Full wwPDB X-ray Structure Validation Report (i)

May 23, 2020 – 10:22 am BST

PDB ID	:	5KOP
Title	:	Arabidopsis thaliana fucosyltransferase 1 (FUT1) in its apo-form
Authors	:	Rocha, J.; de Sanctis, D.; Breton, C.
Deposited on	:	2016-07-01
Resolution	:	2.10 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 (i) symbol.

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

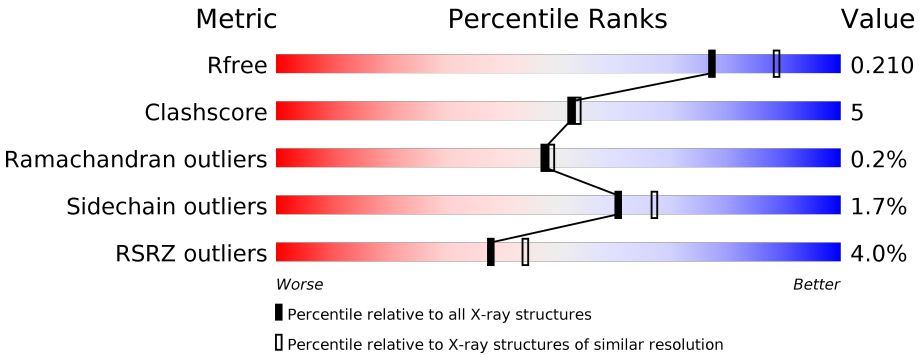
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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 <=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	521	5% 75% 12% • 12%
1	B	521	2% 75% 9% • 15%
1	C	521	2% 76% 9% • 14%
1	D	521	5% 78% 10% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15339 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 Galactoside 2-alpha-L-fucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	4	0
			3705	2383	612	686	24			
1	B	445	Total	C	N	O	S	0	3	0
			3604	2320	599	663	22			
1	C	448	Total	C	N	O	S	0	7	0
			3654	2351	604	675	24			
1	D	457	Total	C	N	O	S	0	3	0
			3696	2377	615	682	22			

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	HIS	-	expression tag	UNP Q9SWH5
A	39	HIS	-	expression tag	UNP Q9SWH5
A	40	HIS	-	expression tag	UNP Q9SWH5
A	41	HIS	-	expression tag	UNP Q9SWH5
A	42	HIS	-	expression tag	UNP Q9SWH5
A	43	HIS	-	expression tag	UNP Q9SWH5
A	44	GLY	-	expression tag	UNP Q9SWH5
A	45	MET	-	expression tag	UNP Q9SWH5
A	46	ALA	-	expression tag	UNP Q9SWH5
A	47	SER	-	expression tag	UNP Q9SWH5
A	48	MET	-	expression tag	UNP Q9SWH5
A	49	THR	-	expression tag	UNP Q9SWH5
A	50	GLY	-	expression tag	UNP Q9SWH5
A	51	GLY	-	expression tag	UNP Q9SWH5
A	52	GLN	-	expression tag	UNP Q9SWH5
A	53	GLN	-	expression tag	UNP Q9SWH5
A	54	MET	-	expression tag	UNP Q9SWH5
A	55	GLY	-	expression tag	UNP Q9SWH5
A	56	ARG	-	expression tag	UNP Q9SWH5
A	57	ASP	-	expression tag	UNP Q9SWH5
A	58	LEU	-	expression tag	UNP Q9SWH5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	TYR	-	expression tag	UNP Q9SWH5
A	60	ASP	-	expression tag	UNP Q9SWH5
A	61	ASP	-	expression tag	UNP Q9SWH5
A	62	ASP	-	expression tag	UNP Q9SWH5
A	63	ASP	-	expression tag	UNP Q9SWH5
A	64	LYS	-	expression tag	UNP Q9SWH5
A	65	SER	-	expression tag	UNP Q9SWH5
A	66	ARG	-	expression tag	UNP Q9SWH5
A	67	LEU	-	expression tag	UNP Q9SWH5
A	68	GLN	-	expression tag	UNP Q9SWH5
B	38	HIS	-	expression tag	UNP Q9SWH5
B	39	HIS	-	expression tag	UNP Q9SWH5
B	40	HIS	-	expression tag	UNP Q9SWH5
B	41	HIS	-	expression tag	UNP Q9SWH5
B	42	HIS	-	expression tag	UNP Q9SWH5
B	43	HIS	-	expression tag	UNP Q9SWH5
B	44	GLY	-	expression tag	UNP Q9SWH5
B	45	MET	-	expression tag	UNP Q9SWH5
B	46	ALA	-	expression tag	UNP Q9SWH5
B	47	SER	-	expression tag	UNP Q9SWH5
B	48	MET	-	expression tag	UNP Q9SWH5
B	49	THR	-	expression tag	UNP Q9SWH5
B	50	GLY	-	expression tag	UNP Q9SWH5
B	51	GLY	-	expression tag	UNP Q9SWH5
B	52	GLN	-	expression tag	UNP Q9SWH5
B	53	GLN	-	expression tag	UNP Q9SWH5
B	54	MET	-	expression tag	UNP Q9SWH5
B	55	GLY	-	expression tag	UNP Q9SWH5
B	56	ARG	-	expression tag	UNP Q9SWH5
B	57	ASP	-	expression tag	UNP Q9SWH5
B	58	LEU	-	expression tag	UNP Q9SWH5
B	59	TYR	-	expression tag	UNP Q9SWH5
B	60	ASP	-	expression tag	UNP Q9SWH5
B	61	ASP	-	expression tag	UNP Q9SWH5
B	62	ASP	-	expression tag	UNP Q9SWH5
B	63	ASP	-	expression tag	UNP Q9SWH5
B	64	LYS	-	expression tag	UNP Q9SWH5
B	65	SER	-	expression tag	UNP Q9SWH5
B	66	ARG	-	expression tag	UNP Q9SWH5
B	67	LEU	-	expression tag	UNP Q9SWH5
B	68	GLN	-	expression tag	UNP Q9SWH5
C	38	HIS	-	expression tag	UNP Q9SWH5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	39	HIS	-	expression tag	UNP Q9SWH5
C	40	HIS	-	expression tag	UNP Q9SWH5
C	41	HIS	-	expression tag	UNP Q9SWH5
C	42	HIS	-	expression tag	UNP Q9SWH5
C	43	HIS	-	expression tag	UNP Q9SWH5
C	44	GLY	-	expression tag	UNP Q9SWH5
C	45	MET	-	expression tag	UNP Q9SWH5
C	46	ALA	-	expression tag	UNP Q9SWH5
C	47	SER	-	expression tag	UNP Q9SWH5
C	48	MET	-	expression tag	UNP Q9SWH5
C	49	THR	-	expression tag	UNP Q9SWH5
C	50	GLY	-	expression tag	UNP Q9SWH5
C	51	GLY	-	expression tag	UNP Q9SWH5
C	52	GLN	-	expression tag	UNP Q9SWH5
C	53	GLN	-	expression tag	UNP Q9SWH5
C	54	MET	-	expression tag	UNP Q9SWH5
C	55	GLY	-	expression tag	UNP Q9SWH5
C	56	ARG	-	expression tag	UNP Q9SWH5
C	57	ASP	-	expression tag	UNP Q9SWH5
C	58	LEU	-	expression tag	UNP Q9SWH5
C	59	TYR	-	expression tag	UNP Q9SWH5
C	60	ASP	-	expression tag	UNP Q9SWH5
C	61	ASP	-	expression tag	UNP Q9SWH5
C	62	ASP	-	expression tag	UNP Q9SWH5
C	63	ASP	-	expression tag	UNP Q9SWH5
C	64	LYS	-	expression tag	UNP Q9SWH5
C	65	SER	-	expression tag	UNP Q9SWH5
C	66	ARG	-	expression tag	UNP Q9SWH5
C	67	LEU	-	expression tag	UNP Q9SWH5
C	68	GLN	-	expression tag	UNP Q9SWH5
D	38	HIS	-	expression tag	UNP Q9SWH5
D	39	HIS	-	expression tag	UNP Q9SWH5
D	40	HIS	-	expression tag	UNP Q9SWH5
D	41	HIS	-	expression tag	UNP Q9SWH5
D	42	HIS	-	expression tag	UNP Q9SWH5
D	43	HIS	-	expression tag	UNP Q9SWH5
D	44	GLY	-	expression tag	UNP Q9SWH5
D	45	MET	-	expression tag	UNP Q9SWH5
D	46	ALA	-	expression tag	UNP Q9SWH5
D	47	SER	-	expression tag	UNP Q9SWH5
D	48	MET	-	expression tag	UNP Q9SWH5
D	49	THR	-	expression tag	UNP Q9SWH5

Continued on next page...

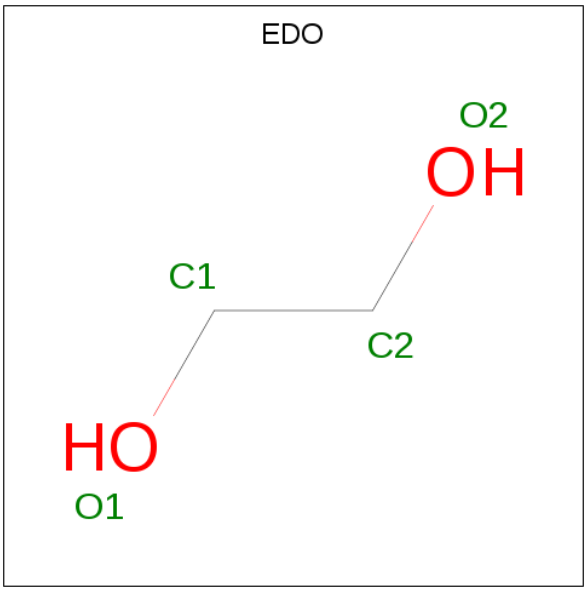
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	50	GLY	-	expression tag	UNP Q9SWH5
D	51	GLY	-	expression tag	UNP Q9SWH5
D	52	GLN	-	expression tag	UNP Q9SWH5
D	53	GLN	-	expression tag	UNP Q9SWH5
D	54	MET	-	expression tag	UNP Q9SWH5
D	55	GLY	-	expression tag	UNP Q9SWH5
D	56	ARG	-	expression tag	UNP Q9SWH5
D	57	ASP	-	expression tag	UNP Q9SWH5
D	58	LEU	-	expression tag	UNP Q9SWH5
D	59	TYR	-	expression tag	UNP Q9SWH5
D	60	ASP	-	expression tag	UNP Q9SWH5
D	61	ASP	-	expression tag	UNP Q9SWH5
D	62	ASP	-	expression tag	UNP Q9SWH5
D	63	ASP	-	expression tag	UNP Q9SWH5
D	64	LYS	-	expression tag	UNP Q9SWH5
D	65	SER	-	expression tag	UNP Q9SWH5
D	66	ARG	-	expression tag	UNP Q9SWH5
D	67	LEU	-	expression tag	UNP Q9SWH5
D	68	GLN	-	expression tag	UNP Q9SWH5

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	D	2	Total Cl 2 2	0	0
2	C	2	Total Cl 2 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is water.

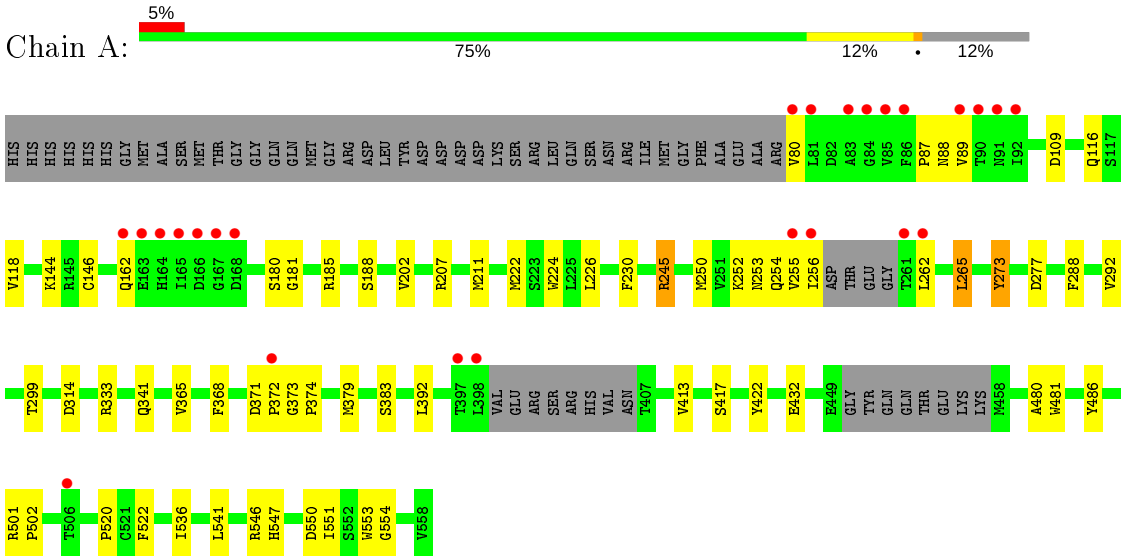
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	179	Total O 179 179	0	0
4	B	159	Total O 159 159	0	0
4	C	194	Total O 194 194	0	0
4	D	123	Total O 123 123	0	0

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

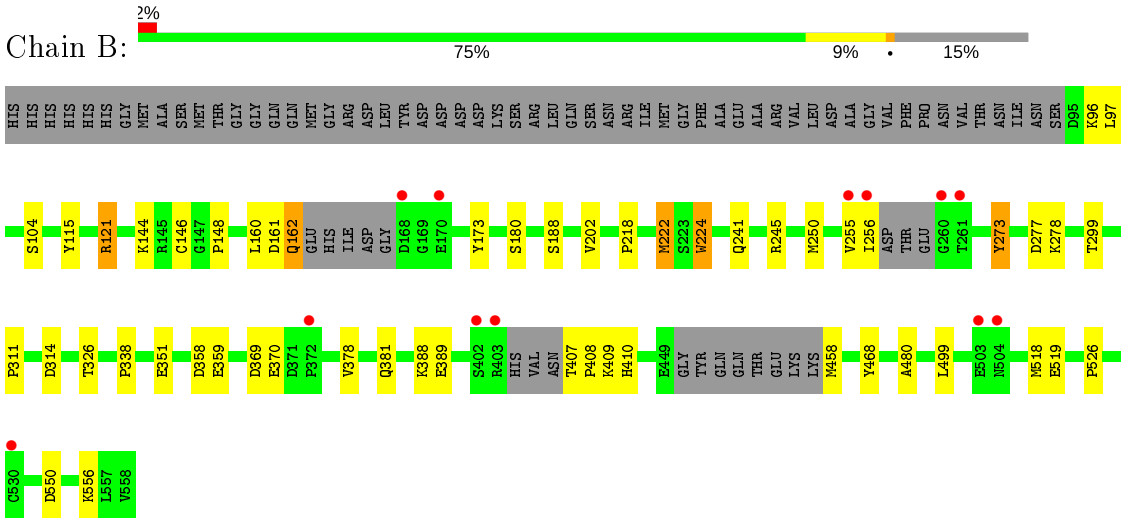
- Molecule 1: Galactoside 2-alpha-L-fucosyltransferase

Chain A:



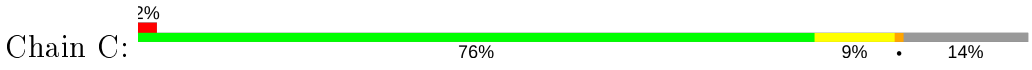
- Molecule 1: Galactoside 2-alpha-L-fucosyltransferase

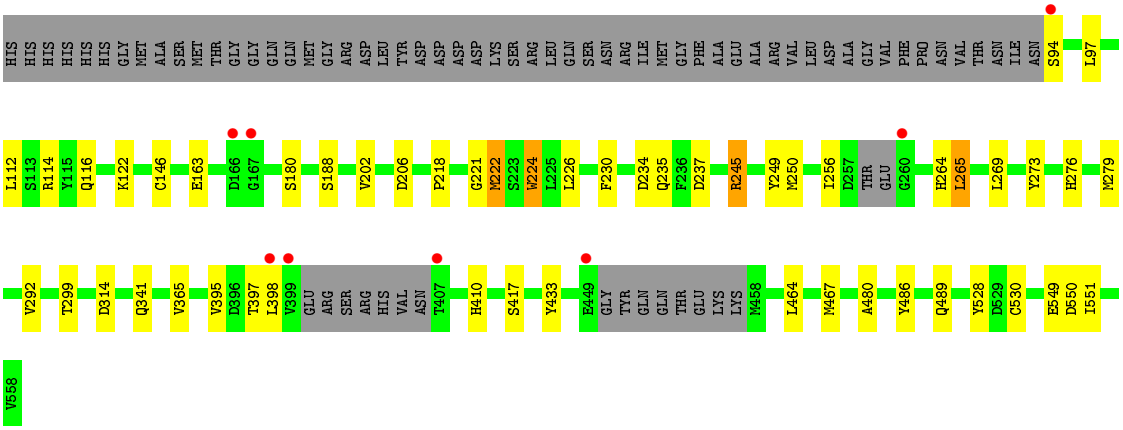
Chain B:



- Molecule 1: Galactoside 2-alpha-L-fucosyltransferase

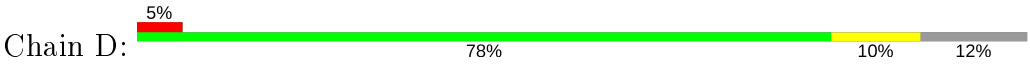
Chain C:

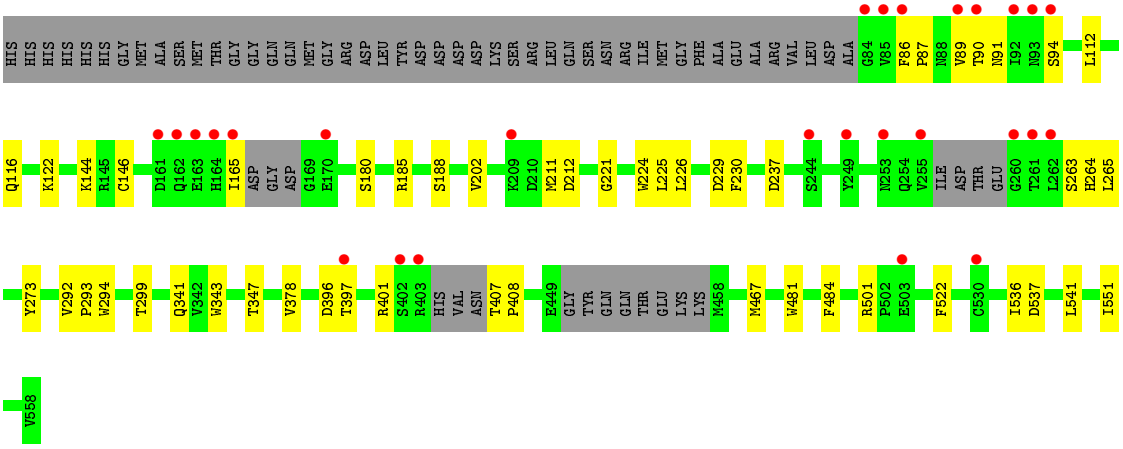




• Molecule 1: Galactoside 2-alpha-L-fucosyltransferase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.84Å 85.86Å 150.47Å 90.00° 96.22° 90.00°	Depositor
Resolution (Å)	43.66 – 2.10 49.24 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.66-2.10) 99.5 (49.24-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.177 , 0.215 0.172 , 0.210	Depositor DCC
R_{free} test set	6452 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.788	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15339	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 10.02% 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, 0.333 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: EDO, CL

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	0.77	1/3809 (0.0%)	0.75	4/5167 (0.1%)
1	B	0.75	0/3705	0.74	0/5020
1	C	0.80	1/3757 (0.0%)	0.78	4/5090 (0.1%)
1	D	0.77	0/3800	0.76	1/5152 (0.0%)
All	All	0.77	2/15071 (0.0%)	0.76	9/20429 (0.0%)

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	553	TRP	CB-CG	-6.34	1.38	1.50
1	C	530	CYS	CB-SG	5.36	1.91	1.82

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	314	ASP	CB-CG-OD1	8.21	125.69	118.30
1	C	314	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	A	265	LEU	CB-CG-CD2	-6.30	100.28	111.00
1	C	265	LEU	CA-CB-CG	5.99	129.06	115.30
1	A	546	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	A	314	ASP	CB-CG-OD1	5.54	123.29	118.30
1	C	206	ASP	CB-CG-OD1	5.30	123.08	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	333	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	D	229	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	410[B]	HIS	Mainchain

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	3705	0	3593	48	0
1	B	3604	0	3503	44	0
1	C	3654	0	3538	35	0
1	D	3696	0	3583	33	0
2	A	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	B	8	0	12	2	0
3	C	8	0	12	0	0
3	D	4	0	6	1	0
4	A	179	0	0	1	0
4	B	159	0	0	1	0
4	C	194	0	0	3	0
4	D	123	0	0	0	0
All	All	15339	0	14247	159	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 5.

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:255:VAL:O	1:A:256:ILE:HG13	1.04	1.22

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:VAL:O	1:A:256:ILE:CG1	1.94	1.14
1:B:407:THR:CG2	1:B:408:PRO:HD2	1.87	1.04
1:A:371:ASP:OD1	1:A:372:PRO:HD2	1.62	0.99
1:B:407:THR:HG23	1:B:408:PRO:HD2	1.46	0.96
1:A:256:ILE:CG2	1:A:288:PHE:CE1	2.53	0.91
1:D:407:THR:HG22	1:D:408:PRO:HD2	1.56	0.86
1:D:91:ASN:HB3	1:D:94:SER:HB3	1.58	0.86
1:C:249:TYR:OH	4:C:701:HOH:O	1.93	0.85
1:A:255:VAL:C	1:A:256:ILE:HG13	1.97	0.84
1:D:397:THR:HG22	1:D:397:THR:O	1.77	0.82
1:D:396:ASP:OD1	1:D:401:ARG:NH2	2.13	0.82
1:B:407:THR:HG22	1:B:408:PRO:HD2	1.63	0.79
1:A:256:ILE:HG23	1:A:288:PHE:CZ	2.19	0.77
1:B:188:SER:HB2	1:B:299:THR:HG23	1.68	0.76
1:D:396:ASP:CG	1:D:401:ARG:HH22	1.90	0.74
1:B:407:THR:CG2	1:B:408:PRO:CD	2.65	0.73
1:A:536:ILE:HD11	1:A:541:LEU:HD21	1.70	0.73
1:D:407:THR:CG2	1:D:408:PRO:HD2	2.18	0.73
1:C:464:LEU:HA	1:C:467:MET:HE3	1.70	0.72
1:D:407:THR:HG22	1:D:408:PRO:CD	2.19	0.72
1:A:256:ILE:HG23	1:A:288:PHE:CE1	2.23	0.72
1:D:407:THR:CG2	1:D:408:PRO:CD	2.67	0.71
1:B:407:THR:HG22	1:B:408:PRO:CD	2.21	0.70
1:A:253:ASN:O	1:A:255:VAL:HG23	1.92	0.69
1:B:218:PRO:HG3	1:B:224:TRP:CE3	2.30	0.67
1:C:234:ASP:OD1	1:C:235:GLN:HG3	1.93	0.67
1:A:245:ARG:HH12	1:A:262:LEU:HD22	1.60	0.66
1:A:87:PRO:C	1:A:89:VAL:H	1.99	0.66
1:D:397:THR:CG2	1:D:397:THR:O	2.46	0.63
1:C:234:ASP:OD1	1:C:235:GLN:N	2.33	0.62
1:D:89:VAL:HG12	1:D:90:THR:N	2.15	0.62
1:C:464:LEU:HA	1:C:467:MET:CE	2.29	0.62
1:A:432:GLU:HG2	1:B:458:MET:SD	2.40	0.61
1:A:368:PHE:HB2	1:A:501:ARG:NH2	2.15	0.61
1:B:121:ARG:CB	1:B:121:ARG:HH21	2.14	0.61
1:B:144:LYS:HA	1:B:222:MET:HG3	1.84	0.60
1:B:121:ARG:NH2	1:B:121:ARG:HB3	2.17	0.59
1:A:80:VAL:HG22	1:A:80:VAL:O	2.02	0.59
1:A:245:ARG:NH1	1:A:262:LEU:HD22	2.17	0.59
1:B:338:PRO:HD3	1:B:468[B]:TYR:OH	2.03	0.58
1:A:188:SER:HB2	1:A:299:THR:HG23	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ILE:CG2	1:A:288:PHE:CZ	2.82	0.58
1:A:256:ILE:HG21	1:A:288:PHE:CE1	2.38	0.57
1:A:87:PRO:C	1:A:89:VAL:N	2.57	0.57
1:B:255:VAL:O	1:B:255:VAL:HG12	2.04	0.57
1:B:96:LYS:HD3	1:B:115:TYR:HB3	1.87	0.56
1:D:536:ILE:HD11	1:D:541:LEU:HD21	1.88	0.56
1:D:89:VAL:CG1	1:D:90:THR:N	2.69	0.56
1:A:250:MET:HE3	1:A:256:ILE:HG12	1.88	0.55
1:B:338:PRO:HD3	1:B:468[B]:TYR:CZ	2.41	0.55
1:B:378:VAL:HG13	3:B:601:EDO:H11	1.88	0.55
1:B:358:ASP:HB2	1:B:409:LYS:HG3	1.88	0.55
1:C:269:LEU:HB2	1:C:299:THR:HB	1.89	0.54
1:C:112:LEU:O	1:C:116:GLN:HB2	2.08	0.54
1:B:407:THR:HG22	1:B:408:PRO:N	2.22	0.53
1:B:311:PRO:HA	1:B:314:ASP:OD2	2.09	0.53
1:D:188:SER:HB2	1:D:299:THR:HG23	1.90	0.53
1:B:161:ASP:O	1:B:162:GLN:HG3	2.09	0.52
1:A:368:PHE:HB2	1:A:501:ARG:HH21	1.74	0.52
1:D:226:LEU:HD11	1:D:230:PHE:CG	2.45	0.52
1:D:89:VAL:O	1:D:90:THR:HB	2.10	0.52
1:C:250:MET:HE1	1:C:265:LEU:HD11	1.91	0.51
1:D:263:SER:O	1:D:293:PRO:HG2	2.11	0.51
1:A:551:ILE:HG23	1:A:551:ILE:O	2.10	0.51
1:A:501:ARG:HD3	1:A:502:PRO:O	2.11	0.51
1:B:160:LEU:C	1:B:162:GLN:H	2.14	0.51
1:B:148:PRO:O	1:B:222:MET:HE1	2.11	0.51
1:C:276:HIS:HA	1:C:279[B]:MET:HG2	1.93	0.50
1:C:250:MET:HE3	1:C:256:ILE:HD13	1.94	0.50
1:A:486:TYR:HB3	1:A:520:PRO:HB3	1.93	0.50
1:C:265:LEU:HD22	1:C:292:VAL:HG21	1.94	0.49
1:D:407:THR:HG23	1:D:408:PRO:CD	2.41	0.49
1:B:245:ARG:HA	1:B:250:MET:HE3	1.93	0.49
1:B:388:LYS:NZ	1:B:389:GLU:OE2	2.45	0.48
1:C:163:GLU:HB3	1:C:245:ARG:HH12	1.79	0.48
1:C:221:GLY:O	1:C:222[A]:MET:HG2	2.14	0.48
1:C:279[B]:MET:HE3	1:C:528:TYR:HE1	1.78	0.48
1:D:112:LEU:O	1:D:116:GLN:HB2	2.14	0.48
1:B:146:CYS:HB2	1:B:202:VAL:HG21	1.95	0.48
1:A:536:ILE:CD1	1:A:541:LEU:HD21	2.40	0.47
1:B:359:GLU:HB2	1:B:409:LYS:HE2	1.96	0.47
1:D:146:CYS:HB2	1:D:202:VAL:HG21	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ARG:NH1	1:D:211:MET:SD	2.88	0.47
1:D:378:VAL:HG13	3:D:601:EDO:H12	1.97	0.46
1:A:226:LEU:HD11	1:A:230:PHE:CG	2.51	0.46
1:B:173:TYR:CD1	1:B:202:VAL:HB	2.50	0.46
1:D:551:ILE:HG23	1:D:551:ILE:O	2.15	0.46
1:A:256:ILE:CG2	1:A:288:PHE:HE1	2.22	0.46
1:D:212:ASP:HB3	1:D:225:LEU:HD11	1.97	0.46
1:C:551:ILE:O	1:C:551:ILE:HG23	2.15	0.46
1:A:501:ARG:CD	1:A:502:PRO:O	2.65	0.45
1:C:226:LEU:HD11	1:C:230:PHE:CD2	2.51	0.45
1:A:146:CYS:HB2	1:A:202:VAL:HG21	1.97	0.45
1:B:161:ASP:C	1:B:162:GLN:HG3	2.37	0.45
1:C:395:VAL:HB	1:C:433:TYR:HB2	1.98	0.45
1:C:549:GLU:H	1:C:549:GLU:CD	2.18	0.45
1:A:365:VAL:HB	1:A:417:SER:HB2	1.98	0.45
1:C:397:THR:C	1:C:398:LEU:HD12	2.37	0.45
1:A:87:PRO:HB2	1:A:89:VAL:HB	1.99	0.45
1:B:519:GLU:O	1:B:556:LYS:HE3	2.17	0.44
1:C:146:CYS:HB2	1:C:202:VAL:HG21	1.99	0.44
1:B:121:ARG:NH2	1:B:121:ARG:CB	2.75	0.44
1:C:365:VAL:HB	1:C:417:SER:HB2	2.00	0.44
1:B:250:MET:HB3	1:B:256:ILE:HG12	1.99	0.44
1:A:144:LYS:HA	1:A:222:MET:HG3	2.00	0.44
1:A:265:LEU:HD22	1:A:292:VAL:HG21	2.00	0.44
1:C:226:LEU:HD11	1:C:230:PHE:CG	2.52	0.43
1:A:109:ASP:HB2	4:A:799:HOH:O	2.19	0.43
1:A:180:SER:OG	1:A:181:GLY:N	2.51	0.43
1:A:480:ALA:HB1	1:A:550:ASP:HB2	1.99	0.43
1:B:97:LEU:HD11	1:B:104:SER:HB3	2.00	0.43
1:C:94:SER:HB3	1:C:97:LEU:HB2	2.01	0.43
1:B:369:ASP:OD1	1:B:370:GLU:N	2.51	0.43
1:D:536:ILE:HG12	1:D:537:ASP:N	2.34	0.43
1:C:188:SER:HB2	1:C:299:THR:HG23	2.01	0.42
1:D:264:HIS:HA	1:D:294:TRP:O	2.20	0.42
1:A:252:LYS:C	1:A:254:GLN:H	2.21	0.42
1:D:122:LYS:H	1:D:122:LYS:HG3	1.54	0.42
1:C:486:TYR:O	1:C:489:GLN:HG2	2.19	0.42
1:A:373:GLY:HA3	1:A:374:PRO:HA	1.71	0.42
1:A:379[B]:MET:HG3	1:A:422:TYR:HD1	1.84	0.42
1:A:547:HIS:HA	1:A:554:GLY:O	2.19	0.42
1:A:87:PRO:O	1:A:89:VAL:N	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:PRO:HD2	1:B:222:MET:HE2	2.02	0.42
1:B:273:TYR:HB2	1:B:277:ASP:CB	2.50	0.42
1:D:467:MET:HE2	1:D:484:PHE:HA	2.02	0.42
1:B:326:THR:HG22	1:B:518:MET:CE	2.50	0.42
1:C:250:MET:HE3	1:C:256:ILE:CD1	2.50	0.41
1:C:256:ILE:HB	4:C:773:HOH:O	2.20	0.41
1:D:343:TRP:O	1:D:347:THR:HG23	2.21	0.41
1:C:218:PRO:HG3	1:C:224:TRP:CE3	2.56	0.41
1:C:250:MET:CE	1:C:265:LEU:HD11	2.50	0.41
1:A:116:GLN:C	1:A:118:VAL:N	2.74	0.41
1:A:392:LEU:HD21	1:A:413:VAL:HG22	2.03	0.41
1:A:481:TRP:CZ2	1:A:501:ARG:HG2	2.56	0.41
1:C:480:ALA:HB1	1:C:550:ASP:HB2	2.03	0.41
1:D:165:ILE:HG23	1:D:263:SER:HA	2.03	0.41
1:B:245:ARG:HA	1:B:245:ARG:HD3	1.83	0.41
1:B:381:GLN:HG2	1:B:499:LEU:HD22	2.02	0.41
1:D:481:TRP:CZ2	1:D:501:ARG:HG2	2.55	0.41
1:C:114:ARG:HD3	4:C:840:HOH:O	2.21	0.41
1:C:279[B]:MET:CE	1:C:528:TYR:CE1	3.03	0.41
1:C:398:LEU:CD1	1:C:398:LEU:N	2.82	0.41
1:D:144:LYS:HE3	1:D:221:GLY:HA3	2.02	0.41
1:A:379[B]:MET:HG3	1:A:422:TYR:CD1	2.55	0.41
1:B:278:LYS:HD3	1:B:526:PRO:HA	2.02	0.41
1:A:273:TYR:HB2	1:A:277:ASP:HB2	2.03	0.41
1:B:245:ARG:HD3	1:B:250:MET:CE	2.51	0.40
1:B:480:ALA:HB1	1:B:550:ASP:HB2	2.03	0.40
1:C:245:ARG:HG3	1:C:264:HIS:NE2	2.36	0.40
1:B:378:VAL:HG13	3:B:601:EDO:C1	2.50	0.40
1:A:181:GLY:O	1:A:185:ARG:HG3	2.22	0.40
1:B:241:GLN:HG3	4:B:760:HOH:O	2.20	0.40
1:A:207:ARG:HA	1:A:211:MET:HB2	2.04	0.40
1:B:160:LEU:C	1:B:162:GLN:N	2.75	0.40
1:D:86:PHE:HA	1:D:87:PRO:HD2	1.84	0.40
1:D:265:LEU:HD22	1:D:292:VAL:HG21	2.03	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	455/521 (87%)	439 (96%)	16 (4%)	0	100	100
1	B	438/521 (84%)	426 (97%)	11 (2%)	1 (0%)	47	49
1	C	446/521 (86%)	433 (97%)	12 (3%)	1 (0%)	47	49
1	D	450/521 (86%)	431 (96%)	18 (4%)	1 (0%)	47	49
All	All	1789/2084 (86%)	1729 (97%)	57 (3%)	3 (0%)	47	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	180	SER
1	B	180	SER
1	D	180	SER

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	412/460 (90%)	403 (98%)	9 (2%)	52	57
1	B	399/460 (87%)	392 (98%)	7 (2%)	59	65
1	C	405/460 (88%)	397 (98%)	8 (2%)	55	60
1	D	410/460 (89%)	405 (99%)	5 (1%)	71	77
All	All	1626/1840 (88%)	1597 (98%)	29 (2%)	60	65

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	162	GLN
1	A	224	TRP
1	A	245	ARG
1	A	273	TYR
1	A	341	GLN
1	A	383[A]	SER
1	A	383[B]	SER
1	A	522	PHE
1	B	121	ARG
1	B	162	GLN
1	B	222	MET
1	B	224	TRP
1	B	273	TYR
1	B	351	GLU
1	B	410	HIS
1	C	122	LYS
1	C	222[A]	MET
1	C	222[B]	MET
1	C	224	TRP
1	C	237	ASP
1	C	245	ARG
1	C	273	TYR
1	C	341	GLN
1	D	224	TRP
1	D	237	ASP
1	D	273	TYR
1	D	341	GLN
1	D	522	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	254	GLN

5.3.3 RNA

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)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	C	601	-	3,3,3	0.59	0	2,2,2	0.60	0
3	EDO	C	602	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	B	601	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	D	601	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	B	602	-	3,3,3	0.46	0	2,2,2	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	601	-	-	0/1/1/1	-
3	EDO	C	602	-	-	1/1/1/1	-
3	EDO	B	601	-	-	1/1/1/1	-
3	EDO	D	601	-	-	1/1/1/1	-
3	EDO	B	602	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	602	EDO	O1-C1-C2-O2
3	D	601	EDO	O1-C1-C2-O2
3	B	602	EDO	O1-C1-C2-O2
3	B	601	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	EDO	2	0
3	D	601	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	459/521 (88%)	0.04	25 (5%)	25	31	20, 35, 75, 113	11 (2%)
1	B	445/521 (85%)	-0.10	12 (2%)	54	60	19, 36, 72, 112	1 (0%)
1	C	448/521 (85%)	-0.14	8 (1%)	68	72	19, 33, 68, 105	0
1	D	457/521 (87%)	0.11	27 (5%)	22	27	20, 40, 77, 124	10 (2%)
All	All	1809/2084 (86%)	-0.02	72 (3%)	38	44	19, 36, 75, 124	22 (1%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	89	VAL	11.6
1	D	165	ILE	7.7
1	D	261	THR	6.8
1	A	166	ASP	5.8
1	D	530	CYS	5.8
1	A	398	LEU	5.6
1	B	256	ILE	5.3
1	D	164	HIS	5.1
1	A	168	ASP	5.1
1	D	260	GLY	4.9
1	A	81	LEU	4.9
1	A	90	THR	4.9
1	C	398	LEU	4.8
1	D	92	ILE	4.8
1	A	164	HIS	4.7
1	B	168	ASP	4.6
1	C	167	GLY	4.5
1	C	166	ASP	4.5
1	D	163	GLU	4.4
1	D	262	LEU	4.3
1	A	256	ILE	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	403	ARG	4.2
1	C	407	THR	3.9
1	A	167	GLY	3.9
1	A	163	GLU	3.9
1	B	260	GLY	3.9
1	B	530	CYS	3.7
1	A	80	VAL	3.7
1	D	84	GLY	3.7
1	A	255	VAL	3.6
1	D	403	ARG	3.5
1	A	89	VAL	3.4
1	D	170	GLU	3.3
1	B	504	ASN	3.3
1	D	255	VAL	3.3
1	B	261	THR	3.2
1	A	85	VAL	3.0
1	C	399	VAL	3.0
1	A	262	LEU	3.0
1	B	255	VAL	3.0
1	A	397	THR	2.9
1	A	86	PHE	2.9
1	A	165	ILE	2.8
1	D	162	GLN	2.8
1	C	260	GLY	2.8
1	D	397	THR	2.7
1	D	94	SER	2.7
1	B	402	SER	2.7
1	A	261	THR	2.6
1	C	94	SER	2.5
1	C	449	GLU	2.5
1	D	503	GLU	2.5
1	D	93	ASN	2.5
1	A	91	ASN	2.5
1	A	92	ILE	2.4
1	D	86	PHE	2.4
1	D	402	SER	2.4
1	D	161	ASP	2.4
1	A	84	GLY	2.3
1	A	162	GLN	2.3
1	B	503	GLU	2.3
1	D	253	ASN	2.2
1	D	90	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	249	TYR	2.2
1	A	372	PRO	2.2
1	B	170	GLU	2.2
1	B	372	PRO	2.2
1	D	85	VAL	2.2
1	A	83	ALA	2.2
1	D	244	SER	2.1
1	A	506	THR	2.0
1	D	209	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. 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	B-factors(Å^2)	Q<0.9
3	EDO	C	602	4/4	0.88	0.17	52,55,58,60	0
3	EDO	B	602	4/4	0.89	0.14	44,51,55,66	0
3	EDO	B	601	4/4	0.91	0.17	33,48,53,56	0
3	EDO	D	601	4/4	0.92	0.20	38,48,56,57	0
2	CL	D	603	1/1	0.95	0.09	45,45,45,45	0
2	CL	A	601	1/1	0.96	0.11	48,48,48,48	0
3	EDO	C	601	4/4	0.96	0.14	38,44,49,52	0
2	CL	C	604	1/1	0.97	0.07	54,54,54,54	0
2	CL	D	602	1/1	0.97	0.09	49,49,49,49	0
2	CL	C	603	1/1	0.98	0.13	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.