Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:22 am BST

PDB ID	:	5IZ1
Title	:	Physcomitrella patens FBPase
Authors	:	Einsle, O.; Guetle, D.
Deposited on	:	2016-03-24
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

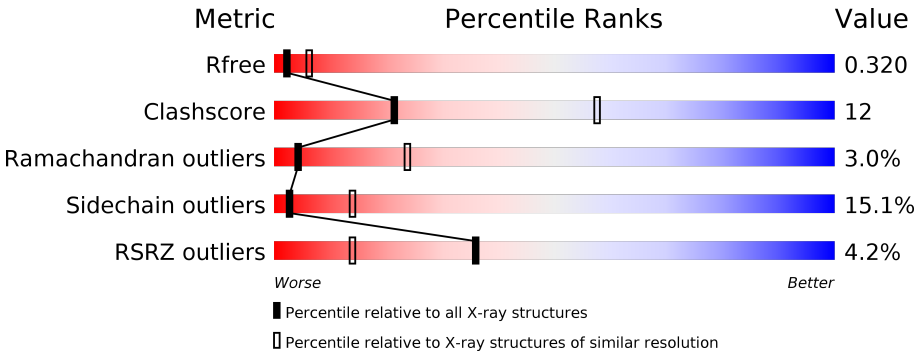
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	337	5% 64% 23% 7% • 5%
1	B	337	2% 64% 23% 7% • 5%
1	C	337	2% 67% 20% 7% • 5%
1	D	337	7% 65% 24% 6% • 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9856 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 fructose-1,6-bisphosphatase.

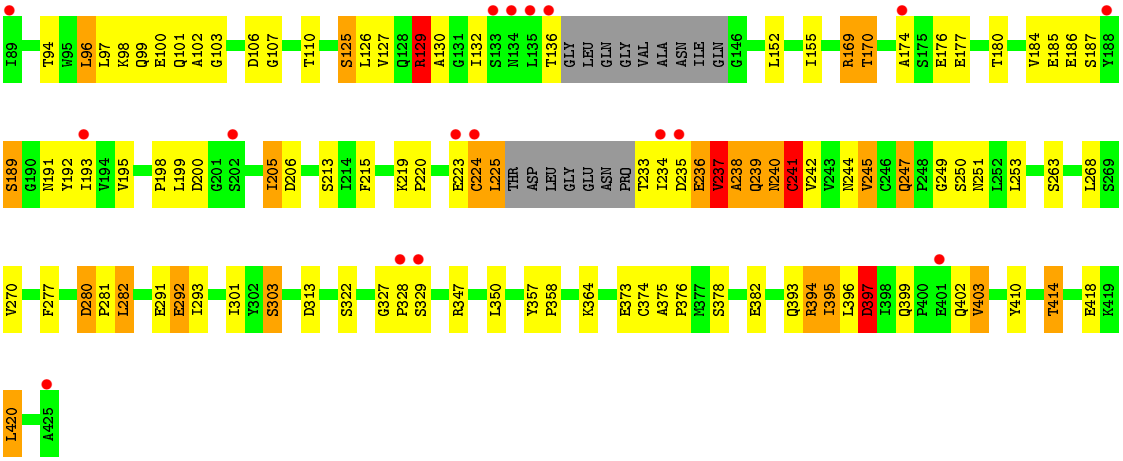
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2464	1561	402	491	10			
1	B	321	Total	C	N	O	S	0	0	0
			2464	1561	402	491	10			
1	C	321	Total	C	N	O	S	0	0	0
			2464	1561	402	491	10			
1	D	321	Total	C	N	O	S	0	0	0
			2464	1561	402	491	10			

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 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.

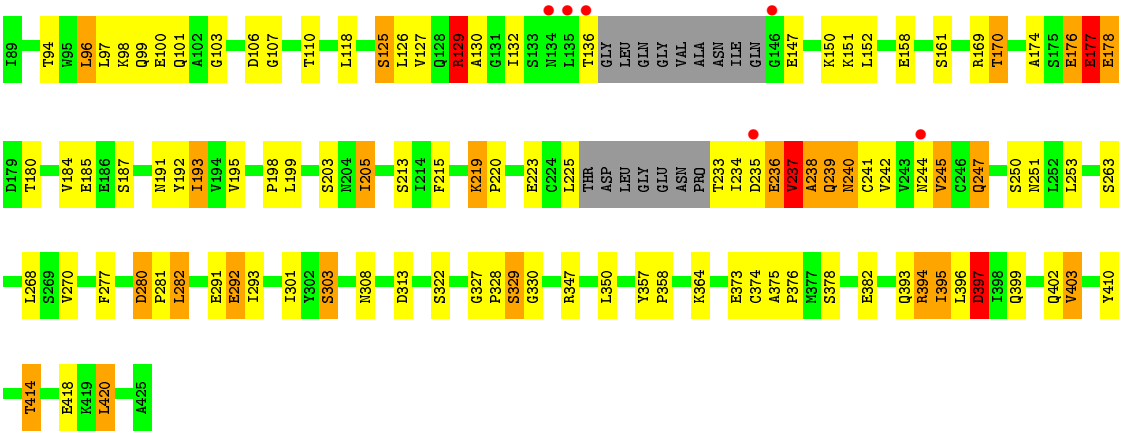
- Molecule 1: fructose-1,6-bisphosphatase

Chain A:



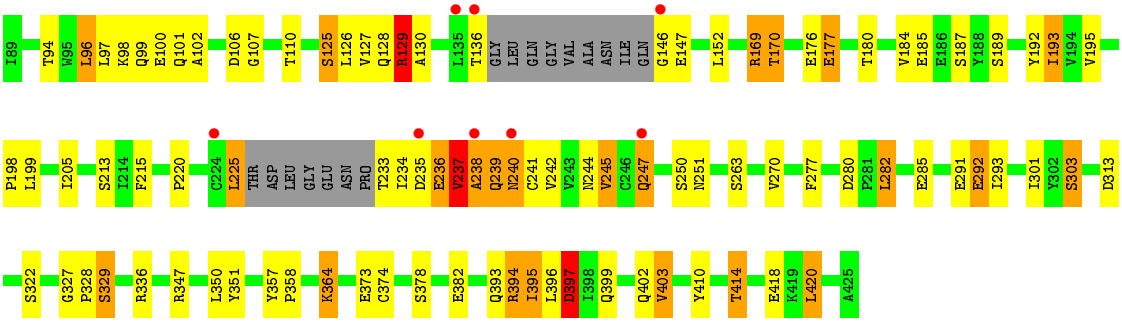
- Molecule 1: fructose-1,6-bisphosphatase

Chain B:

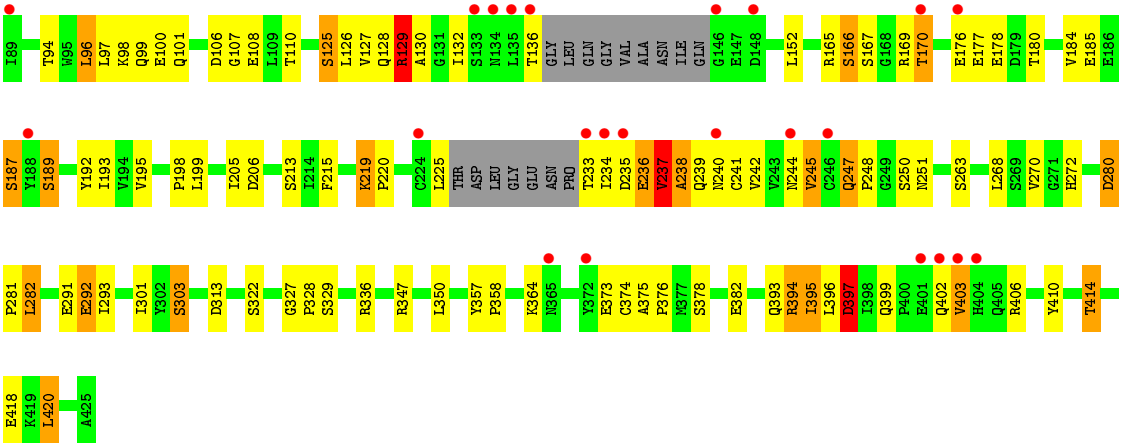


- Molecule 1: fructose-1,6-bisphosphatase

Chain C:



- Molecule 1: fructose-1,6-bisphosphatase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.08Å 84.80Å 105.75Å 90.00° 104.59° 90.00°	Depositor
Resolution (Å)	102.34 – 3.00 44.82 – 3.00	Depositor EDS
% Data completeness (in resolution range)	73.0 (102.34-3.00) 73.0 (44.82-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.50 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.254 , 0.315 0.256 , 0.320	Depositor DCC
R_{free} test set	931 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	48.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	9856	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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

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	0.52	0/2510	0.73	3/3395 (0.1%)
1	B	0.55	0/2510	0.74	1/3395 (0.0%)
1	C	0.54	0/2510	0.72	0/3395
1	D	0.50	0/2510	0.72	2/3395 (0.1%)
All	All	0.53	0/10040	0.73	6/13580 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	280	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	241	CYS	CA-CB-SG	-5.99	103.22	114.00
1	B	280	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	169	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	D	129	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	280	ASP	CB-CG-OD2	5.41	123.17	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2464	0	2425	70	1
1	B	2464	0	2424	70	2
1	C	2464	0	2424	63	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2464	0	2424	64	1
All	All	9856	0	9697	234	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (234) 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:C:129:ARG:NH2	1:D:280:ASP:OD1	1.56	1.35
1:A:129:ARG:NH2	1:B:280:ASP:OD1	1.62	1.33
1:C:129:ARG:NH2	1:D:280:ASP:CG	2.21	0.93
1:C:351:TYR:CD1	1:D:205:ILE:HD11	2.10	0.87
1:A:129:ARG:CZ	1:B:280:ASP:OD1	2.26	0.84
1:C:129:ARG:CZ	1:D:280:ASP:OD1	2.27	0.83
1:A:129:ARG:NH2	1:B:280:ASP:CG	2.35	0.79
1:A:223:GLU:O	1:A:223:GLU:HG3	1.82	0.78
1:A:241:CYS:SG	1:A:242:VAL:N	2.57	0.77
1:D:198:PRO:O	1:D:199:LEU:HD23	1.87	0.75
1:C:241:CYS:O	1:C:245:VAL:HG23	1.87	0.74
1:A:198:PRO:O	1:A:199:LEU:HD23	1.87	0.74
1:A:241:CYS:O	1:A:245:VAL:HG23	1.88	0.74
1:B:241:CYS:O	1:B:245:VAL:HG23	1.88	0.74
1:C:198:PRO:O	1:C:199:LEU:HD23	1.88	0.73
1:B:198:PRO:O	1:B:199:LEU:HD23	1.88	0.73
1:D:241:CYS:O	1:D:245:VAL:HG23	1.89	0.73
1:A:174:ALA:O	1:A:176:GLU:OE1	2.06	0.72
1:C:244:ASN:O	1:C:247:GLN:NE2	2.23	0.72
1:B:244:ASN:O	1:B:247:GLN:NE2	2.24	0.70
1:B:235:ASP:O	1:B:238:ALA:HB3	1.92	0.70
1:D:244:ASN:O	1:D:247:GLN:NE2	2.24	0.70
1:A:235:ASP:O	1:A:238:ALA:HB3	1.92	0.69
1:A:244:ASN:O	1:A:247:GLN:NE2	2.25	0.69
1:C:235:ASP:O	1:C:238:ALA:HB3	1.93	0.69
1:D:235:ASP:O	1:D:238:ALA:HB3	1.93	0.69
1:C:129:ARG:CZ	1:D:280:ASP:CG	2.61	0.68
1:A:97:LEU:HD21	1:D:97:LEU:HD21	1.74	0.68
1:C:282:LEU:HB2	1:D:129:ARG:NH2	2.09	0.68
1:C:351:TYR:CG	1:D:205:ILE:HD11	2.29	0.68
1:A:129:ARG:NH2	1:B:282:LEU:HB2	2.09	0.68
1:C:176:GLU:HG2	1:C:177:GLU:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:TYR:CD1	1:D:205:ILE:CD1	2.76	0.67
1:C:327:GLY:HA3	1:C:328:PRO:C	2.16	0.65
1:C:100:GLU:OE2	1:C:107:GLY:HA2	1.97	0.64
1:B:327:GLY:HA3	1:B:328:PRO:C	2.17	0.64
1:D:239:GLN:O	1:D:242:VAL:N	2.29	0.64
1:B:177:GLU:N	1:B:177:GLU:OE1	2.30	0.64
1:A:100:GLU:OE2	1:A:107:GLY:HA2	1.98	0.64
1:D:177:GLU:OE1	1:D:406:ARG:NH2	2.31	0.63
1:C:169:ARG:HH21	1:C:225:LEU:HA	1.63	0.63
1:B:193:ILE:CG1	1:B:220:PRO:HG3	2.28	0.63
1:A:129:ARG:CZ	1:B:280:ASP:CG	2.67	0.63
1:A:239:GLN:O	1:A:242:VAL:N	2.29	0.63
1:D:100:GLU:OE2	1:D:107:GLY:HA2	1.98	0.63
1:A:282:LEU:HB2	1:B:129:ARG:NH2	2.14	0.62
1:B:100:GLU:OE2	1:B:107:GLY:HA2	1.99	0.62
1:A:280:ASP:OD2	1:B:132:ILE:HG21	1.99	0.62
1:C:414:THR:O	1:C:418:GLU:HG3	2.00	0.62
1:A:414:THR:O	1:A:418:GLU:HG3	2.00	0.61
1:C:106:ASP:OD1	1:C:192:TYR:OH	2.16	0.61
1:B:106:ASP:OD1	1:B:192:TYR:OH	2.17	0.61
1:C:169:ARG:NH2	1:C:225:LEU:HA	2.16	0.61
1:D:106:ASP:OD1	1:D:192:TYR:OH	2.17	0.61
1:D:327:GLY:HA3	1:D:328:PRO:C	2.20	0.61
1:D:414:THR:O	1:D:418:GLU:HG3	2.01	0.61
1:A:97:LEU:HD21	1:D:97:LEU:CD2	2.30	0.60
1:A:282:LEU:HB2	1:B:129:ARG:CZ	2.31	0.60
1:D:108:GLU:OE2	1:D:189:SER:OG	2.16	0.60
1:A:327:GLY:HA3	1:A:328:PRO:C	2.22	0.60
1:D:394:ARG:HG2	1:D:397:ASP:HB2	1.83	0.60
1:A:106:ASP:OD1	1:A:192:TYR:OH	2.18	0.60
1:A:394:ARG:HG2	1:A:397:ASP:HB2	1.84	0.60
1:B:394:ARG:HG2	1:B:397:ASP:HB2	1.83	0.60
1:B:414:THR:O	1:B:418:GLU:HG3	2.02	0.60
1:C:394:ARG:HG2	1:C:397:ASP:HB2	1.84	0.60
1:D:127:VAL:O	1:D:130:ALA:HB2	2.02	0.59
1:A:127:VAL:O	1:A:130:ALA:HB2	2.03	0.59
1:C:127:VAL:O	1:C:130:ALA:HB2	2.03	0.59
1:B:127:VAL:O	1:B:130:ALA:HB2	2.03	0.58
1:D:187:SER:OG	1:D:192:TYR:O	2.17	0.58
1:A:129:ARG:CZ	1:B:282:LEU:HB2	2.34	0.58
1:A:129:ARG:HE	1:B:281:PRO:HD2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:GLU:O	1:B:161:SER:OG	2.20	0.58
1:C:239:GLN:O	1:C:242:VAL:N	2.31	0.58
1:B:174:ALA:O	1:B:176:GLU:OE1	2.22	0.57
1:D:219:LYS:NZ	1:D:220:PRO:O	2.32	0.57
1:D:410:TYR:CD1	1:D:420:LEU:CD1	2.87	0.57
1:A:193:ILE:CG1	1:A:220:PRO:HG3	2.35	0.56
1:B:239:GLN:O	1:B:242:VAL:N	2.33	0.56
1:A:281:PRO:HD2	1:B:129:ARG:HE	1.71	0.55
1:B:410:TYR:CD1	1:B:420:LEU:CD1	2.90	0.55
1:A:410:TYR:CD1	1:A:420:LEU:CD1	2.89	0.55
1:A:189:SER:OG	1:A:191:ASN:ND2	2.41	0.54
1:C:410:TYR:CD1	1:C:420:LEU:CD1	2.91	0.54
1:A:224:CYS:SG	1:A:245:VAL:HG21	2.47	0.54
1:A:193:ILE:HG12	1:A:220:PRO:HG3	1.89	0.53
1:C:129:ARG:NH2	1:D:282:LEU:HB2	2.22	0.53
1:A:280:ASP:OD2	1:B:132:ILE:HD13	2.07	0.53
1:C:293:ILE:HD11	1:C:350:LEU:HD23	1.91	0.53
1:B:94:THR:HG22	1:B:98:LYS:HE3	1.92	0.52
1:D:293:ILE:HD11	1:D:350:LEU:HD23	1.92	0.52
1:C:193:ILE:CG1	1:C:220:PRO:HG3	2.39	0.52
1:B:293:ILE:HD11	1:B:350:LEU:HD23	1.92	0.51
1:D:378:SER:OG	1:D:395:ILE:HG21	2.11	0.51
1:A:293:ILE:HD11	1:A:350:LEU:HD23	1.92	0.51
1:C:94:THR:HG22	1:C:98:LYS:HE3	1.92	0.51
1:B:176:GLU:HG2	1:B:177:GLU:OE1	2.11	0.51
1:C:129:ARG:HE	1:D:281:PRO:HD2	1.76	0.51
1:A:125:SER:O	1:A:126:LEU:C	2.50	0.51
1:C:239:GLN:O	1:C:241:CYS:N	2.44	0.51
1:A:291:GLU:O	1:A:292:GLU:C	2.49	0.50
1:A:378:SER:OG	1:A:395:ILE:HG21	2.11	0.50
1:D:291:GLU:O	1:D:292:GLU:C	2.49	0.50
1:C:291:GLU:O	1:C:292:GLU:C	2.50	0.50
1:A:94:THR:HG22	1:A:98:LYS:HE3	1.93	0.50
1:B:378:SER:OG	1:B:395:ILE:HG21	2.11	0.50
1:C:378:SER:OG	1:C:395:ILE:HG21	2.11	0.50
1:A:199:LEU:O	1:A:200:ASP:C	2.51	0.49
1:D:236:GLU:O	1:D:239:GLN:N	2.45	0.49
1:B:239:GLN:O	1:B:241:CYS:N	2.44	0.49
1:B:291:GLU:O	1:B:292:GLU:C	2.51	0.49
1:D:94:THR:HG22	1:D:98:LYS:HE3	1.93	0.49
1:A:239:GLN:O	1:A:241:CYS:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:CYS:O	1:A:378:SER:OG	2.29	0.48
1:D:245:VAL:O	1:D:251:ASN:ND2	2.43	0.48
1:A:192:TYR:O	1:A:193:ILE:HD13	2.14	0.48
1:B:193:ILE:HD11	1:B:220:PRO:HG3	1.96	0.48
1:D:125:SER:O	1:D:126:LEU:C	2.53	0.48
1:B:150:LYS:NZ	1:B:178:GLU:OE2	2.39	0.48
1:B:402:GLN:HG3	1:B:403:VAL:H	1.79	0.48
1:B:97:LEU:HD21	1:C:97:LEU:HD21	1.97	0.47
1:C:239:GLN:O	1:C:240:ASN:C	2.53	0.47
1:C:351:TYR:CG	1:D:205:ILE:CD1	2.97	0.47
1:C:402:GLN:HG3	1:C:403:VAL:H	1.79	0.47
1:D:165:ARG:O	1:D:166:SER:O	2.32	0.47
1:A:132:ILE:HG21	1:B:280:ASP:OD2	2.13	0.47
1:A:245:VAL:O	1:A:251:ASN:ND2	2.44	0.47
1:A:402:GLN:HG3	1:A:403:VAL:H	1.79	0.47
1:C:126:LEU:HB3	1:C:152:LEU:HD11	1.97	0.47
1:C:280:ASP:OD2	1:D:132:ILE:HD13	2.14	0.47
1:D:126:LEU:HB3	1:D:152:LEU:HD11	1.97	0.47
1:B:239:GLN:O	1:B:240:ASN:C	2.53	0.46
1:D:374:CYS:O	1:D:378:SER:OG	2.30	0.46
1:D:239:GLN:O	1:D:240:ASN:C	2.52	0.46
1:B:125:SER:O	1:B:126:LEU:C	2.53	0.46
1:D:166:SER:OG	1:D:167:SER:N	2.48	0.46
1:A:126:LEU:HB3	1:A:152:LEU:HD11	1.97	0.46
1:D:402:GLN:HG3	1:D:403:VAL:H	1.80	0.46
1:A:239:GLN:O	1:A:240:ASN:C	2.54	0.45
1:A:223:GLU:OE1	1:A:225:LEU:HD13	2.17	0.45
1:C:382:GLU:OE1	1:C:396:LEU:HD12	2.16	0.45
1:B:126:LEU:HB3	1:B:152:LEU:HD11	1.97	0.45
1:B:237:VAL:HG13	1:B:238:ALA:H	1.82	0.45
1:B:303:SER:OG	1:B:347:ARG:NH2	2.50	0.45
1:B:220:PRO:HB3	1:B:245:VAL:CG1	2.46	0.45
1:A:224:CYS:SG	1:A:245:VAL:CG2	3.05	0.45
1:B:236:GLU:O	1:B:237:VAL:C	2.55	0.45
1:B:382:GLU:OE1	1:B:396:LEU:HD12	2.17	0.45
1:C:146:GLY:C	1:C:147:GLU:HG3	2.37	0.45
1:C:374:CYS:O	1:C:378:SER:OG	2.30	0.45
1:D:177:GLU:CG	1:D:178:GLU:H	2.29	0.45
1:A:132:ILE:HD13	1:B:280:ASP:OD2	2.16	0.45
1:D:96:LEU:HD13	1:D:110:THR:HG23	1.99	0.45
1:D:236:GLU:O	1:D:237:VAL:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLU:O	1:A:237:VAL:C	2.55	0.44
1:C:237:VAL:HG13	1:C:238:ALA:H	1.81	0.44
1:A:240:ASN:O	1:A:241:CYS:C	2.56	0.44
1:B:236:GLU:O	1:B:239:GLN:N	2.48	0.44
1:C:277:PHE:CD1	1:C:277:PHE:N	2.85	0.44
1:D:382:GLU:OE1	1:D:396:LEU:HD12	2.17	0.44
1:C:236:GLU:O	1:C:239:GLN:N	2.50	0.44
1:D:220:PRO:HB3	1:D:245:VAL:CG1	2.48	0.44
1:A:293:ILE:CD1	1:A:350:LEU:HD23	2.48	0.44
1:A:195:VAL:O	1:A:215:PHE:HA	2.18	0.44
1:C:125:SER:O	1:C:126:LEU:C	2.55	0.44
1:C:327:GLY:HA3	1:C:329:SER:N	2.33	0.44
1:B:203:SER:OG	1:B:205:ILE:HG22	2.18	0.44
1:A:205:ILE:HG22	1:A:206:ASP:N	2.33	0.44
1:A:382:GLU:OE1	1:A:396:LEU:HD12	2.17	0.44
1:C:96:LEU:HD13	1:C:110:THR:HG23	1.99	0.44
1:A:96:LEU:HD13	1:A:110:THR:HG23	2.00	0.43
1:B:293:ILE:CD1	1:B:350:LEU:HD23	2.48	0.43
1:B:358:PRO:HB3	1:B:410:TYR:OH	2.17	0.43
1:A:237:VAL:HG13	1:A:238:ALA:H	1.83	0.43
1:B:308:ASN:N	1:B:308:ASN:HD22	2.16	0.43
1:C:293:ILE:CD1	1:C:350:LEU:HD23	2.48	0.43
1:A:236:GLU:O	1:A:239:GLN:N	2.50	0.43
1:B:277:PHE:CD1	1:B:277:PHE:N	2.86	0.43
1:C:245:VAL:O	1:C:251:ASN:ND2	2.44	0.43
1:A:220:PRO:HB3	1:A:245:VAL:CG1	2.49	0.43
1:C:236:GLU:O	1:C:237:VAL:C	2.56	0.43
1:A:129:ARG:NH1	1:B:280:ASP:OD1	2.52	0.43
1:C:193:ILE:HG13	1:C:220:PRO:HG3	2.01	0.43
1:C:358:PRO:HB3	1:C:410:TYR:OH	2.18	0.43
1:D:303:SER:OG	1:D:336:ARG:O	2.29	0.43
1:D:170:THR:HA	1:D:184:VAL:O	2.18	0.43
1:D:195:VAL:O	1:D:215:PHE:HA	2.18	0.43
1:B:245:VAL:O	1:B:251:ASN:ND2	2.45	0.43
1:C:170:THR:HA	1:C:184:VAL:O	2.19	0.43
1:C:303:SER:OG	1:C:347:ARG:NH2	2.51	0.42
1:B:96:LEU:HD13	1:B:110:THR:HG23	2.00	0.42
1:A:358:PRO:HB3	1:A:410:TYR:OH	2.19	0.42
1:B:327:GLY:HA3	1:B:329:SER:N	2.34	0.42
1:D:358:PRO:HB3	1:D:410:TYR:OH	2.19	0.42
1:A:375:ALA:HB3	1:A:376:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:PRO:HB3	1:B:245:VAL:HG11	2.02	0.42
1:C:98:LYS:HA	1:C:101:GLN:HB2	2.02	0.42
1:D:247:GLN:HA	1:D:248:PRO:HD2	1.89	0.42
1:A:234:ILE:HG22	1:A:239:GLN:HG3	2.02	0.42
1:D:293:ILE:CD1	1:D:350:LEU:HD23	2.49	0.42
1:D:375:ALA:HB3	1:D:376:PRO:HD3	2.02	0.42
1:B:374:CYS:O	1:B:378:SER:OG	2.30	0.42
1:C:303:SER:OG	1:C:336:ARG:O	2.27	0.42
1:C:234:ILE:HG22	1:C:239:GLN:HG3	2.01	0.42
1:A:303:SER:OG	1:A:347:ARG:NH2	2.53	0.42
1:C:129:ARG:CZ	1:D:282:LEU:HB2	2.50	0.41
1:C:195:VAL:O	1:C:215:PHE:HA	2.20	0.41
1:D:234:ILE:HG22	1:D:239:GLN:HG3	2.02	0.41
1:D:410:TYR:CD1	1:D:420:LEU:HD11	2.55	0.41
1:B:193:ILE:CD1	1:B:220:PRO:HG3	2.50	0.41
1:B:234:ILE:HG22	1:B:239:GLN:HG3	2.02	0.41
1:C:327:GLY:CA	1:C:329:SER:N	2.83	0.41
1:D:303:SER:OG	1:D:347:ARG:NH2	2.53	0.41
1:C:220:PRO:HB3	1:C:245:VAL:CG1	2.50	0.41
1:B:170:THR:HA	1:B:184:VAL:O	2.21	0.41
1:A:101:GLN:C	1:A:103:GLY:H	2.23	0.41
1:A:170:THR:HA	1:A:184:VAL:O	2.20	0.41
1:B:101:GLN:C	1:B:103:GLY:H	2.23	0.41
1:D:128:GLN:C	1:D:130:ALA:N	2.74	0.41
1:D:239:GLN:O	1:D:241:CYS:N	2.54	0.41
1:B:195:VAL:O	1:B:215:PHE:HA	2.20	0.41
1:C:125:SER:O	1:C:128:GLN:N	2.54	0.41
1:C:282:LEU:HB2	1:D:129:ARG:CZ	2.51	0.41
1:A:98:LYS:HA	1:A:101:GLN:HB2	2.03	0.41
1:B:327:GLY:CA	1:B:329:SER:N	2.84	0.41
1:B:375:ALA:HB3	1:B:376:PRO:HD3	2.02	0.41
1:D:205:ILE:HG22	1:D:206:ASP:N	2.36	0.40
1:B:328:PRO:C	1:B:330:GLY:H	2.24	0.40
1:A:219:LYS:HB2	1:A:253:LEU:HD11	2.01	0.40
1:B:219:LYS:HB3	1:B:253:LEU:HD11	2.03	0.40
1:B:118:LEU:HD13	1:C:285:GLU:HG3	2.02	0.40
1:D:98:LYS:HA	1:D:101:GLN:HB2	2.03	0.40
1:A:277:PHE:N	1:A:277:PHE:CD1	2.90	0.40

All (3) 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)
1:C:328:PRO:O	1:D:272:HIS:CE1[2_656]	1.72	0.48
1:A:249:GLY:O	1:B:147:GLU:OE1[2_647]	2.02	0.18
1:B:191:ASN:CG	1:C:364:LYS:NZ[2_556]	2.18	0.02

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	315/337 (94%)	274 (87%)	31 (10%)	10 (3%)	4	22
1	B	315/337 (94%)	276 (88%)	29 (9%)	10 (3%)	4	22
1	C	315/337 (94%)	277 (88%)	28 (9%)	10 (3%)	4	22
1	D	315/337 (94%)	273 (87%)	34 (11%)	8 (2%)	5	28
All	All	1260/1348 (94%)	1100 (87%)	122 (10%)	38 (3%)	4	24

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	GLU
1	A	329	SER
1	B	236	GLU
1	B	238	ALA
1	B	329	SER
1	C	236	GLU
1	C	329	SER
1	D	236	GLU
1	D	329	SER
1	A	129	ARG
1	A	238	ALA
1	A	292	GLU
1	B	129	ARG
1	B	292	GLU
1	B	397	ASP

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Mol	Chain	Res	Type
1	C	129	ARG
1	C	238	ALA
1	C	292	GLU
1	C	397	ASP
1	D	129	ARG
1	D	166	SER
1	D	238	ALA
1	D	292	GLU
1	A	237	VAL
1	A	239	GLN
1	A	397	ASP
1	B	237	VAL
1	B	239	GLN
1	B	240	ASN
1	C	237	VAL
1	C	239	GLN
1	C	240	ASN
1	D	237	VAL
1	D	397	ASP
1	A	240	ASN
1	C	102	ALA
1	A	102	ALA
1	B	177	GLU

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	274/286 (96%)	231 (84%)	43 (16%)	2 13
1	B	274/286 (96%)	230 (84%)	44 (16%)	2 12
1	C	274/286 (96%)	235 (86%)	39 (14%)	3 16
1	D	274/286 (96%)	234 (85%)	40 (15%)	3 15
All	All	1096/1144 (96%)	930 (85%)	166 (15%)	3 14

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LEU
1	A	99	GLN
1	A	125	SER
1	A	129	ARG
1	A	136	THR
1	A	155	ILE
1	A	169	ARG
1	A	170	THR
1	A	177	GLU
1	A	180	THR
1	A	185	GLU
1	A	186	GLU
1	A	187	SER
1	A	189	SER
1	A	205	ILE
1	A	213	SER
1	A	224	CYS
1	A	225	LEU
1	A	233	THR
1	A	237	VAL
1	A	241	CYS
1	A	245	VAL
1	A	247	GLN
1	A	250	SER
1	A	263	SER
1	A	268	LEU
1	A	270	VAL
1	A	282	LEU
1	A	301	ILE
1	A	303	SER
1	A	313	ASP
1	A	322	SER
1	A	357	TYR
1	A	364	LYS
1	A	373	GLU
1	A	393	GLN
1	A	394	ARG
1	A	395	ILE
1	A	397	ASP
1	A	399	GLN
1	A	403	VAL
1	A	414	THR
1	A	420	LEU

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Mol	Chain	Res	Type
1	B	96	LEU
1	B	99	GLN
1	B	125	SER
1	B	129	ARG
1	B	136	THR
1	B	151	LYS
1	B	169	ARG
1	B	170	THR
1	B	176	GLU
1	B	177	GLU
1	B	178	GLU
1	B	180	THR
1	B	185	GLU
1	B	187	SER
1	B	193	ILE
1	B	205	ILE
1	B	213	SER
1	B	219	LYS
1	B	223	GLU
1	B	225	LEU
1	B	233	THR
1	B	237	VAL
1	B	245	VAL
1	B	247	GLN
1	B	250	SER
1	B	263	SER
1	B	268	LEU
1	B	270	VAL
1	B	282	LEU
1	B	301	ILE
1	B	303	SER
1	B	313	ASP
1	B	322	SER
1	B	357	TYR
1	B	364	LYS
1	B	373	GLU
1	B	393	GLN
1	B	394	ARG
1	B	395	ILE
1	B	397	ASP
1	B	399	GLN
1	B	403	VAL

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Mol	Chain	Res	Type
1	B	414	THR
1	B	420	LEU
1	C	96	LEU
1	C	99	GLN
1	C	125	SER
1	C	129	ARG
1	C	136	THR
1	C	169	ARG
1	C	170	THR
1	C	177	GLU
1	C	180	THR
1	C	185	GLU
1	C	187	SER
1	C	189	SER
1	C	193	ILE
1	C	205	ILE
1	C	213	SER
1	C	225	LEU
1	C	233	THR
1	C	237	VAL
1	C	245	VAL
1	C	247	GLN
1	C	250	SER
1	C	263	SER
1	C	270	VAL
1	C	282	LEU
1	C	301	ILE
1	C	303	SER
1	C	313	ASP
1	C	322	SER
1	C	357	TYR
1	C	364	LYS
1	C	373	GLU
1	C	393	GLN
1	C	394	ARG
1	C	395	ILE
1	C	397	ASP
1	C	399	GLN
1	C	403	VAL
1	C	414	THR
1	C	420	LEU
1	D	96	LEU

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Mol	Chain	Res	Type
1	D	99	GLN
1	D	125	SER
1	D	129	ARG
1	D	136	THR
1	D	169	ARG
1	D	170	THR
1	D	176	GLU
1	D	180	THR
1	D	185	GLU
1	D	187	SER
1	D	189	SER
1	D	193	ILE
1	D	213	SER
1	D	219	LYS
1	D	225	LEU
1	D	233	THR
1	D	237	VAL
1	D	245	VAL
1	D	247	GLN
1	D	250	SER
1	D	263	SER
1	D	268	LEU
1	D	270	VAL
1	D	282	LEU
1	D	301	ILE
1	D	303	SER
1	D	313	ASP
1	D	322	SER
1	D	357	TYR
1	D	364	LYS
1	D	373	GLU
1	D	393	GLN
1	D	394	ARG
1	D	395	ILE
1	D	397	ASP
1	D	399	GLN
1	D	403	VAL
1	D	414	THR
1	D	420	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	101	GLN
1	A	191	ASN
1	A	221	ASN
1	A	272	HIS
1	A	308	ASN
1	A	393	GLN
1	B	99	GLN
1	B	101	GLN
1	B	191	ASN
1	B	221	ASN
1	B	272	HIS
1	B	308	ASN
1	B	393	GLN
1	C	101	GLN
1	C	221	ASN
1	C	272	HIS
1	C	308	ASN
1	C	393	GLN
1	D	99	GLN
1	D	101	GLN
1	D	221	ASN
1	D	272	HIS
1	D	308	ASN
1	D	393	GLN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	321/337 (95%)	0.08	17 (5%) 26 10	21, 58, 112, 156	0
1	B	321/337 (95%)	-0.17	6 (1%) 66 37	17, 45, 101, 148	0
1	C	321/337 (95%)	-0.25	8 (2%) 57 29	14, 39, 92, 148	0
1	D	321/337 (95%)	0.32	23 (7%) 15 4	20, 62, 113, 146	0
All	All	1284/1348 (95%)	-0.00	54 (4%) 36 14	14, 52, 108, 156	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	136	THR	8.9
1	D	136	THR	5.9
1	B	134	ASN	5.4
1	B	136	THR	4.5
1	C	146	GLY	4.5
1	A	235	ASP	4.2
1	D	401	GLU	3.7
1	B	235	ASP	3.7
1	D	224	CYS	3.7
1	C	238	ALA	3.7
1	B	135	LEU	3.6
1	C	224	CYS	3.6
1	A	328	PRO	3.6
1	C	240	ASN	3.5
1	A	401	GLU	3.5
1	C	135	LEU	3.5
1	D	234	ILE	3.4
1	A	136	THR	3.3
1	D	134	ASN	3.3
1	C	235	ASP	3.2
1	D	133	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	133	SER	3.2
1	D	235	ASP	3.2
1	A	135	LEU	3.0
1	A	425	ALA	2.9
1	A	89	ILE	2.9
1	D	246	CYS	2.9
1	D	402	GLN	2.8
1	D	135	LEU	2.8
1	D	148	ASP	2.8
1	A	224	CYS	2.7
1	A	234	ILE	2.6
1	D	233	THR	2.6
1	D	146	GLY	2.6
1	D	244	ASN	2.5
1	D	372	TYR	2.5
1	A	134	ASN	2.5
1	D	170	THR	2.4
1	D	403	VAL	2.4
1	A	174	ALA	2.4
1	D	176	GLU	2.3
1	D	404	HIS	2.3
1	B	146	GLY	2.3
1	D	89	ILE	2.3
1	D	240	ASN	2.2
1	D	365	ASN	2.2
1	B	244	ASN	2.2
1	C	247	GLN	2.2
1	A	223	GLU	2.1
1	A	193	ILE	2.1
1	A	202	SER	2.1
1	A	329	SER	2.1
1	A	188	TYR	2.0
1	D	188	TYR	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.