Full wwPDB X-ray Structure Validation Report (i)

Feb 20, 2024 – 10:38 AM EST

PDB ID	:	4LDP
Title	:	Spinosyn Forosaminyltransferase SpnP
Authors	:	Isiorho, E.A.; Liu, H.-W.; Keatinge-Clay, A.K.
Deposited on	:	2013-06-24
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 (i) 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 (1)) were used in the production of this report:

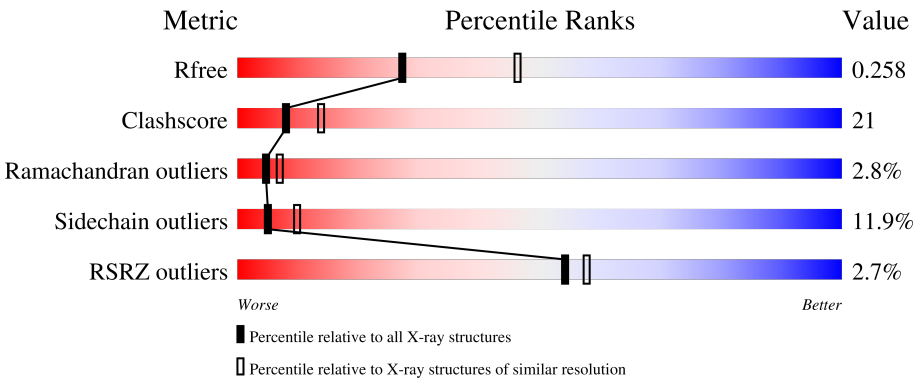
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	455	2% 58% 20% • • 18%
1	B	455	2% 51% 22% 6% • 19%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5856 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 NDP-forosamyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	373	2899	1835	509	542	13	0	0	0
1	B	369	2873	1821	504	535	13	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP Q9ALN7
A	-14	HIS	-	expression tag	UNP Q9ALN7
A	-13	HIS	-	expression tag	UNP Q9ALN7
A	-12	HIS	-	expression tag	UNP Q9ALN7
A	-11	HIS	-	expression tag	UNP Q9ALN7
A	-10	HIS	-	expression tag	UNP Q9ALN7
A	-9	SER	-	expression tag	UNP Q9ALN7
A	-8	SER	-	expression tag	UNP Q9ALN7
A	-7	GLY	-	expression tag	UNP Q9ALN7
A	-6	LEU	-	expression tag	UNP Q9ALN7
A	-5	VAL	-	expression tag	UNP Q9ALN7
A	-4	PRO	-	expression tag	UNP Q9ALN7
A	-3	ARG	-	expression tag	UNP Q9ALN7
A	-2	GLY	-	expression tag	UNP Q9ALN7
A	-1	SER	-	expression tag	UNP Q9ALN7
A	0	HIS	-	expression tag	UNP Q9ALN7
B	-15	HIS	-	expression tag	UNP Q9ALN7
B	-14	HIS	-	expression tag	UNP Q9ALN7
B	-13	HIS	-	expression tag	UNP Q9ALN7
B	-12	HIS	-	expression tag	UNP Q9ALN7
B	-11	HIS	-	expression tag	UNP Q9ALN7
B	-10	HIS	-	expression tag	UNP Q9ALN7
B	-9	SER	-	expression tag	UNP Q9ALN7
B	-8	SER	-	expression tag	UNP Q9ALN7
B	-7	GLY	-	expression tag	UNP Q9ALN7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	LEU	-	expression tag	UNP Q9ALN7
B	-5	VAL	-	expression tag	UNP Q9ALN7
B	-4	PRO	-	expression tag	UNP Q9ALN7
B	-3	ARG	-	expression tag	UNP Q9ALN7
B	-2	GLY	-	expression tag	UNP Q9ALN7
B	-1	SER	-	expression tag	UNP Q9ALN7
B	0	HIS	-	expression tag	UNP Q9ALN7

- Molecule 2 is water.

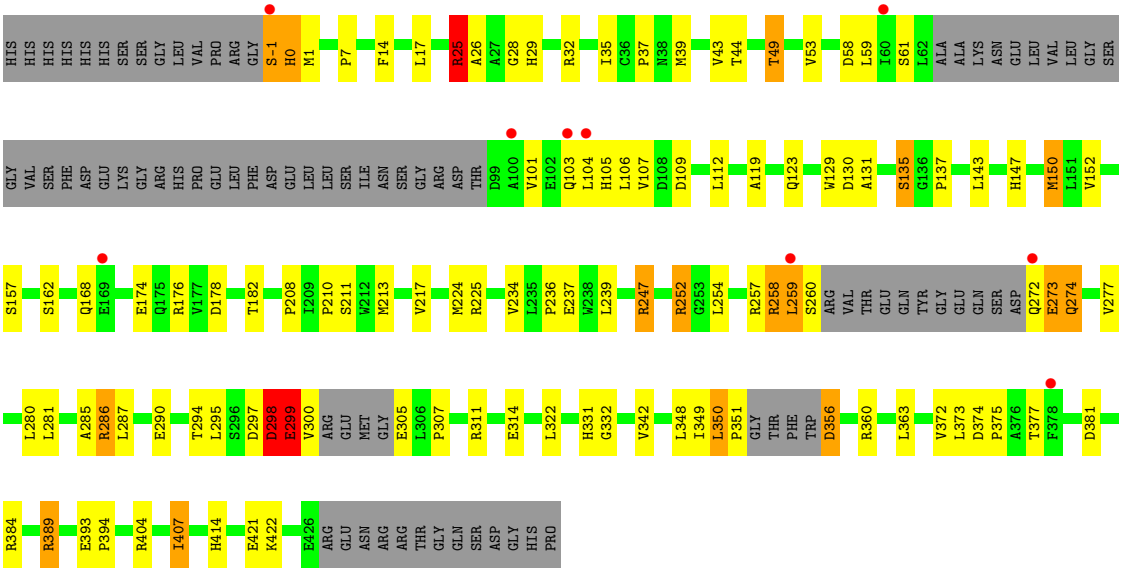
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	36	36	36	0	0
			Total	O		
2	B	48	48	48	0	0

3 Residue-property plots (i)

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

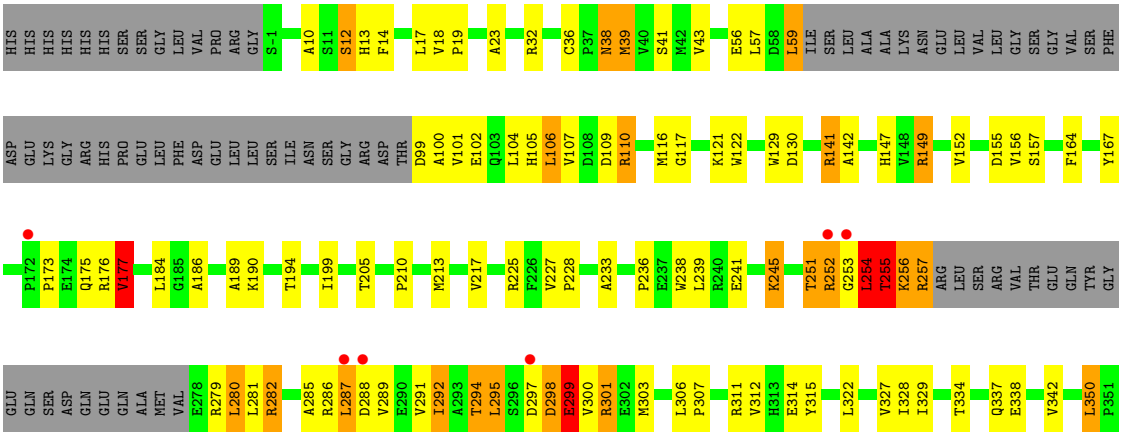
- Molecule 1: NDP-forosamyltransferase

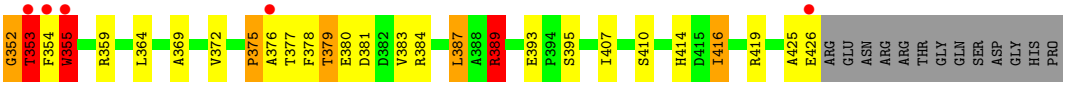
Chain A:



- Molecule 1: NDP-forosamyltransferase

Chain B:




G352
T353
F354
W355
R359
L364
A369
V372
P375
A376
T377
F378
T379
E380
D381
D382
V383
R384
L387
A388
R389
E393
P394
S395
I407
S410
H414
D415
I416
R419
A425
E426
ARG
GLU
ASN
ARG
ARG
THR
GLY
GLN
SER
ASP
GLY
HIS
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	162.42Å 162.42Å 81.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.93 – 2.50 46.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.93-2.50) 99.7 (46.89-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.09 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.200 , 0.257 0.200 , 0.258	Depositor DCC
R_{free} test set	1912 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	57.2	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5856	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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 (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.76	0/2958	0.94	4/4030 (0.1%)
1	B	0.82	0/2937	1.04	12/4005 (0.3%)
All	All	0.79	0/5895	0.99	16/8035 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	149	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	A	25	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	B	149	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	389	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	B	280	LEU	CA-CB-CG	6.71	130.74	115.30
1	B	225	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	B	350	LEU	CA-CB-CG	-6.65	100.00	115.30
1	B	416	ILE	CG1-CB-CG2	-6.15	97.87	111.40
1	A	32	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	B	177	VAL	CB-CA-C	-5.66	100.64	111.40
1	B	149	ARG	CB-CG-CD	-5.42	97.51	111.60
1	B	389	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	B	387	LEU	CA-CB-CG	-5.23	103.28	115.30
1	A	130	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	135	SER	N-CA-CB	-5.04	102.95	110.50
1	B	287	LEU	CB-CG-CD2	-5.00	102.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	299	GLU	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	2899	0	2909	101	0
1	B	2873	0	2870	149	0
2	A	36	0	0	5	0
2	B	48	0	0	3	1
All	All	5856	0	5779	247	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (247) 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:287:LEU:HD21	1:B:380:GLU:O	1.21	1.29
1:B:287:LEU:CD2	1:B:380:GLU:O	1.78	1.28
1:B:301:ARG:HA	1:B:301:ARG:NE	1.38	1.25
1:B:287:LEU:HD22	1:B:380:GLU:CA	1.66	1.24
1:B:287:LEU:CD2	1:B:383:VAL:HB	1.73	1.18
1:B:287:LEU:HD23	1:B:383:VAL:CB	1.75	1.14
1:A:273:GLU:HA	1:A:274:GLN:HB3	1.12	1.12
1:A:299:GLU:HB2	1:A:300:VAL:HB	1.32	1.10
1:B:352:GLY:HA3	1:B:353:THR:CG2	1.84	1.07
1:B:352:GLY:HA3	1:B:353:THR:CB	1.83	1.06
1:A:389:ARG:HG2	1:A:389:ARG:HH11	1.19	1.05
1:B:287:LEU:CD2	1:B:380:GLU:HA	1.88	1.04
1:A:247:ARG:HG3	1:A:247:ARG:HH11	1.19	1.02
1:A:389:ARG:NH1	1:A:393:GLU:OE2	1.90	1.02
1:B:352:GLY:HA3	1:B:353:THR:HG23	1.39	1.01
1:B:287:LEU:CD2	1:B:380:GLU:C	2.33	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LEU:HD22	1:B:380:GLU:HA	0.96	0.96
1:B:301:ARG:NE	1:B:301:ARG:CA	2.30	0.95
1:B:287:LEU:HD23	1:B:383:VAL:HB	0.98	0.94
1:B:287:LEU:HD21	1:B:380:GLU:C	1.88	0.93
1:A:299:GLU:HB2	1:A:300:VAL:CB	1.97	0.93
1:B:301:ARG:HA	1:B:301:ARG:HE	0.98	0.93
1:A:273:GLU:CA	1:A:274:GLN:HB3	1.98	0.91
1:B:252:ARG:HG3	1:B:252:ARG:HH11	1.35	0.90
1:B:354:PHE:O	1:B:355:TRP:HB2	1.70	0.90
1:A:1:MET:H	1:A:29:HIS:HD2	1.15	0.90
1:A:259:LEU:HA	1:A:260:SER:O	1.74	0.88
1:B:289:VAL:HG21	1:B:307:PRO:HG2	1.56	0.87
1:B:379:THR:HG23	1:B:381:ASP:H	1.37	0.87
1:A:389:ARG:HH11	1:A:389:ARG:CG	1.88	0.87
1:A:273:GLU:HA	1:A:274:GLN:CB	2.01	0.87
1:B:295:LEU:N	1:B:295:LEU:HD23	1.88	0.87
1:B:287:LEU:CD1	1:B:380:GLU:O	2.24	0.85
1:A:1:MET:H	1:A:29:HIS:CD2	1.95	0.84
1:A:49:THR:HG22	2:A:512:HOH:O	1.76	0.84
1:A:389:ARG:HH12	1:A:393:GLU:CD	1.79	0.84
1:A:17:LEU:HD23	1:A:150:MET:HE3	1.58	0.84
1:B:129:TRP:HE1	1:B:147:HIS:HD2	1.26	0.84
1:A:123:GLN:HG3	2:A:521:HOH:O	1.77	0.83
1:A:259:LEU:HA	1:A:260:SER:C	1.97	0.83
1:B:252:ARG:O	1:B:254:LEU:N	2.12	0.82
1:B:352:GLY:HA3	1:B:353:THR:OG1	1.79	0.82
1:B:298:ASP:O	1:B:299:GLU:HB2	1.79	0.81
1:B:285:ALA:O	1:B:289:VAL:HG13	1.81	0.80
1:A:298:ASP:C	1:A:299:GLU:HG3	2.03	0.79
1:B:38:ASN:HD22	1:B:38:ASN:H	1.30	0.79
1:A:286:ARG:HG2	1:A:286:ARG:HH11	1.48	0.79
1:B:210:PRO:HG3	1:B:407:ILE:HD11	1.64	0.78
1:A:25:ARG:HH11	1:A:25:ARG:CG	1.97	0.78
1:B:352:GLY:CA	1:B:353:THR:OG1	2.32	0.77
2:A:502:HOH:O	1:B:414:HIS:HD2	1.68	0.77
1:B:287:LEU:CG	1:B:380:GLU:O	2.34	0.76
1:A:298:ASP:O	1:A:299:GLU:HG3	1.85	0.76
1:B:287:LEU:CG	1:B:383:VAL:HB	2.16	0.75
1:B:300:VAL:HG22	1:B:301:ARG:NH2	2.01	0.75
1:B:256:LYS:HA	1:B:257:ARG:C	2.08	0.75
1:B:286:ARG:O	1:B:289:VAL:HG22	1.86	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:VAL:HG22	1:A:305:GLU:N	2.02	0.74
1:B:352:GLY:CA	1:B:353:THR:HG23	2.17	0.74
1:B:287:LEU:HD22	1:B:380:GLU:C	2.02	0.74
1:B:141:ARG:NH1	1:B:194:THR:O	2.20	0.74
1:A:29:HIS:HE1	1:A:421:GLU:OE2	1.71	0.73
1:B:287:LEU:HD11	1:B:380:GLU:O	1.89	0.72
1:B:375:PRO:O	1:B:377:THR:N	2.22	0.72
1:A:17:LEU:HD23	1:A:150:MET:CE	2.21	0.71
1:A:210:PRO:HG3	1:A:407:ILE:CD1	2.21	0.71
1:A:25:ARG:HH11	1:A:25:ARG:HG3	1.56	0.70
1:B:129:TRP:HE1	1:B:147:HIS:CD2	2.08	0.70
1:A:247:ARG:HG3	1:A:247:ARG:NH1	1.97	0.70
1:A:298:ASP:C	1:A:299:GLU:CG	2.61	0.70
1:B:213:MET:CE	1:B:364:LEU:CD2	2.69	0.70
1:A:374:ASP:OD2	1:A:377:THR:HG23	1.91	0.69
1:B:352:GLY:CA	1:B:353:THR:CB	2.68	0.69
1:B:10:ALA:HB1	1:B:256:LYS:HE2	1.73	0.69
1:B:301:ARG:CA	1:B:301:ARG:HE	1.92	0.69
1:B:116:MET:HE1	1:B:142:ALA:HB3	1.75	0.69
1:A:106:LEU:HB2	1:A:135:SER:HB2	1.76	0.67
1:A:356:ASP:OD2	1:A:360:ARG:HD3	1.94	0.67
1:B:256:LYS:N	1:B:257:ARG:HG2	2.10	0.67
1:A:213:MET:CE	1:A:360:ARG:HG2	2.25	0.67
1:B:287:LEU:HD23	1:B:383:VAL:CG2	2.24	0.66
1:A:213:MET:HE2	1:A:360:ARG:HG2	1.78	0.66
1:B:252:ARG:HH12	1:B:257:ARG:H	1.44	0.65
1:B:213:MET:CE	1:B:364:LEU:HD22	2.26	0.65
1:B:117:GLY:O	1:B:121:LYS:HE2	1.97	0.65
1:A:286:ARG:HH11	1:A:286:ARG:CG	2.09	0.65
1:A:300:VAL:HG13	1:A:305:GLU:N	2.12	0.65
1:B:12:SER:H	1:B:256:LYS:NZ	1.94	0.65
1:A:17:LEU:CD2	1:A:150:MET:HE3	2.27	0.64
1:B:295:LEU:N	1:B:295:LEU:CD2	2.61	0.64
1:B:12:SER:H	1:B:256:LYS:HZ3	1.43	0.64
1:B:287:LEU:CD2	1:B:380:GLU:CA	2.50	0.64
1:B:364:LEU:HD12	1:B:369:ALA:HB3	1.79	0.64
1:B:282:ARG:NH2	1:B:303:MET:O	2.31	0.63
1:A:0:HIS:HB3	2:A:523:HOH:O	1.98	0.63
1:B:288:ASP:CG	1:B:387:LEU:HD22	2.19	0.63
1:B:213:MET:HE3	1:B:364:LEU:HD22	1.81	0.62
1:B:299:GLU:HG2	1:B:300:VAL:O	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ARG:HG2	1:A:257:ARG:HD3	1.82	0.62
1:B:141:ARG:HG3	1:B:199:ILE:HD11	1.82	0.62
1:A:129:TRP:HE1	1:A:147:HIS:HD2	1.48	0.61
1:B:379:THR:HG23	1:B:381:ASP:N	2.11	0.61
1:A:210:PRO:HG3	1:A:407:ILE:HD13	1.81	0.60
1:B:252:ARG:HH11	1:B:252:ARG:CG	2.10	0.60
1:A:298:ASP:C	1:A:298:ASP:OD2	2.39	0.60
1:B:141:ARG:CG	1:B:199:ILE:HD11	2.32	0.59
1:B:186:ALA:O	1:B:189:ALA:HB3	2.02	0.59
1:A:300:VAL:CG2	1:A:305:GLU:N	2.64	0.59
1:B:254:LEU:HG	1:B:255:THR:N	2.17	0.59
1:B:213:MET:HE1	1:B:364:LEU:CD2	2.32	0.58
1:A:7:PRO:HB3	1:A:17:LEU:CD1	2.34	0.58
1:B:110:ARG:HH11	1:B:110:ARG:HB3	1.68	0.58
1:B:156:VAL:HG21	1:B:355:TRP:CZ2	2.38	0.58
1:B:288:ASP:OD2	1:B:329:ILE:HD11	2.03	0.57
1:A:252:ARG:HH11	1:A:331:HIS:CD2	2.23	0.57
1:B:300:VAL:O	1:B:301:ARG:HG2	2.04	0.56
1:A:294:THR:O	1:A:295:LEU:HD23	2.05	0.56
1:B:289:VAL:HG21	1:B:307:PRO:CG	2.32	0.56
1:B:104:LEU:HD22	1:B:105:HIS:CD2	2.41	0.56
1:A:101:VAL:O	1:A:105:HIS:HD2	1.89	0.55
1:B:152:VAL:O	1:B:334:THR:HG21	2.07	0.55
1:B:99:ASP:O	1:B:101:VAL:N	2.40	0.55
1:A:257:ARG:O	1:A:260:SER:HB3	2.07	0.55
1:B:59:LEU:N	1:B:59:LEU:HD12	2.22	0.55
1:B:254:LEU:HD21	1:B:256:LYS:HD2	1.89	0.55
1:B:295:LEU:HD23	1:B:295:LEU:H	1.70	0.54
1:A:29:HIS:CE1	1:A:421:GLU:OE2	2.57	0.54
1:B:38:ASN:H	1:B:38:ASN:ND2	2.00	0.54
1:B:149:ARG:NH2	1:B:155:ASP:OD1	2.40	0.54
1:A:389:ARG:NH1	1:A:389:ARG:CG	2.58	0.54
1:B:255:THR:O	1:B:256:LYS:HG3	2.07	0.53
1:B:301:ARG:HA	1:B:301:ARG:CZ	2.28	0.53
1:A:273:GLU:CA	1:A:274:GLN:CB	2.73	0.53
1:A:414:HIS:CD2	1:B:414:HIS:CD2	2.97	0.53
1:B:173:PRO:HA	1:B:176:ARG:HG3	1.89	0.53
1:A:300:VAL:CG1	1:A:305:GLU:N	2.72	0.52
1:B:99:ASP:HB3	1:B:102:GLU:HB2	1.90	0.52
1:B:414:HIS:HE1	2:B:524:HOH:O	1.91	0.52
1:A:7:PRO:HB3	1:A:17:LEU:HD11	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ARG:HG3	1:A:25:ARG:NH1	2.23	0.52
1:A:129:TRP:CD2	1:A:137:PRO:HD3	2.45	0.52
1:A:174:GLU:H	1:A:174:GLU:CD	2.13	0.51
1:A:389:ARG:HG2	1:A:389:ARG:NH1	2.03	0.51
1:B:156:VAL:HG23	1:B:157:SER:H	1.75	0.51
1:B:256:LYS:H	1:B:257:ARG:HG2	1.74	0.51
1:A:210:PRO:HG3	1:A:407:ILE:HD11	1.92	0.51
1:B:252:ARG:CG	1:B:252:ARG:NH1	2.71	0.50
1:A:58:ASP:OD1	1:A:61:SER:HB3	2.11	0.50
1:A:35:ILE:HG13	1:A:39:MET:HB2	1.93	0.50
1:B:372:VAL:HG12	2:B:541:HOH:O	2.11	0.50
1:A:299:GLU:HB2	1:A:300:VAL:CG2	2.42	0.50
1:B:342:VAL:HG12	1:B:407:ILE:HG21	1.94	0.50
1:A:348:LEU:HD11	1:A:373:LEU:HG	1.94	0.49
1:B:13:HIS:HB3	1:B:130:ASP:OD2	2.12	0.49
1:B:106:LEU:CD1	1:B:106:LEU:N	2.76	0.49
1:B:252:ARG:C	1:B:254:LEU:H	2.13	0.49
1:B:300:VAL:HG13	1:B:301:ARG:NH1	2.28	0.49
1:B:12:SER:HB3	1:B:254:LEU:HD11	1.95	0.49
1:A:298:ASP:OD2	1:A:299:GLU:N	2.46	0.49
1:B:149:ARG:O	1:B:205:THR:HA	2.13	0.49
1:A:129:TRP:HE1	1:A:147:HIS:CD2	2.29	0.48
1:B:32:ARG:HG2	1:B:122:TRP:CH2	2.48	0.48
1:A:225:ARG:HG3	1:A:407:ILE:HG22	1.95	0.48
1:A:286:ARG:CG	1:A:286:ARG:NH1	2.72	0.48
1:A:119:ALA:HB1	1:A:143:LEU:HD11	1.95	0.48
1:A:287:LEU:CD1	1:A:384:ARG:HG2	2.44	0.48
1:B:38:ASN:HD21	1:B:57:LEU:H	1.61	0.48
1:B:175:GLN:O	1:B:177:VAL:HG22	2.14	0.48
1:A:372:VAL:HG12	1:A:373:LEU:N	2.30	0.47
1:B:389:ARG:HG2	1:B:393:GLU:OE2	2.14	0.47
1:A:49:THR:HG23	2:A:503:HOH:O	2.13	0.47
1:B:156:VAL:HG21	1:B:355:TRP:CE2	2.49	0.47
1:B:41:SER:HB3	2:B:544:HOH:O	2.15	0.47
1:B:389:ARG:CG	1:B:393:GLU:OE2	2.62	0.47
1:A:26:ALA:HB1	1:B:23:ALA:HB2	1.96	0.47
1:B:287:LEU:HD13	1:B:380:GLU:HB3	1.97	0.47
1:B:252:ARG:HG3	1:B:252:ARG:NH1	2.13	0.47
1:B:352:GLY:N	1:B:353:THR:OG1	2.48	0.47
1:B:12:SER:HB3	1:B:254:LEU:CD1	2.45	0.46
1:A:389:ARG:NH1	1:A:393:GLU:CD	2.53	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:VAL:HB	1:B:19:PRO:HD3	1.98	0.46
1:B:291:VAL:HG12	1:B:292:ILE:N	2.31	0.46
1:B:245:LYS:HG3	1:B:294:THR:HG22	1.97	0.46
1:B:375:PRO:HA	1:B:378:PHE:HD1	1.80	0.46
1:B:287:LEU:CB	1:B:383:VAL:HB	2.46	0.46
1:A:35:ILE:CG1	1:A:39:MET:HB2	2.46	0.45
1:A:252:ARG:HG3	1:A:257:ARG:HG2	1.98	0.45
1:A:298:ASP:O	1:A:299:GLU:CG	2.61	0.45
1:B:116:MET:CE	1:B:142:ALA:HB3	2.45	0.45
1:A:208:PRO:HA	1:A:224:MET:O	2.16	0.45
1:A:299:GLU:HB2	1:A:300:VAL:CA	2.46	0.45
1:B:327:VAL:HG12	1:B:328:ILE:N	2.31	0.45
1:B:282:ARG:HH12	1:B:286:ARG:CZ	2.30	0.45
1:B:287:LEU:HB2	1:B:380:GLU:HG2	1.99	0.45
1:B:353:THR:HB	1:B:354:PHE:H	1.29	0.45
1:B:213:MET:HE3	1:B:364:LEU:CD2	2.44	0.45
1:A:281:LEU:HD12	1:A:281:LEU:HA	1.65	0.45
1:B:164:PHE:C	1:B:164:PHE:CD2	2.89	0.45
1:A:280:LEU:HD21	1:A:350:LEU:HD13	1.99	0.45
1:B:334:THR:O	1:B:338:GLU:HG2	2.16	0.44
1:B:254:LEU:O	1:B:256:LYS:N	2.51	0.44
1:A:49:THR:HB	1:B:233:ALA:HB3	2.00	0.44
1:A:373:LEU:O	1:A:375:PRO:HD3	2.18	0.44
1:B:38:ASN:ND2	1:B:56:GLU:HA	2.33	0.44
1:B:337:GLN:OE1	1:B:364:LEU:HD23	2.17	0.44
1:A:322:LEU:HD23	1:A:322:LEU:HA	1.83	0.44
1:B:110:ARG:HB3	1:B:110:ARG:NH1	2.32	0.44
1:A:247:ARG:NH1	1:A:290:GLU:OE1	2.51	0.43
1:A:258:ARG:H	1:A:258:ARG:HG2	1.68	0.43
1:B:282:ARG:HH12	1:B:286:ARG:NH1	2.16	0.43
1:A:14:PHE:CZ	1:A:43:VAL:HA	2.54	0.43
1:B:106:LEU:N	1:B:106:LEU:HD12	2.33	0.43
1:A:107:VAL:HG23	1:A:112:LEU:HD22	2.00	0.43
1:A:234:VAL:O	1:A:236:PRO:HD3	2.19	0.43
1:B:104:LEU:HD23	1:B:104:LEU:O	2.19	0.43
1:B:241:GLU:OE1	1:B:241:GLU:HA	2.19	0.43
1:A:393:GLU:HA	1:A:394:PRO:HD3	1.85	0.43
1:B:306:LEU:HD22	1:B:306:LEU:H	1.84	0.42
1:B:251:THR:HG22	1:B:298:ASP:OD2	2.19	0.42
1:B:227:VAL:HA	1:B:228:PRO:HD3	1.85	0.42
1:A:332:GLY:O	1:A:360:ARG:NH2	2.41	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LEU:HB3	1:B:383:VAL:CG1	2.49	0.42
1:A:168:GLN:HG3	1:A:176:ARG:HB3	2.01	0.42
1:A:178:ASP:O	1:A:182:THR:HG23	2.20	0.42
1:B:14:PHE:CZ	1:B:43:VAL:HA	2.54	0.42
1:B:141:ARG:O	1:B:141:ARG:HD3	2.20	0.42
1:A:287:LEU:HD13	1:A:384:ARG:HG2	2.01	0.42
1:B:282:ARG:HG3	1:B:282:ARG:HH11	1.85	0.42
1:B:425:ALA:O	1:B:426:GLU:C	2.59	0.41
1:A:104:LEU:HD12	1:A:105:HIS:CD2	2.55	0.41
1:A:213:MET:HE1	1:A:360:ARG:HG2	2.02	0.41
1:B:281:LEU:HD11	1:B:303:MET:SD	2.61	0.41
1:A:-1:SER:HA	1:A:28:GLY:O	2.20	0.41
1:A:272:GLN:N	1:A:274:GLN:HG2	2.35	0.41
1:A:274:GLN:O	1:A:277:VAL:HG22	2.20	0.41
1:B:19:PRO:HG2	1:B:227:VAL:O	2.19	0.41
1:A:285:ALA:CB	1:A:307:PRO:HG2	2.51	0.41
1:B:287:LEU:HG	1:B:384:ARG:N	2.35	0.41
1:B:322:LEU:HD23	1:B:322:LEU:HA	1.84	0.41
1:A:349:ILE:O	1:A:351:PRO:HD3	2.21	0.41
1:B:213:MET:HE1	1:B:364:LEU:HD23	2.00	0.41
1:B:236:PRO:HD2	1:B:239:LEU:HD12	2.02	0.41
1:A:297:ASP:O	1:A:298:ASP:HB3	2.20	0.40
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.93	0.40
1:B:297:ASP:OD2	1:B:312:VAL:HA	2.21	0.40
1:B:300:VAL:HG22	1:B:301:ARG:HH22	1.85	0.40
1:B:36:CYS:SG	1:B:39:MET:HG3	2.62	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:532:HOH:O	2:B:532:HOH:O[7_556]	1.21	0.99

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	363/455 (80%)	338 (93%)	17 (5%)	8 (2%)	6 10
1	B	363/455 (80%)	337 (93%)	14 (4%)	12 (3%)	4 5
All	All	726/910 (80%)	675 (93%)	31 (4%)	20 (3%)	5 7

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	LEU
1	A	274	GLN
1	B	100	ALA
1	B	253	GLY
1	B	254	LEU
1	B	256	LYS
1	B	353	THR
1	B	355	TRP
1	A	131	ALA
1	A	299	GLU
1	B	255	THR
1	B	299	GLU
1	A	286	ARG
1	A	298	ASP
1	B	376	ALA
1	A	109	ASP
1	B	190	LYS
1	B	375	PRO
1	A	211	SER
1	B	352	GLY

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	317/386 (82%)	284 (90%)	33 (10%)	7 13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	312/386 (81%)	270 (86%)	42 (14%)	4 7
All	All	629/772 (82%)	554 (88%)	75 (12%)	5 10

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	0	HIS
1	A	25	ARG
1	A	37	PRO
1	A	44	THR
1	A	49	THR
1	A	53	VAL
1	A	59	LEU
1	A	103	GLN
1	A	150	MET
1	A	152	VAL
1	A	157	SER
1	A	162	SER
1	A	217	VAL
1	A	237	GLU
1	A	247	ARG
1	A	252	ARG
1	A	254	LEU
1	A	258	ARG
1	A	273	GLU
1	A	298	ASP
1	A	299	GLU
1	A	311	ARG
1	A	314	GLU
1	A	342	VAL
1	A	350	LEU
1	A	356	ASP
1	A	363	LEU
1	A	381	ASP
1	A	389	ARG
1	A	404	ARG
1	A	407	ILE
1	A	422	LYS
1	B	12	SER
1	B	17	LEU
1	B	38	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	39	MET
1	B	59	LEU
1	B	106	LEU
1	B	107	VAL
1	B	109	ASP
1	B	110	ARG
1	B	141	ARG
1	B	167	TYR
1	B	177	VAL
1	B	184	LEU
1	B	217	VAL
1	B	238	TRP
1	B	245	LYS
1	B	251	THR
1	B	252	ARG
1	B	254	LEU
1	B	255	THR
1	B	257	ARG
1	B	279	ARG
1	B	280	LEU
1	B	282	ARG
1	B	292	ILE
1	B	294	THR
1	B	295	LEU
1	B	298	ASP
1	B	301	ARG
1	B	311	ARG
1	B	314	GLU
1	B	315	TYR
1	B	350	LEU
1	B	353	THR
1	B	355	TRP
1	B	359	ARG
1	B	379	THR
1	B	389	ARG
1	B	395	SER
1	B	410	SER
1	B	416	ILE
1	B	419	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	105	HIS
1	A	147	HIS
1	A	230	ASN
1	A	343	ASN
1	B	0	HIS
1	B	38	ASN
1	B	103	GLN
1	B	105	HIS
1	B	147	HIS
1	B	414	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	373/455 (81%)	0.02	9 (2%)	59	62	34, 59, 96, 125	0
1	B	369/455 (81%)	-0.02	11 (2%)	50	53	33, 53, 102, 135	0
All	All	742/910 (81%)	-0.00	20 (2%)	54	58	33, 56, 101, 135	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	354	PHE	6.2
1	A	60	ILE	5.2
1	A	259	LEU	4.2
1	B	355	TRP	3.6
1	A	104	LEU	3.3
1	A	378	PHE	3.3
1	B	252	ARG	3.2
1	B	288	ASP	3.0
1	B	426	GLU	2.9
1	B	287	LEU	2.9
1	B	297	ASP	2.8
1	A	100	ALA	2.7
1	A	169	GLU	2.7
1	B	353	THR	2.6
1	A	103	GLN	2.4
1	B	376	ALA	2.4
1	A	-1	SER	2.2
1	B	253	GLY	2.1
1	B	172	PRO	2.0
1	A	272	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.