
1:C:401:ASN:C	1:C:401:ASN:ND2	2.71	0.43
1:D:401:ASN:HA	1:D:402:PRO:HD2	1.91	0.43
1:C:50:GLN:HA	1:C:51:PRO:HD3	1.85	0.43
1:A:9:ARG:HD3	5:A:2017:HOH:O	2.18	0.43
1:D:173:LEU:HD21	1:D:196:CYS:HB3	2.01	0.42
1:C:71:ASP:O	1:C:75:TYR:HB3	2.19	0.42
1:A:311:HIS:HD2	5:A:2116:HOH:O	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:LEU:CG	1:D:343:LEU:HD11	2.38	0.42
1:D:134:LEU:N	1:D:135:PRO:CD	2.82	0.42
1:A:26:GLY:HA3	1:A:225:ILE:HD11	2.01	0.42
1:C:261:GLU:O	1:C:296:ALA:HA	2.19	0.42
1:A:92:LEU:HA	1:A:95:VAL:HG13	2.01	0.42
1:C:203:VAL:HG12	1:C:213:ALA:HB2	2.01	0.42
1:D:75:TYR:CG	1:D:108:VAL:CG1	2.98	0.42
1:D:37:LEU:CD2	1:D:61:THR:HB	2.47	0.42
1:B:48:GLU:OE2	1:B:71:ASP:OD1	2.37	0.42
1:C:3:LEU:HD23	1:C:31:LEU:HA	2.02	0.42
1:D:247:LEU:HG	1:D:251:LEU:HD22	2.02	0.42
1:C:382:LEU:HD23	1:C:397:ALA:HB2	2.01	0.41
1:C:371:VAL:CG2	1:C:434:ILE:HD12	2.49	0.41
1:C:168:THR:O	1:C:168:THR:HG23	2.20	0.41
1:A:454:VAL:O	1:A:454:VAL:HG23	2.20	0.41
1:A:315:ASN:HD22	1:D:315:ASN:HD22	1.69	0.41
1:B:340:ASP:OD2	1:B:342:LYS:HB2	2.21	0.41
1:C:61:THR:HG23	5:C:2003:HOH:O	2.20	0.41
1:C:148:ARG:NH2	1:C:451:LYS:HA	2.32	0.41
1:B:48:GLU:HG3	1:B:68:SER:N	2.36	0.41
1:D:261:GLU:CD	1:D:272:ARG:NH2	2.65	0.41
1:A:219[A]:ARG:HD3	1:A:453:ILE:HD11	2.03	0.41
1:A:261:GLU:CD	1:A:272:ARG:HH22	2.24	0.41
4:D:1459:VDO:HAM	4:D:1459:VDO:OAO	2.20	0.41
1:B:99:ARG:N	1:B:100:PRO:CD	2.84	0.41
1:A:247:LEU:HD21	1:A:350:TYR:HH	1.83	0.41
1:C:231:GLU:O	1:C:235:GLN:HG2	2.21	0.41
1:D:401:ASN:HD22	1:D:403:TYR:H	1.69	0.40
1:B:162:ILE:CD1	1:B:162:ILE:N	2.83	0.40
1:C:174:GLU:HA	1:C:214:TRP:CZ3	2.55	0.40
1:C:141:ARG:NH2	1:C:180:ASP:OD1	2.55	0.40
2:A:1458:EDO:C2	5:A:2036:HOH:O	2.67	0.40
1:D:137:ALA:HB2	1:D:179:TYR:CE1	2.56	0.40
1:A:382:LEU:HD23	1:A:397:ALA:HB2	2.02	0.40
1:B:50:GLN:HG3	1:B:51:PRO:CD	2.48	0.40
1:C:227:ILE:HD13	1:C:232:ILE:HD12	2.03	0.40
1:D:117:LEU:HD11	1:D:143:ARG:HB3	2.04	0.40
1:B:405:ARG:HD2	2:B:1459:EDO:H11	2.04	0.40
1:D:2:ARG:NH2	1:D:124:ASP:OD2	2.52	0.40
1:A:54:LYS:HA	1:A:62:TRP:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	457/474 (96%)	441 (96%)	15 (3%)	1 (0%)	52 59
1	B	451/474 (95%)	429 (95%)	21 (5%)	1 (0%)	52 59
1	C	433/474 (91%)	417 (96%)	16 (4%)	0	100 100
1	D	455/474 (96%)	437 (96%)	15 (3%)	3 (1%)	26 25
All	All	1796/1896 (95%)	1724 (96%)	67 (4%)	5 (0%)	46 50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	208	ALA
1	B	364	ASN
1	A	364	ASN
1	D	364	ASN
1	D	438	ASP

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	387/399 (97%)	342 (88%)	45 (12%)	7 6
1	B	384/399 (96%)	342 (89%)	42 (11%)	8 7
1	C	373/399 (94%)	326 (87%)	47 (13%)	5 4
1	D	385/399 (96%)	347 (90%)	38 (10%)	10 9
All	All	1529/1596 (96%)	1357 (89%)	172 (11%)	7 6

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	44	GLU
1	A	50	GLN
1	A	52	LEU
1	A	67	LEU
1	A	75	TYR
1	A	92	LEU
1	A	94	LEU
1	A	99	ARG
1	A	108	VAL
1	A	111	LEU
1	A	116	LEU
1	A	117	LEU
1	A	130	ASP
1	A	145	VAL
1	A	148	ARG
1	A	166	LEU
1	A	168	THR
1	A	172	LEU
1	A	191	LEU
1	A	194	LEU
1	A	200	LEU
1	A	203	VAL
1	A	212	THR
1	A	243	LYS
1	A	250	GLU
1	A	251	LEU
1	A	261	GLU
1	A	269	LEU
1	A	280	LEU
1	A	287[A]	HIS
1	A	287[B]	HIS
1	A	315	ASN
1	A	350	TYR
1	A	355	LEU
1	A	359	LEU
1	A	360	ARG
1	A	361	ASP
1	A	371	VAL
1	A	395	THR
1	A	398	LEU
1	A	401	ASN

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Mol	Chain	Res	Type
1	A	405	ARG
1	A	443	GLN
1	A	456	ARG
1	B	14	ASP
1	B	19	SER
1	B	37	LEU
1	B	44	GLU
1	B	47	ASN
1	B	48	GLU
1	B	52	LEU
1	B	53	LYS
1	B	56	LYS
1	B	57	LYS
1	B	67	LEU
1	B	92	LEU
1	B	94	LEU
1	B	111	LEU
1	B	112	LEU
1	B	116	LEU
1	B	117	LEU
1	B	130	ASP
1	B	145	VAL
1	B	148	ARG
1	B	166	LEU
1	B	168	THR
1	B	172	LEU
1	B	173	LEU
1	B	191	LEU
1	B	194	LEU
1	B	200	LEU
1	B	206	ARG
1	B	229	PRO
1	B	244	LEU
1	B	248	LYS
1	B	251	LEU
1	B	261	GLU
1	B	269	LEU
1	B	280	LEU
1	B	355	LEU
1	B	359	LEU
1	B	371	VAL
1	B	384	LEU

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Mol	Chain	Res	Type
1	B	395	THR
1	B	401	ASN
1	B	405	ARG
1	C	27	ILE
1	C	28	LEU
1	C	31	LEU
1	C	37	LEU
1	C	45	THR
1	C	52	LEU
1	C	56	LYS
1	C	60	ILE
1	C	67	LEU
1	C	75	TYR
1	C	92	LEU
1	C	94	LEU
1	C	98	GLN
1	C	99	ARG
1	C	108	VAL
1	C	115	LYS
1	C	116	LEU
1	C	117	LEU
1	C	130	ASP
1	C	145	VAL
1	C	166	LEU
1	C	168	THR
1	C	172	LEU
1	C	173	LEU
1	C	186	THR
1	C	194	LEU
1	C	195	ASP
1	C	200	LEU
1	C	252	LYS
1	C	253	ASN
1	C	261	GLU
1	C	269	LEU
1	C	272	ARG
1	C	280	LEU
1	C	313	LEU
1	C	342	LYS
1	C	355	LEU
1	C	359	LEU
1	C	371	VAL

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Mol	Chain	Res	Type
1	C	384	LEU
1	C	398	LEU
1	C	401	ASN
1	C	405	ARG
1	C	438	ASP
1	C	440	ASN
1	C	443	GLN
1	C	456	ARG
1	D	28	LEU
1	D	37	LEU
1	D	48	GLU
1	D	94	LEU
1	D	99	ARG
1	D	108	VAL
1	D	111	LEU
1	D	116	LEU
1	D	123	ASP
1	D	130	ASP
1	D	142	LYS
1	D	159	THR
1	D	166	LEU
1	D	172	LEU
1	D	173	LEU
1	D	191	LEU
1	D	194	LEU
1	D	202	ARG
1	D	203	VAL
1	D	244	LEU
1	D	246	GLN
1	D	248	LYS
1	D	251	LEU
1	D	253	ASN
1	D	261	GLU
1	D	269	LEU
1	D	272	ARG
1	D	280	LEU
1	D	313	LEU
1	D	355	LEU
1	D	359	LEU
1	D	361	ASP
1	D	384	LEU
1	D	398	LEU

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Mol	Chain	Res	Type
1	D	401	ASN
1	D	405	ARG
1	D	443	GLN
1	D	454	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	16	HIS
1	A	50	GLN
1	A	66	ASN
1	A	77	ASN
1	A	78	GLN
1	A	175	GLN
1	A	235	GLN
1	A	315	ASN
1	A	326	GLN
1	A	338	HIS
1	A	401	ASN
1	B	8	ASN
1	B	47	ASN
1	B	77	ASN
1	B	78	GLN
1	B	146	ASN
1	B	175	GLN
1	B	315	ASN
1	B	401	ASN
1	C	8	ASN
1	C	77	ASN
1	C	146	ASN
1	C	386	GLN
1	C	401	ASN
1	D	8	ASN
1	D	50	GLN
1	D	78	GLN
1	D	98	GLN
1	D	146	ASN
1	D	235	GLN
1	D	256	ASN
1	D	401	ASN
1	D	441	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

13 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	EDO	A	1457	-	3,3,3	0.66	0	2,2,2	0.10	0
2	EDO	A	1458	-	3,3,3	0.70	0	2,2,2	0.25	0
2	EDO	A	1459	-	3,3,3	0.40	0	2,2,2	0.56	0
3	UDP	A	1460	-	18,26,26	1.09	1 (5%)	26,40,40	1.58	1 (3%)
4	VDO	A	1461	-	28,28,28	1.59	4 (14%)	29,42,42	1.40	4 (13%)
2	EDO	B	1459	-	3,3,3	0.42	0	2,2,2	0.42	0
2	EDO	B	1460	-	3,3,3	0.55	0	2,2,2	0.48	0
3	UDP	B	1461	-	18,26,26	1.25	2 (11%)	26,40,40	1.65	3 (11%)
4	VDO	B	1462	-	28,28,28	1.62	4 (14%)	29,42,42	1.46	5 (17%)
3	UDP	C	1457	-	18,26,26	1.16	1 (5%)	26,40,40	1.41	2 (7%)
4	VDO	C	1458	-	28,28,28	1.44	5 (17%)	29,42,42	1.39	4 (13%)
3	UDP	D	1458	-	18,26,26	1.29	1 (5%)	26,40,40	1.51	1 (3%)
4	VDO	D	1459	-	28,28,28	1.53	4 (14%)	29,42,42	1.11	3 (10%)

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	EDO	A	1457	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1458	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1459	-	-	0/1/1/1	0/0/0/0
3	UDP	A	1460	-	-	0/12/32/32	0/2/2/2
4	VDO	A	1461	-	-	0/12/52/52	0/2/2/2
2	EDO	B	1459	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1460	-	-	0/1/1/1	0/0/0/0
3	UDP	B	1461	-	-	0/12/32/32	0/2/2/2
4	VDO	B	1462	-	-	0/12/52/52	0/2/2/2
3	UDP	C	1457	-	-	0/12/32/32	0/2/2/2
4	VDO	C	1458	-	-	0/12/52/52	0/2/2/2
3	UDP	D	1458	-	-	0/12/32/32	0/2/2/2
4	VDO	D	1459	-	-	0/12/52/52	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1461	UDP	PA-O2A	-2.04	1.46	1.54
4	D	1459	VDO	CAJ-CAM	2.12	1.56	1.53
4	C	1458	VDO	CAB-CAA	2.17	1.57	1.52
4	D	1459	VDO	PBA-OAY	2.24	1.62	1.54
3	A	1460	UDP	C4-N3	2.33	1.37	1.33
4	A	1461	VDO	CAA-NAN	2.40	1.52	1.47
4	C	1458	VDO	PBA-OAZ	2.52	1.63	1.54
4	B	1462	VDO	CAM-CAL	2.56	1.54	1.50
4	D	1459	VDO	CAM-CAL	2.57	1.54	1.50
4	C	1458	VDO	CAM-CAL	2.70	1.54	1.50
4	B	1462	VDO	CAM-NAN	2.74	1.52	1.47
4	C	1458	VDO	CAJ-CAM	2.79	1.57	1.53
4	A	1461	VDO	CAM-NAN	2.85	1.52	1.47
3	D	1458	UDP	C4-N3	2.91	1.38	1.33
3	C	1457	UDP	C4-N3	3.06	1.38	1.33
3	B	1461	UDP	C4-N3	3.17	1.39	1.33
4	A	1461	VDO	CAJ-CAM	3.41	1.57	1.53
4	B	1462	VDO	CAJ-CAM	4.05	1.58	1.53
4	C	1458	VDO	CAL-CAK	4.26	1.39	1.32
4	B	1462	VDO	CAL-CAK	4.53	1.39	1.32
4	A	1461	VDO	CAL-CAK	4.76	1.40	1.32
4	D	1459	VDO	CAL-CAK	4.88	1.40	1.32

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1461	VDO	OAS-CAI-CAH	-3.03	104.02	109.49
4	C	1458	VDO	CAF-CAE-CAC	-2.76	108.20	111.93
4	D	1459	VDO	OAS-CAI-CAH	-2.74	104.54	109.49
4	B	1462	VDO	OAS-CAI-CAH	-2.59	104.82	109.49
4	A	1461	VDO	OAQ-CAD-CAK	-2.37	106.39	112.12
3	C	1457	UDP	PA-O3A-PB	-2.03	125.84	132.67
3	B	1461	UDP	O3A-PA-O5'	2.03	108.33	102.94
4	C	1458	VDO	CAJ-CAI-CAH	2.27	113.50	110.73
4	B	1462	VDO	CAJ-CAI-CAH	2.28	113.51	110.73
3	B	1461	UDP	O3B-PB-O3A	2.30	115.52	105.09
4	D	1459	VDO	CAC-CAB-CAA	2.45	115.04	111.23
4	B	1462	VDO	OAW-PBA-OAX	2.76	114.16	107.14
4	A	1461	VDO	CAV-CAF-CAE	2.80	112.28	109.86
4	C	1458	VDO	CAC-CAB-CAA	2.90	115.73	111.23
4	D	1459	VDO	CAJ-CAI-CAH	3.14	114.56	110.73
4	A	1461	VDO	CAF-CAV-CAA	3.34	112.97	108.50
4	C	1458	VDO	CAF-CAV-CAA	3.40	113.05	108.50
4	B	1462	VDO	CAV-CAF-CAE	3.78	113.13	109.86
4	B	1462	VDO	CAF-CAV-CAA	3.83	113.63	108.50
3	C	1457	UDP	C4-N3-C2	5.45	119.54	114.14
3	D	1458	UDP	C4-N3-C2	5.93	120.02	114.14
3	B	1461	UDP	C4-N3-C2	6.67	120.75	114.14
3	A	1460	UDP	C4-N3-C2	6.71	120.78	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1458	EDO	4	0
2	A	1459	EDO	5	0
4	A	1461	VDO	3	0
2	B	1459	EDO	4	0
3	B	1461	UDP	1	0
4	B	1462	VDO	3	0
4	C	1458	VDO	2	0
4	D	1459	VDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	456/474 (96%)	-0.35	3 (0%) 89 88	9, 19, 39, 63	0
1	B	454/474 (95%)	-0.17	7 (1%) 76 75	11, 26, 53, 65	0
1	C	440/474 (92%)	0.30	26 (5%) 26 25	20, 37, 76, 88	0
1	D	457/474 (96%)	-0.24	4 (0%) 85 85	13, 25, 48, 62	0
All	All	1807/1896 (95%)	-0.12	40 (2%) 65 64	9, 26, 62, 88	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	206	ARG	6.0
1	C	52	LEU	5.2
1	C	251	LEU	4.4
1	C	36	GLY	4.2
1	B	33	ALA	4.0
1	C	53	LYS	4.0
1	A	246	GLN	3.9
1	C	32	LYS	3.8
1	C	41	TRP	3.7
1	C	252	LYS	3.7
1	C	112	LEU	3.3
1	C	123	ASP	3.3
1	C	2	ARG	3.3
1	B	14	ASP	3.1
1	C	350	TYR	3.1
1	B	251	LEU	3.1
1	C	1	SER	3.1
1	C	71	ASP	3.0
1	D	350	TYR	3.0
1	D	46	GLY	2.9
1	C	65	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	207	SER	2.9
1	C	253	ASN	2.8
1	B	19	SER	2.6
1	C	249	ALA	2.5
1	C	4	VAL	2.4
1	C	148	ARG	2.4
1	C	450	LEU	2.4
1	C	64	SER	2.3
1	C	30	ALA	2.2
1	A	206	ARG	2.1
1	C	25	VAL	2.1
1	C	67	LEU	2.1
1	B	253	ASN	2.1
1	C	219	ARG	2.1
1	B	49	ASP	2.1
1	A	456	ARG	2.0
1	D	47	ASN	2.0
1	C	250	GLU	2.0
1	B	57	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	EDO	A	1458	4/4	0.71	0.47	34.27	33,40,40,43	0
2	EDO	A	1459	4/4	0.93	0.28	10.53	23,25,25,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	EDO	A	1457	4/4	0.82	0.21	7.50	35,36,37,37	0
2	EDO	B	1459	4/4	0.95	0.25	4.56	25,30,30,32	0
2	EDO	B	1460	4/4	0.88	0.27	3.12	33,37,38,40	0
4	VDO	A	1461	27/27	0.95	0.13	1.47	13,17,20,27	0
4	VDO	B	1462	27/27	0.94	0.12	0.16	15,23,31,32	0
4	VDO	C	1458	27/27	0.92	0.13	-0.01	35,40,42,44	0
4	VDO	D	1459	27/27	0.95	0.11	-0.08	15,23,28,30	0
3	UDP	A	1460	25/25	0.99	0.10	-0.33	12,15,17,19	0
3	UDP	B	1461	25/25	0.99	0.10	-0.85	16,25,28,28	0
3	UDP	C	1457	25/25	0.97	0.11	-1.01	31,37,38,39	0
3	UDP	D	1458	25/25	0.98	0.10	-1.09	16,20,24,25	0

6.5 Other polymers (i)

There are no such residues in this entry.