Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:42 PM GMT

PDB ID	:	4MH1
Title	:	Crystal structure and functional studies of quinoprotein L-sorbose dehydrogenase from Ketogulonicigenium vulgare Y25
Authors	:	Han, X.; Liu, X.
Deposited on	:	2013-08-29
Resolution	:	2.70 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:

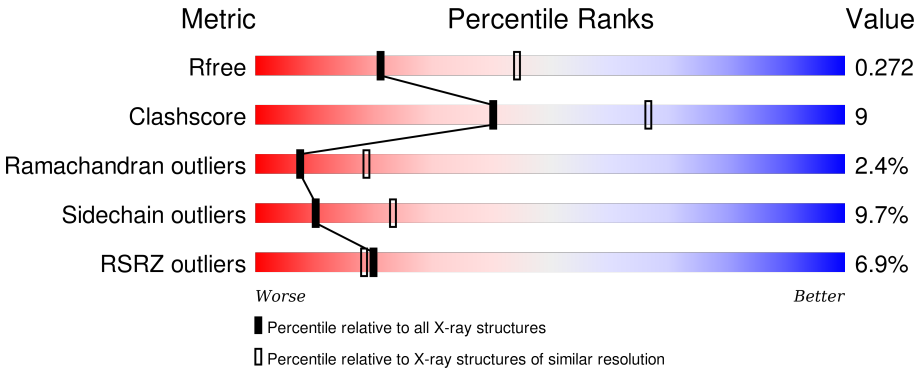
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	560	6% 73% 15% • 9%
1	B	560	7% 67% 19% • • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7710 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.

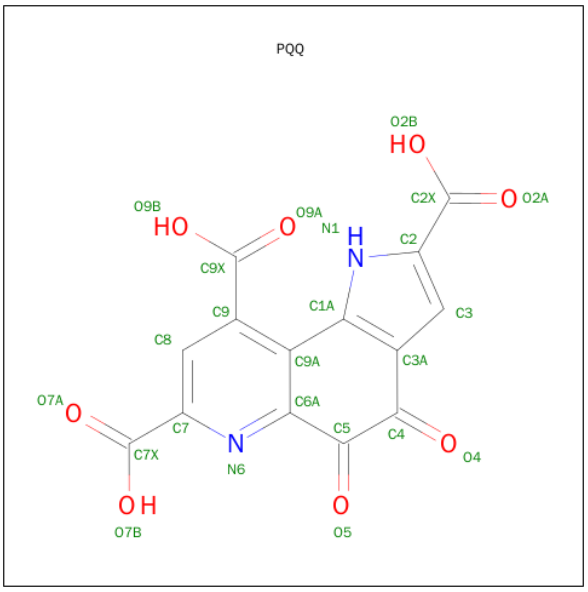
- Molecule 1 is a protein called Sorbose dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			3818	2392	655	753	18			
1	B	514	Total	C	N	O	S	0	0	0
			3867	2420	660	768	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	TYR	-	EXPRESSION TAG	UNP E3F069
A	-3	PHE	-	EXPRESSION TAG	UNP E3F069
A	-2	GLN	-	EXPRESSION TAG	UNP E3F069
A	-1	SER	-	EXPRESSION TAG	UNP E3F069
B	-4	TYR	-	EXPRESSION TAG	UNP E3F069
B	-3	PHE	-	EXPRESSION TAG	UNP E3F069
B	-2	GLN	-	EXPRESSION TAG	UNP E3F069
B	-1	SER	-	EXPRESSION TAG	UNP E3F069

- Molecule 2 is PYRROLOQUINOLINE QUINONE (three-letter code: PQQ) (formula: $C_{14}H_6N_2O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 24 14 2 8	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

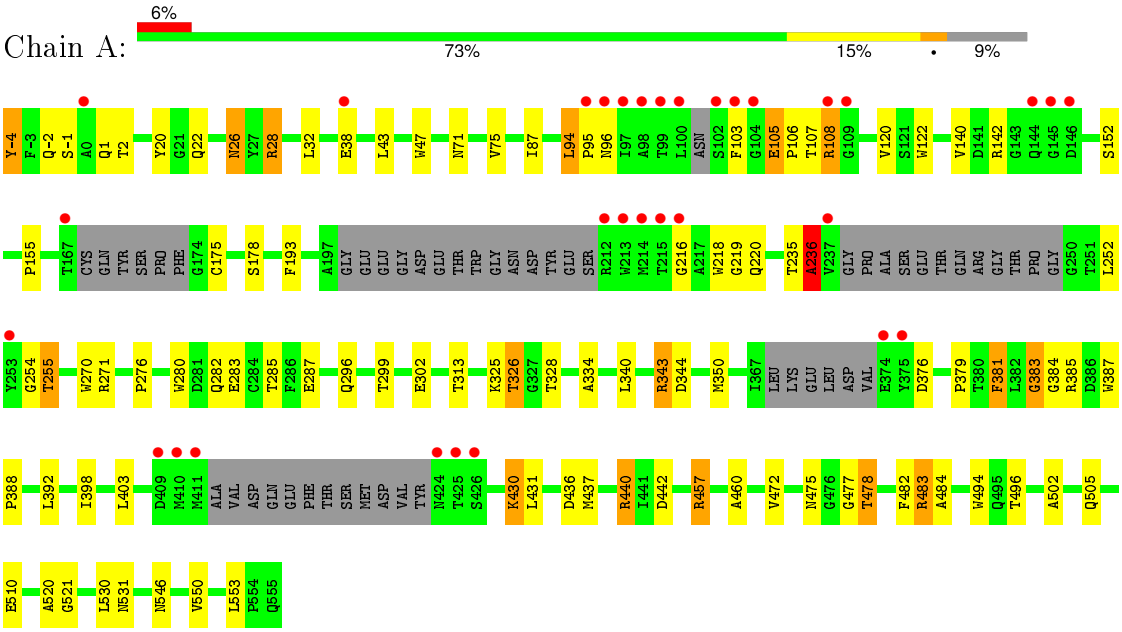
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0

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.

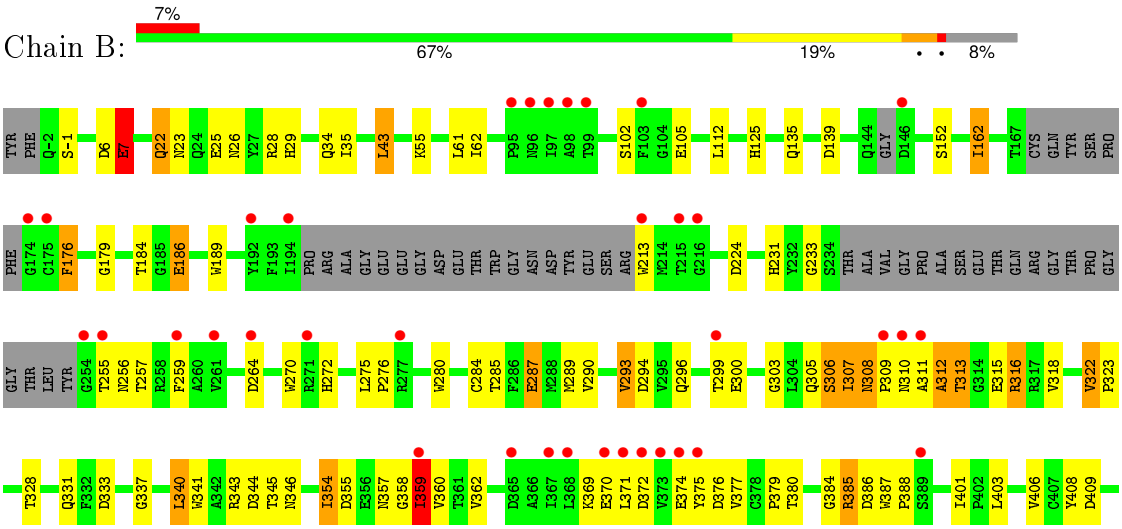
- Molecule 1: Sorbose dehydrogenase

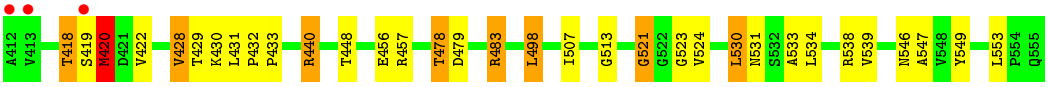
Chain A:



- Molecule 1: Sorbose dehydrogenase

Chain B:




A412
V413
T418
S419
K420
D421
V422
V428
T429
K430
L431
P432
P433
R440
T448
E456
R457
T478
D479
R483
L498
I507
G513
G521
G522
G523
V524
L530
N531
S532
A533
L534
R538
V539
N546
A547
V548
Y549
L553
F554
Q555

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 3 2	Depositor
Cell constants a, b, c, α, β, γ	201.53Å 201.53Å 201.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.14 – 2.70 41.14 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.14-2.70) 99.1 (41.14-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.16 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.226 , 0.232 0.221 , 0.272	Depositor DCC
R_{free} test set	1943 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 38755 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7710	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: PQQ, CA

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	0.48	0/3903	0.69	3/5333 (0.1%)
1	B	0.44	0/3951	0.66	0/5399
All	All	0.46	0/7854	0.67	3/10732 (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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	236	ALA	N-CA-C	-7.44	90.91	111.00
1	A	94	LEU	C-N-CD	-5.91	107.60	120.60
1	A	384	GLY	N-CA-C	-5.23	100.03	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	383	GLY	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	3818	0	3541	51	0
1	B	3867	0	3604	78	0
2	B	24	0	3	0	0
3	B	1	0	0	0	0
All	All	7710	0	7148	129	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 9.

All (129) 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:359:ILE:HB	1:B:360:VAL:HA	1.50	0.93
1:A:235:THR:C	1:A:236:ALA:O	2.09	0.83
1:B:305:GLN:HG3	1:B:354:ILE:HB	1.62	0.81
1:B:308:ASN:HB3	1:B:311:ALA:HB2	1.63	0.79
1:A:142:ARG:HH21	1:A:178:SER:HB3	1.49	0.78
1:B:315:GLU:HA	1:B:316:ARG:HB2	1.64	0.77
1:B:306:SER:HB3	1:B:354:ILE:HG22	1.68	0.75
1:A:403:LEU:HB2	1:A:440:ARG:HG2	1.70	0.72
1:A:343:ARG:NH1	1:A:344:ASP:O	2.24	0.71
1:A:105:GLU:HG2	1:A:106:PRO:HD2	1.73	0.71
1:A:381:PHE:H	1:A:381:PHE:HD2	1.40	0.70
1:B:354:ILE:HA	1:B:359:ILE:HG21	1.75	0.69
1:A:105:GLU:HB2	1:A:122:TRP:CZ2	2.30	0.67
1:B:316:ARG:HH11	1:B:333:ASP:HB2	1.59	0.67
1:A:252:LEU:O	1:A:255:THR:HB	1.95	0.66
1:B:403:LEU:HB2	1:B:440:ARG:HG2	1.78	0.66
1:B:315:GLU:HA	1:B:316:ARG:CB	2.25	0.66
1:B:318:VAL:HG21	1:B:331:GLN:HE21	1.59	0.66
1:B:359:ILE:CB	1:B:360:VAL:HA	2.25	0.65
1:B:287:GLU:OE2	1:B:385:ARG:NH2	2.19	0.65
1:A:270:TRP:NE1	1:A:334:ALA:O	2.28	0.65
1:A:478:THR:CG2	1:A:531:ASN:HD21	2.11	0.63
1:B:355:ASP:N	1:B:359:ILE:HG12	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ASP:OD2	1:B:430:LYS:NZ	2.25	0.61
1:B:380:THR:HG23	1:B:406:VAL:HG13	1.83	0.61
1:A:475:ASN:O	1:A:483:ARG:HG3	2.01	0.61
1:B:233:GLY:HA3	1:B:285:THR:HA	1.84	0.59
1:A:440:ARG:HD2	1:A:442:ASP:OD1	2.02	0.59
1:B:213:TRP:N	1:B:256:ASN:OD1	2.36	0.59
1:B:385:ARG:HG3	1:B:401:ILE:HD11	1.85	0.58
1:B:358:GLY:C	1:B:359:ILE:HD12	2.23	0.58
1:B:355:ASP:H	1:B:359:ILE:CG2	2.17	0.58
1:B:440:ARG:HB2	1:B:456:GLU:HG2	1.86	0.58
1:A:28:ARG:HD3	1:A:505:GLN:OE1	2.04	0.58
1:B:354:ILE:HG12	1:B:359:ILE:HD13	1.87	0.57
1:A:521:GLY:O	1:A:546:ASN:HA	2.05	0.56
1:B:369:LYS:O	1:B:375:TYR:OH	2.23	0.56
1:B:316:ARG:NH1	1:B:333:ASP:HB2	2.21	0.56
1:B:409:ASP:HB2	1:B:428:VAL:HG13	1.88	0.56
1:B:521:GLY:HA3	1:B:547:ALA:O	2.06	0.55
1:B:418:THR:HG22	1:B:419:SER:HA	1.88	0.55
1:A:478:THR:HG21	1:A:531:ASN:HD21	1.72	0.55
1:B:420:MET:HB3	1:B:422:VAL:HG12	1.88	0.54
1:B:184:THR:HG22	1:B:186:GLU:H	1.72	0.54
1:A:236:ALA:HA	1:A:255:THR:HG23	1.88	0.54
1:B:429:THR:HG22	1:B:533:ALA:HB2	1.90	0.54
1:A:120:VAL:HG23	1:A:155:PRO:HD3	1.91	0.53
1:B:270:TRP:CE3	1:B:337:GLY:HA3	2.44	0.53
1:A:254:GLY:HA3	1:A:271:ARG:HH22	1.72	0.53
1:B:478:THR:HG21	1:B:531:ASN:HD21	1.74	0.52
1:B:478:THR:CG2	1:B:531:ASN:HD21	2.22	0.52
1:A:47:TRP:CZ2	1:A:550:VAL:HG21	2.46	0.51
1:B:312:ALA:O	1:B:313:THR:HB	2.11	0.51
1:A:-4:TYR:HB3	1:A:87:ILE:O	2.10	0.51
1:B:310:ASN:HA	1:B:311:ALA:HB3	1.93	0.51
1:A:460:ALA:O	1:A:478:THR:HB	2.11	0.51
1:B:284:CYS:HA	1:B:323:PRO:O	2.11	0.50
1:B:305:GLN:HG2	1:B:354:ILE:HD12	1.93	0.50
1:B:406:VAL:HG21	1:B:530:LEU:HG	1.92	0.50
1:A:26:ASN:OD1	1:A:28:ARG:NH2	2.45	0.50
1:A:108:ARG:HH22	1:A:218:TRP:HZ3	1.59	0.50
1:B:341:TRP:HZ3	1:B:343:ARG:HG2	1.77	0.50
1:B:355:ASP:H	1:B:359:ILE:HG21	1.77	0.50
1:B:62:ILE:HD13	1:B:507:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ASN:O	1:A:28:ARG:N	2.44	0.49
1:A:220:GLN:HB2	1:A:287:GLU:HB3	1.93	0.49
1:B:61:LEU:HD13	1:B:112:LEU:HG	1.95	0.49
1:A:219:GLY:HA3	1:A:285:THR:O	2.13	0.49
1:B:521:GLY:O	1:B:546:ASN:HA	2.13	0.48
1:A:1:GLN:HG3	1:A:2:THR:HA	1.95	0.48
1:B:371:LEU:HD13	1:B:372:ASP:N	2.29	0.48
1:A:392:LEU:HD12	1:A:398:ILE:O	2.12	0.48
1:B:272:HIS:HE1	1:B:358:GLY:O	1.97	0.48
1:B:322:VAL:HG22	1:B:385:ARG:HD2	1.96	0.47
1:B:479:ASP:OD1	1:B:483:ARG:NH2	2.47	0.47
1:A:430:LYS:HG2	1:A:431:LEU:N	2.30	0.47
1:B:331:GLN:HG2	1:B:340:LEU:HD23	1.96	0.46
1:B:354:ILE:HG23	1:B:359:ILE:CD1	2.45	0.46
1:A:28:ARG:HB2	1:A:28:ARG:HH11	1.80	0.46
1:A:477:GLY:H	1:A:502:ALA:HB3	1.81	0.46
1:A:235:THR:O	1:A:236:ALA:O	2.34	0.45
1:B:55:LYS:HA	1:B:523:GLY:HA3	1.98	0.45
1:B:290:VAL:HA	1:B:318:VAL:O	2.16	0.45
1:A:254:GLY:HA3	1:A:271:ARG:NH2	2.31	0.45
1:B:179:GLY:HA3	1:B:189:TRP:NE1	2.32	0.44
1:B:224:ASP:HB2	1:B:290:VAL:HG21	1.99	0.44
1:A:437:MET:HB3	1:A:457:ARG:O	2.17	0.44
1:A:108:ARG:HG3	1:A:152:SER:O	2.18	0.44
1:B:431:LEU:HA	1:B:432:PRO:HD3	1.79	0.44
1:B:23:ASN:ND2	1:B:25:GLU:HB2	2.33	0.44
1:B:22:GLN:HG2	1:B:29:HIS:O	2.18	0.44
1:B:299:THR:HA	1:B:307:ILE:HD11	1.99	0.44
1:B:386:ASP:HB3	1:B:388:PRO:HD2	1.99	0.44
1:B:354:ILE:CG1	1:B:359:ILE:HD13	2.48	0.43
1:B:345:THR:OG1	1:B:346:ASN:N	2.50	0.43
1:A:71:ASN:HB2	1:A:75:VAL:HB	2.00	0.43
1:B:498:LEU:HG	1:B:549:TYR:CE2	2.53	0.43
1:B:275:LEU:HA	1:B:275:LEU:HD12	1.90	0.43
1:A:283:GLU:OE2	1:A:325:LYS:NZ	2.50	0.43
1:A:383:GLY:HA3	1:A:385:ARG:O	2.19	0.43
1:B:293:VAL:O	1:B:315:GLU:CB	2.67	0.42
1:A:20:TYR:HE2	1:A:28:ARG:HH21	1.64	0.42
1:B:387:TRP:CG	1:B:388:PRO:HD3	2.54	0.42
1:A:282:GLN:HB3	1:A:326:THR:HG22	2.01	0.42
1:B:162:ILE:H	1:B:162:ILE:HG12	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:VAL:HB	1:B:408:TYR:CE1	2.55	0.42
1:B:272:HIS:NE2	1:B:358:GLY:HA3	2.35	0.41
1:B:231:HIS:HA	1:B:259:PHE:O	2.20	0.41
1:A:478:THR:HG23	1:A:531:ASN:HD21	1.82	0.41
1:A:484:ALA:HB3	1:A:494:TRP:HB3	2.03	0.41
1:B:312:ALA:CB	1:B:316:ARG:HH21	2.32	0.41
1:A:302:GLU:HG2	1:A:343:ARG:NH2	2.36	0.41
1:A:520:ALA:HB1	1:A:521:GLY:HA3	2.02	0.41
1:A:387:TRP:CD1	1:A:388:PRO:HD3	2.54	0.41
1:B:303:GLY:HA3	1:B:344:ASP:HB2	2.02	0.41
1:A:302:GLU:O	1:A:343:ARG:HG3	2.19	0.41
1:A:193:PHE:HE2	1:A:216:GLY:HA2	1.85	0.41
1:A:32:LEU:HD11	1:A:510:GLU:HB2	2.03	0.41
1:B:374:GLU:OE1	1:B:409:ASP:HB3	2.21	0.41
1:B:34:GLN:NE2	1:B:513:GLY:O	2.52	0.41
1:A:280:TRP:CZ3	1:A:350:MET:HB3	2.55	0.41
1:B:380:THR:CG2	1:B:406:VAL:HG13	2.50	0.41
1:B:61:LEU:C	1:B:62:ILE:HD12	2.41	0.41
1:A:482:PHE:HB3	1:A:496:THR:HG22	2.03	0.41
1:A:437:MET:HB3	1:A:457:ARG:C	2.41	0.40
1:B:384:GLY:O	1:B:403:LEU:HA	2.20	0.40
1:B:125:HIS:ND1	1:B:139:ASP:OD2	2.47	0.40
1:B:6:ASP:O	1:B:7:GLU:HB2	2.20	0.40
1:B:35:ILE:HD13	1:B:43:LEU:HD11	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	495/560 (88%)	451 (91%)	35 (7%)	9 (2%)	11 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	504/560 (90%)	446 (88%)	43 (8%)	15 (3%)	5 13
All	All	999/1120 (89%)	897 (90%)	78 (8%)	24 (2%)	7 19

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	B	7	GLU
1	B	276	PRO
1	B	316	ARG
1	B	370	GLU
1	A	26	ASN
1	A	96	ASN
1	A	103	PHE
1	A	175	CYS
1	A	236	ALA
1	B	307	ILE
1	B	420	MET
1	B	309	PRO
1	B	313	THR
1	B	359	ILE
1	B	433	PRO
1	A	95	PRO
1	B	176	PHE
1	B	294	ASP
1	B	312	ALA
1	A	276	PRO
1	B	379	PRO
1	B	521	GLY
1	A	379	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	390/458 (85%)	360 (92%)	30 (8%)	16 36
1	B	401/458 (88%)	354 (88%)	47 (12%)	7 15
All	All	791/916 (86%)	714 (90%)	77 (10%)	10 23

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-4	TYR
1	A	-2	GLN
1	A	-1	SER
1	A	22	GLN
1	A	28	ARG
1	A	38	GLU
1	A	43	LEU
1	A	105	GLU
1	A	107	THR
1	A	108	ARG
1	A	140	VAL
1	A	255	THR
1	A	296	GLN
1	A	299	THR
1	A	313	THR
1	A	326	THR
1	A	328	THR
1	A	340	LEU
1	A	343	ARG
1	A	376	ASP
1	A	381	PHE
1	A	430	LYS
1	A	436	ASP
1	A	440	ARG
1	A	457	ARG
1	A	472	VAL
1	A	478	THR
1	A	483	ARG
1	A	530	LEU
1	A	553	LEU
1	B	-1	SER
1	B	7	GLU
1	B	22	GLN
1	B	26	ASN
1	B	28	ARG

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Mol	Chain	Res	Type
1	B	43	LEU
1	B	102	SER
1	B	105	GLU
1	B	135	GLN
1	B	152	SER
1	B	162	ILE
1	B	176	PHE
1	B	186	GLU
1	B	255	THR
1	B	257	THR
1	B	264	ASP
1	B	280	TRP
1	B	287	GLU
1	B	289	MET
1	B	293	VAL
1	B	296	GLN
1	B	300	GLU
1	B	306	SER
1	B	308	ASN
1	B	322	VAL
1	B	328	THR
1	B	340	LEU
1	B	354	ILE
1	B	357	ASN
1	B	359	ILE
1	B	362	VAL
1	B	385	ARG
1	B	418	THR
1	B	420	MET
1	B	428	VAL
1	B	440	ARG
1	B	448	THR
1	B	457	ARG
1	B	478	THR
1	B	483	ARG
1	B	498	LEU
1	B	524	VAL
1	B	530	LEU
1	B	534	LEU
1	B	538	ARG
1	B	539	VAL
1	B	553	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	GLN
1	A	531	ASN
1	B	296	GLN
1	B	331	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

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
2	PQQ	B	601	3	16,26,26	2.82	8 (50%)	17,40,40	1.74	4 (23%)

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	PQQ	B	601	3	-	0/0/28/28	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	PQQ	C5-C4	-2.92	1.44	1.53
2	B	601	PQQ	C9A-C6A	2.71	1.43	1.40
2	B	601	PQQ	C2-N1	2.79	1.46	1.37
2	B	601	PQQ	C3-C3A	3.48	1.47	1.40
2	B	601	PQQ	C3-C2	3.53	1.46	1.40
2	B	601	PQQ	C1A-N1	4.18	1.47	1.37
2	B	601	PQQ	C3A-C4	4.68	1.57	1.48
2	B	601	PQQ	C3A-C1A	6.18	1.49	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	PQQ	C3A-C4-C5	-2.64	114.67	118.08
2	B	601	PQQ	C6A-N6-C7	2.56	122.07	118.38
2	B	601	PQQ	O4-C4-C5	2.94	123.77	119.29
2	B	601	PQQ	C9A-C1A-N1	3.32	130.75	124.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	509/560 (90%)	-0.01	32 (6%)	23	22	10, 25, 83, 125	0
1	B	514/560 (91%)	0.23	39 (7%)	17	15	9, 39, 94, 137	0
All	All	1023/1120 (91%)	0.11	71 (6%)	20	18	9, 30, 89, 137	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	THR	8.7
1	A	145	GLY	6.4
1	A	102	SER	5.5
1	A	375	TYR	5.4
1	A	0	ALA	4.9
1	A	426	SER	4.9
1	A	146	ASP	4.8
1	A	374	GLU	4.4
1	B	373	VAL	4.4
1	B	412	ALA	4.2
1	A	98	ALA	4.1
1	A	97	ILE	3.9
1	B	99	THR	3.9
1	B	419	SER	3.6
1	B	146	ASP	3.5
1	B	372	ASP	3.5
1	B	98	ALA	3.5
1	B	375	TYR	3.5
1	A	411	MET	3.4
1	B	95	PRO	3.3
1	A	167	THR	3.3
1	B	97	ILE	3.2
1	A	213	TRP	3.2
1	A	425	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	109	GLY	3.2
1	B	365	ASP	3.2
1	A	103	PHE	3.2
1	B	311	ALA	3.1
1	A	108	ARG	3.0
1	B	413	VAL	3.0
1	B	192	TYR	2.9
1	A	95	PRO	2.9
1	B	277	ARG	2.9
1	A	96	ASN	2.9
1	A	99	THR	2.8
1	A	216	GLY	2.8
1	A	100	LEU	2.7
1	B	309	PRO	2.7
1	A	144	GLN	2.7
1	B	259	PHE	2.7
1	B	264	ASP	2.7
1	B	374	GLU	2.7
1	B	194	ILE	2.6
1	B	299	THR	2.6
1	A	424	ASN	2.6
1	A	409	ASP	2.6
1	B	175	CYS	2.6
1	B	370	GLU	2.6
1	B	368	LEU	2.5
1	A	212	ARG	2.5
1	B	213	TRP	2.5
1	A	104	GLY	2.5
1	B	310	ASN	2.5
1	B	371	LEU	2.5
1	A	237	VAL	2.5
1	B	271	ARG	2.4
1	A	214	MET	2.3
1	B	174	GLY	2.3
1	A	38	GLU	2.3
1	B	359	ILE	2.3
1	B	216	GLY	2.2
1	B	254	GLY	2.2
1	A	410	MET	2.2
1	B	261	VAL	2.2
1	B	96	ASN	2.1
1	A	253	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	367	ILE	2.1
1	A	215	THR	2.1
1	B	255	THR	2.1
1	B	389	SER	2.1
1	B	103	PHE	2.1

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

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

6.3 Carbohydrates (i)

There are no 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	PQQ	B	601	24/24	0.81	0.25	0.10	62,77,86,86	0
3	CA	B	602	1/1	0.69	0.16	-	107,107,107,107	0

6.5 Other polymers (i)

There are no such residues in this entry.