Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:07 PM GMT

PDB ID	:	1E5L
Title	:	APO SACCHAROPINE REDUCTASE FROM MAGNAPORTHE GRISEA
Authors	:	Johansson, E.; Steffens, J.J.; Lindqvist, Y.; Schneider, G.
Deposited on	:	2000-07-27
Resolution	:	2.40 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:

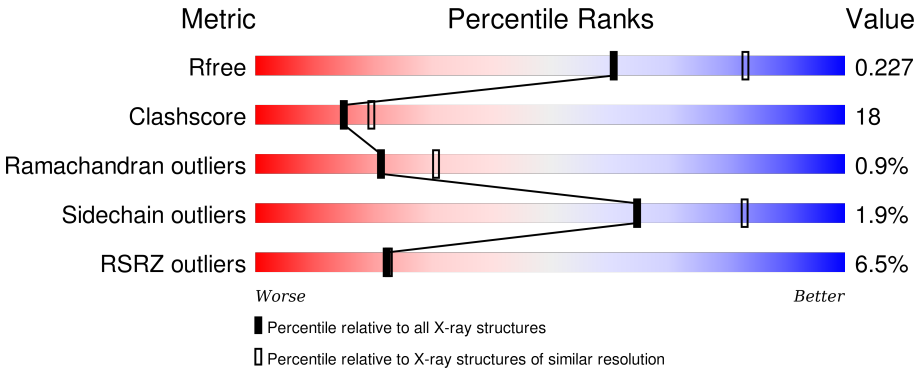
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	450	7% 66% 33%
1	B	450	6% 69% 29%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7055 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 SACCHAROPINE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3442	2191	572	663	16			
1	B	449	Total	C	N	O	S	0	0	0
			3442	2191	572	663	16			

- Molecule 2 is water.

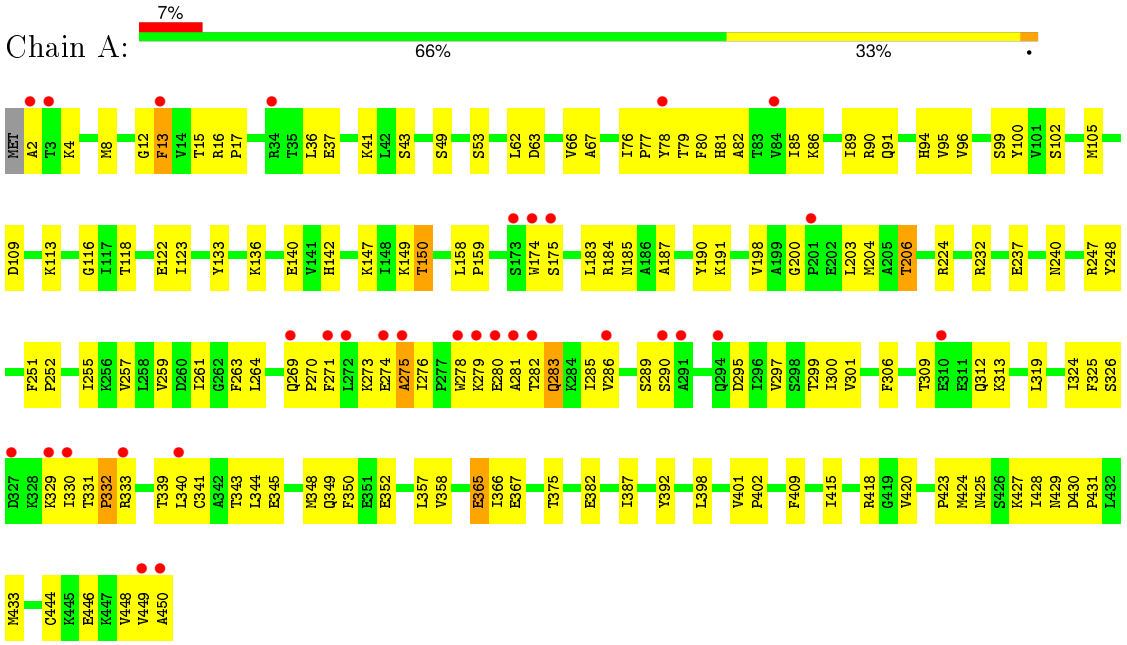
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	83	Total	O	0	0
			83	83		
2	B	88	Total	O	0	0
			88	88		

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.

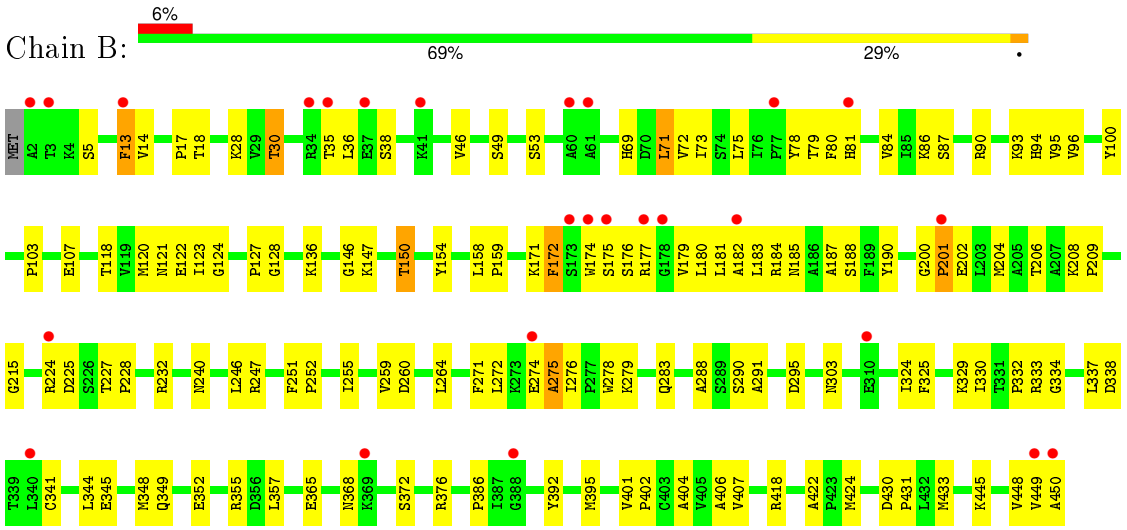
- Molecule 1: SACCHAROPINE REDUCTASE

Chain A:



- Molecule 1: SACCHAROPINE REDUCTASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	89.33Å 119.00Å 195.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.40 19.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.1 (19.91-2.40) 97.2 (19.91-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 2.41Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.222 , 0.259 0.221 , 0.227	Depositor DCC
R_{free} test set	2011 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 39932 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7055	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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

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	0.35	0/3508	0.63	0/4747
1	B	0.39	2/3508 (0.1%)	0.65	1/4747 (0.0%)
All	All	0.37	2/7016 (0.0%)	0.64	1/9494 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	LYS	C-N	5.28	1.46	1.34
1	B	172	PHE	N-CA	5.03	1.56	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	171	LYS	O-C-N	-5.12	114.50	122.70

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	3442	0	3483	133	0
1	B	3442	0	3483	112	0
2	A	83	0	0	1	0
2	B	88	0	0	2	0
All	All	7055	0	6966	243	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 18.

All (243) 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:123:ILE:HD13	1:B:406:ALA:HB2	1.45	0.97
1:A:330:ILE:HG22	1:A:331:THR:H	1.31	0.96
1:A:150:THR:HG23	1:A:365:GLU:HB2	1.52	0.91
1:A:150:THR:HB	1:A:240:ASN:HB2	1.54	0.88
1:A:232:ARG:HB3	1:A:424:MET:CE	2.04	0.87
1:A:341:CYS:O	1:A:345:GLU:HG2	1.82	0.80
1:B:150:THR:HB	1:B:240:ASN:HB2	1.63	0.80
1:B:71:LEU:HD12	1:B:72:VAL:N	1.97	0.79
1:B:251:PHE:HB3	1:B:252:PRO:HD3	1.66	0.77
1:B:30:THR:HG21	1:B:69:HIS:NE2	2.01	0.76
1:B:368:ASN:HD22	1:B:372:SER:HB2	1.52	0.75
1:B:208:LYS:HG3	1:B:209:PRO:HD2	1.68	0.75
1:A:149:LYS:HA	1:A:149:LYS:HE2	1.69	0.74
1:B:184:ARG:HH11	1:B:259:VAL:HG13	1.50	0.73
1:B:120:MET:HA	1:B:120:MET:HE3	1.70	0.73
1:B:123:ILE:CD1	1:B:406:ALA:HB2	2.18	0.73
1:A:263:PHE:HZ	1:A:282:THR:HG22	1.54	0.72
1:A:187:ALA:HB3	1:A:198:VAL:CG1	2.21	0.70
1:A:183:LEU:HD13	1:A:204:MET:HE1	1.74	0.69
1:A:269:GLN:HE21	1:A:270:PRO:HD2	1.57	0.69
1:A:345:GLU:O	1:A:349:GLN:HG3	1.92	0.69
1:A:259:VAL:HG22	1:A:264:LEU:HD12	1.74	0.69
1:A:375:THR:H	1:A:450:ALA:HA	1.58	0.69
1:A:344:LEU:HD22	1:A:348:MET:CE	2.23	0.69
1:B:175:SER:OG	1:B:175:SER:O	2.08	0.68
1:A:142:HIS:HE1	1:A:237:GLU:OE2	1.76	0.67
1:B:94:HIS:HD2	1:B:118:THR:H	1.41	0.67
1:A:232:ARG:HB3	1:A:424:MET:HE1	1.75	0.67
1:B:275:ALA:O	1:B:329:LYS:HD2	1.95	0.67
1:B:344:LEU:HD22	1:B:348:MET:CE	2.25	0.67
1:A:150:THR:HG23	1:A:365:GLU:CB	2.25	0.66
1:B:30:THR:HG21	1:B:69:HIS:CE1	2.31	0.66
1:B:94:HIS:CD2	1:B:118:THR:H	2.13	0.65
1:A:428:ILE:O	1:A:431:PRO:HD2	1.97	0.65
1:A:204:MET:CE	1:A:252:PRO:HB3	2.27	0.65
1:A:259:VAL:CG2	1:A:264:LEU:HD12	2.26	0.65
1:A:281:ALA:HB2	1:A:330:ILE:HD11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:PRO:O	1:A:273:LYS:HG2	1.96	0.65
1:A:116:GLY:O	1:A:418:ARG:HD2	1.96	0.64
1:B:172:PHE:CD2	1:B:176:SER:HB3	2.31	0.64
1:B:279:LYS:HE3	1:B:291:ALA:O	1.98	0.64
1:A:429:ASN:N	1:A:429:ASN:HD22	1.96	0.62
1:A:183:LEU:HD22	1:A:204:MET:HE3	1.79	0.62
1:B:180:LEU:HA	1:B:183:LEU:HD12	1.82	0.62
1:B:259:VAL:HG22	1:B:264:LEU:HD22	1.83	0.61
1:B:17:PRO:HG3	1:B:392:TYR:CD1	2.36	0.61
1:A:261:ILE:HG21	1:A:300:ILE:HG23	1.81	0.61
1:B:35:THR:HB	1:B:38:SER:OG	2.01	0.61
1:A:2:ALA:O	1:A:4:LYS:HG3	2.01	0.60
1:A:281:ALA:O	1:A:285:ILE:HG13	2.01	0.60
1:A:330:ILE:HG22	1:A:331:THR:N	2.10	0.60
1:B:278:TRP:CD2	1:B:330:ILE:HG22	2.37	0.60
1:B:150:THR:HG22	1:B:240:ASN:HD22	1.67	0.60
1:B:13:PHE:CD1	1:B:13:PHE:N	2.70	0.60
1:A:136:LYS:HD2	1:A:433:MET:SD	2.42	0.60
1:A:251:PHE:HB3	1:A:252:PRO:HD3	1.83	0.59
1:B:13:PHE:HD1	1:B:13:PHE:N	2.00	0.59
1:A:136:LYS:O	1:A:140:GLU:HG3	2.02	0.59
1:B:345:GLU:O	1:B:349:GLN:HG2	2.02	0.59
1:B:279:LYS:HG2	1:B:291:ALA:HB1	1.82	0.59
1:A:276:ILE:O	1:A:330:ILE:HG13	2.02	0.59
1:A:280:GLU:O	1:A:283:GLN:HG3	2.03	0.58
1:B:175:SER:C	1:B:177:ARG:N	2.52	0.58
1:A:105:MET:O	1:A:420:VAL:HG21	2.02	0.58
1:B:180:LEU:HD12	1:B:341:CYS:SG	2.43	0.58
1:A:344:LEU:HD22	1:A:348:MET:HE2	1.84	0.58
1:A:306:PHE:CD2	1:A:312:GLN:HA	2.39	0.58
1:A:184:ARG:HH11	1:A:184:ARG:HB3	1.69	0.57
1:B:79:THR:HG22	1:B:80:PHE:N	2.19	0.57
1:B:187:ALA:HA	1:B:224:ARG:O	2.03	0.57
1:A:204:MET:HE2	1:A:252:PRO:HB3	1.85	0.57
1:B:150:THR:CG2	1:B:240:ASN:HD22	2.17	0.57
1:A:401:VAL:HB	1:A:402:PRO:HD3	1.85	0.57
1:A:183:LEU:HD13	1:A:204:MET:CE	2.35	0.57
1:A:16:ARG:HB3	1:A:17:PRO:HD3	1.86	0.57
1:B:344:LEU:HD22	1:B:348:MET:HE1	1.85	0.56
1:B:184:ARG:O	1:B:200:GLY:HA3	2.05	0.56
1:B:175:SER:C	1:B:177:ARG:H	2.07	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:HB3	1:A:184:ARG:NH1	2.20	0.56
1:B:202:GLU:O	1:B:206:THR:HG23	2.05	0.56
1:B:103:PRO:O	1:B:107:GLU:HG3	2.06	0.56
1:A:350:PHE:HB3	1:A:387:ILE:HG13	1.87	0.56
1:A:94:HIS:CD2	1:A:118:THR:H	2.24	0.56
1:A:309:THR:O	1:A:313:LYS:HG2	2.05	0.56
1:B:204:MET:HE2	1:B:252:PRO:HA	1.88	0.55
1:A:330:ILE:C	1:A:332:PRO:HD3	2.27	0.55
1:B:204:MET:CE	1:B:252:PRO:HA	2.37	0.55
1:A:109:ASP:OD1	1:A:113:LYS:HE3	2.07	0.55
1:B:5:SER:HB3	1:B:28:LYS:HE3	1.88	0.55
1:B:330:ILE:O	1:B:332:PRO:HD3	2.07	0.55
1:B:79:THR:HG22	1:B:81:HIS:H	1.71	0.54
1:A:282:THR:HG21	1:A:324:ILE:O	2.07	0.54
1:A:281:ALA:CB	1:A:330:ILE:HD11	2.37	0.54
1:B:200:GLY:C	1:B:202:GLU:H	2.11	0.54
1:B:123:ILE:O	1:B:123:ILE:HG12	2.08	0.53
1:A:204:MET:HE3	1:A:204:MET:HA	1.91	0.53
1:B:190:TYR:O	1:B:240:ASN:HA	2.08	0.53
1:A:297:VAL:O	1:A:301:VAL:HG23	2.09	0.53
1:A:203:LEU:O	1:A:206:THR:HG22	2.09	0.53
1:A:275:ALA:HA	1:A:332:PRO:HG2	1.90	0.53
1:A:344:LEU:HD22	1:A:348:MET:HE1	1.88	0.53
1:A:79:THR:HG23	1:A:80:PHE:CD1	2.43	0.53
1:A:330:ILE:HG21	1:A:339:THR:CG2	2.38	0.52
1:B:183:LEU:HD21	2:B:2046:HOH:O	2.09	0.52
1:B:179:VAL:O	1:B:183:LEU:HG	2.09	0.52
1:B:86:LYS:O	1:B:90:ARG:HG3	2.09	0.52
1:A:116:GLY:C	1:A:418:ARG:HD2	2.30	0.52
1:B:355:ARG:NE	1:B:386:PRO:HG3	2.23	0.52
1:A:409:PHE:HB3	1:A:415:ILE:HG13	1.91	0.52
1:A:331:THR:O	1:A:333:ARG:HG3	2.09	0.52
1:A:357:LEU:HD12	1:A:382:GLU:O	2.10	0.52
1:B:150:THR:OG1	1:B:365:GLU:HG2	2.10	0.52
1:A:102:SER:H	1:A:105:MET:HE3	1.75	0.51
1:B:36:LEU:HB2	1:B:53:SER:OG	2.10	0.51
1:A:319:LEU:HB3	1:A:324:ILE:HD11	1.92	0.51
1:B:172:PHE:CE2	1:B:176:SER:HB3	2.44	0.51
1:A:429:ASN:N	1:A:429:ASN:ND2	2.58	0.51
1:A:8:MET:SD	1:A:15:THR:HG23	2.50	0.51
1:A:147:LYS:HB3	1:A:237:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:VAL:HB	1:B:402:PRO:HD3	1.93	0.51
1:B:174:TRP:CD1	1:B:175:SER:O	2.63	0.51
1:B:344:LEU:HD22	1:B:348:MET:HE2	1.93	0.51
1:A:17:PRO:HG3	1:A:392:TYR:CD1	2.46	0.50
1:B:14:VAL:HG13	1:B:75:LEU:HD13	1.93	0.50
1:B:274:GLU:O	1:B:276:ILE:N	2.45	0.50
1:B:200:GLY:O	1:B:202:GLU:N	2.43	0.50
1:A:286:VAL:O	1:A:286:VAL:HG12	2.11	0.50
1:B:288:ALA:HB1	1:B:295:ASP:OD1	2.11	0.50
1:A:81:HIS:O	1:A:85:ILE:HG13	2.11	0.50
1:A:282:THR:HG21	1:A:324:ILE:HB	1.92	0.50
1:A:67:ALA:HB2	1:A:91:GLN:NE2	2.27	0.50
1:B:188:SER:HB2	1:B:225:ASP:OD1	2.12	0.50
1:B:158:LEU:HB3	1:B:159:PRO:CD	2.41	0.49
1:B:182:ALA:HA	1:B:185:ASN:OD1	2.11	0.49
1:A:63:ASP:OD1	1:A:90:ARG:NH1	2.45	0.49
1:B:376:ARG:NH1	1:B:448:VAL:HG22	2.28	0.49
1:A:251:PHE:O	1:A:255:ILE:HG12	2.13	0.49
1:A:204:MET:HE1	1:A:252:PRO:HB3	1.93	0.49
1:B:150:THR:HG23	1:B:365:GLU:HB2	1.94	0.49
1:A:81:HIS:HE1	1:A:99:SER:OG	1.96	0.49
1:A:425:ASN:OD1	1:A:427:LYS:HB3	2.12	0.49
1:A:174:TRP:CD1	1:A:175:SER:N	2.81	0.49
1:A:248:TYR:CD1	1:B:215:GLY:HA2	2.48	0.48
1:B:227:THR:OG1	1:B:228:PRO:HD3	2.14	0.48
1:A:330:ILE:CG2	1:A:331:THR:H	2.12	0.48
1:A:290:SER:HB3	1:A:295:ASP:OD2	2.13	0.48
1:A:150:THR:CG2	1:A:365:GLU:HG3	2.44	0.48
1:B:208:LYS:HG3	1:B:209:PRO:CD	2.41	0.48
1:A:78:TYR:HA	1:A:81:HIS:CE1	2.49	0.47
1:A:358:VAL:HG11	1:A:398:LEU:HD12	1.96	0.47
1:B:136:LYS:HD2	1:B:433:MET:SD	2.54	0.47
1:A:232:ARG:HB3	1:A:424:MET:HE3	1.94	0.47
1:B:120:MET:HE3	1:B:121:ASN:H	1.80	0.47
1:B:271:PHE:CE1	1:B:272:LEU:HG	2.49	0.47
1:B:120:MET:HE2	1:B:121:ASN:O	2.15	0.47
1:A:158:LEU:HB3	1:A:159:PRO:CD	2.45	0.47
1:B:204:MET:HE2	1:B:255:ILE:HB	1.97	0.47
1:B:333:ARG:HB3	1:B:338:ASP:HB3	1.96	0.47
1:A:430:ASP:HB2	1:A:431:PRO:HD3	1.97	0.47
1:A:158:LEU:HD21	1:A:247:ARG:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASN:O	1:A:200:GLY:HA2	2.14	0.47
1:B:14:VAL:O	1:B:17:PRO:HD2	2.15	0.47
1:B:120:MET:HE1	1:B:422:ALA:N	2.30	0.47
1:B:278:TRP:CE2	1:B:330:ILE:HG22	2.50	0.46
1:A:290:SER:HB3	1:A:295:ASP:HB2	1.96	0.46
1:B:376:ARG:HG3	1:B:376:ARG:HH11	1.80	0.46
1:A:283:GLN:HE21	1:A:283:GLN:HB2	1.55	0.46
1:B:100:TYR:HA	1:B:122:GLU:CG	2.45	0.46
1:A:150:THR:HG23	1:A:365:GLU:HG3	1.97	0.46
1:A:133:TYR:CD2	1:A:444:CYS:HB2	2.51	0.46
1:B:430:ASP:HB2	1:B:431:PRO:HD3	1.98	0.46
1:B:46:VAL:HG23	1:B:49:SER:HB3	1.96	0.46
1:A:275:ALA:O	1:A:329:LYS:HD3	2.15	0.46
1:B:181:LEU:HG	1:B:337:LEU:HD21	1.97	0.46
1:A:198:VAL:HG13	1:A:198:VAL:O	2.16	0.45
1:A:286:VAL:HG12	1:A:299:THR:CG2	2.46	0.45
1:B:395:MET:HE1	2:B:2002:HOH:O	2.15	0.45
1:B:260:ASP:HB3	1:B:303:ASN:O	2.16	0.45
1:B:73:ILE:CD1	1:B:407:VAL:HG21	2.47	0.45
1:A:278:TRP:HE3	1:A:282:THR:HG23	1.81	0.45
1:A:270:PRO:HG2	1:A:271:PHE:HD1	1.82	0.45
1:A:263:PHE:HB3	1:A:340:LEU:HD22	1.99	0.45
1:A:278:TRP:HZ2	1:A:343:THR:HG1	1.64	0.45
1:B:445:LYS:NZ	1:B:445:LYS:HB2	2.32	0.45
1:A:280:GLU:HA	1:A:283:GLN:HG2	1.99	0.44
1:B:100:TYR:CZ	1:B:127:PRO:HD3	2.52	0.44
1:A:95:VAL:HG12	1:A:96:VAL:N	2.33	0.44
1:A:100:TYR:HA	1:A:122:GLU:CG	2.48	0.44
1:A:423:PRO:CA	1:A:429:ASN:HD21	2.31	0.44
1:B:445:LYS:NZ	1:B:445:LYS:CB	2.81	0.44
1:A:13:PHE:CD1	1:A:13:PHE:N	2.78	0.44
1:B:283:GLN:HG3	1:B:290:SER:O	2.16	0.44
1:A:123:ILE:HG13	1:A:123:ILE:O	2.18	0.43
1:A:136:LYS:NZ	1:A:446:GLU:OE2	2.51	0.43
1:A:62:LEU:O	1:A:66:VAL:HG23	2.18	0.43
1:A:36:LEU:HB2	1:A:53:SER:HB2	2.00	0.43
1:A:150:THR:HG23	1:A:365:GLU:CG	2.48	0.43
1:B:324:ILE:HG13	1:B:325:PHE:CD1	2.54	0.43
1:A:275:ALA:CA	1:A:332:PRO:HG2	2.49	0.43
1:B:87:SER:HA	1:B:90:ARG:HH11	1.83	0.43
1:A:76:ILE:HB	1:A:77:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:TYR:HB3	1:B:246:LEU:HG	2.01	0.43
1:A:257:VAL:O	1:A:261:ILE:HG12	2.18	0.43
1:B:448:VAL:HG12	1:B:449:VAL:N	2.33	0.43
1:A:449:VAL:O	1:A:449:VAL:HG12	2.19	0.43
1:A:324:ILE:HG13	1:A:325:PHE:CD1	2.54	0.43
1:A:448:VAL:CG1	1:A:450:ALA:HB2	2.48	0.43
1:A:340:LEU:O	1:A:344:LEU:HG	2.19	0.42
1:A:94:HIS:HD2	1:A:118:THR:H	1.66	0.42
1:B:333:ARG:HG3	1:B:333:ARG:HH11	1.84	0.42
1:A:85:ILE:O	1:A:89:ILE:HG13	2.19	0.42
1:B:124:GLY:O	1:B:128:GLY:HA3	2.19	0.42
1:A:279:LYS:HG3	1:A:326:SER:O	2.19	0.42
1:B:232:ARG:HG2	1:B:424:MET:HE2	2.02	0.42
1:B:146:GLY:O	1:B:147:LYS:HD3	2.19	0.42
1:A:274:GLU:O	1:A:276:ILE:HG23	2.20	0.42
1:A:190:TYR:O	1:A:240:ASN:HA	2.19	0.42
1:A:12:GLY:O	1:A:15:THR:HB	2.19	0.42
1:B:158:LEU:HD21	1:B:247:ARG:HA	2.02	0.42
1:B:120:MET:HE3	1:B:120:MET:CA	2.45	0.42
1:A:43:SER:HB2	1:A:49:SER:OG	2.19	0.42
1:A:248:TYR:CE1	1:B:215:GLY:HA2	2.55	0.41
1:A:290:SER:HB3	1:A:295:ASP:CB	2.49	0.41
1:B:120:MET:HE1	1:B:422:ALA:CA	2.50	0.41
1:B:95:VAL:HG12	1:B:96:VAL:N	2.35	0.41
1:A:191:LYS:HA	1:A:240:ASN:OD1	2.19	0.41
1:B:69:HIS:O	1:B:93:LYS:HD2	2.20	0.41
1:B:87:SER:HA	1:B:90:ARG:NH1	2.35	0.41
1:A:247:ARG:NH2	2:A:2059:HOH:O	2.54	0.41
1:A:275:ALA:N	1:A:332:PRO:HG2	2.35	0.41
1:B:79:THR:CG2	1:B:80:PHE:N	2.83	0.41
1:B:100:TYR:CE2	1:B:127:PRO:HD3	2.56	0.41
1:B:227:THR:N	1:B:228:PRO:CD	2.84	0.41
1:B:18:THR:HG23	1:B:404:ALA:HB2	2.02	0.41
1:B:200:GLY:N	1:B:201:PRO:CD	2.84	0.41
1:B:251:PHE:HB3	1:B:252:PRO:CD	2.46	0.40
1:B:449:VAL:HG12	1:B:450:ALA:N	2.35	0.40
1:A:448:VAL:HG12	1:A:450:ALA:HB2	2.02	0.40
1:A:37:GLU:OE2	1:A:41:LYS:HE3	2.22	0.40
1:B:333:ARG:NH1	1:B:333:ARG:HG3	2.37	0.40
1:A:133:TYR:CG	1:A:444:CYS:HB2	2.57	0.40
1:A:366:ILE:CG2	1:A:367:GLU:N	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ALA:O	1:A:86:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	447/450 (99%)	410 (92%)	33 (7%)	4 (1%)	21	30
1	B	447/450 (99%)	419 (94%)	24 (5%)	4 (1%)	21	30
All	All	894/900 (99%)	829 (93%)	57 (6%)	8 (1%)	21	30

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	ALA
1	A	289	SER
1	B	275	ALA
1	B	201	PRO
1	A	352	GLU
1	B	84	VAL
1	A	332	PRO
1	B	334	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	375/376 (100%)	369 (98%)	6 (2%)	70 86
1	B	375/376 (100%)	367 (98%)	8 (2%)	61 80
All	All	750/752 (100%)	736 (98%)	14 (2%)	65 83

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PHE
1	A	150	THR
1	A	206	THR
1	A	224	ARG
1	A	283	GLN
1	A	365	GLU
1	B	13	PHE
1	B	30	THR
1	B	71	LEU
1	B	78	TYR
1	B	150	THR
1	B	352	GLU
1	B	357	LEU
1	B	418	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	81	HIS
1	A	91	GLN
1	A	94	HIS
1	A	142	HIS
1	A	197	ASN
1	A	223	ASN
1	A	269	GLN
1	A	368	ASN
1	A	429	ASN
1	B	48	HIS
1	B	69	HIS
1	B	94	HIS
1	B	197	ASN
1	B	234	GLN
1	B	368	ASN

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	449/450 (99%)	0.19	32 (7%)	19	19	14, 36, 76, 95	0
1	B	449/450 (99%)	0.11	26 (5%)	26	27	13, 34, 68, 90	0
All	All	898/900 (99%)	0.15	58 (6%)	22	22	13, 35, 73, 95	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	174	TRP	10.0
1	A	174	TRP	8.0
1	A	2	ALA	7.1
1	B	173	SER	6.9
1	A	271	PHE	6.4
1	A	450	ALA	6.2
1	B	2	ALA	5.6
1	B	450	ALA	5.3
1	B	177	ARG	4.8
1	A	327	ASP	4.8
1	B	41	LYS	4.7
1	B	13	PHE	4.6
1	A	13	PHE	3.7
1	B	3	THR	3.4
1	A	78	TYR	3.4
1	A	449	VAL	3.3
1	A	281	ALA	3.3
1	B	77	PRO	3.2
1	B	182	ALA	3.2
1	B	388	GLY	3.2
1	B	201	PRO	3.2
1	A	275	ALA	3.1
1	A	282	THR	3.1
1	A	272	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	274	GLU	3.0
1	A	274	GLU	3.0
1	A	201	PRO	3.0
1	A	333	ARG	2.9
1	A	280	GLU	2.9
1	B	310	GLU	2.8
1	A	290	SER	2.8
1	B	37	GLU	2.8
1	B	224	ARG	2.8
1	B	449	VAL	2.7
1	B	34	ARG	2.4
1	B	61	ALA	2.4
1	A	291	ALA	2.4
1	A	278	TRP	2.3
1	A	340	LEU	2.3
1	B	175	SER	2.3
1	A	3	THR	2.3
1	A	34	ARG	2.3
1	B	60	ALA	2.3
1	A	175	SER	2.3
1	B	81	HIS	2.3
1	A	286	VAL	2.2
1	B	369	LYS	2.2
1	A	269	GLN	2.2
1	A	294	GLN	2.2
1	A	330	ILE	2.1
1	B	35	THR	2.1
1	B	178	GLY	2.1
1	B	340	LEU	2.1
1	A	84	VAL	2.1
1	A	310	GLU	2.1
1	A	329	LYS	2.1
1	A	279	LYS	2.1
1	A	173	SER	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.