Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 06:43 am GMT

PDB ID	:	1QLV
Title	:	Pyrone synthase (PYS) from Gerbera hybrida
Authors	:	Ferrer, J.-L.; Jez, J.M.; Bowman, M.E.; Schroder, J.; Noel, J.P.
Deposited on	:	1999-09-16
Resolution	:	2.10 Å(reported)

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

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

The 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:

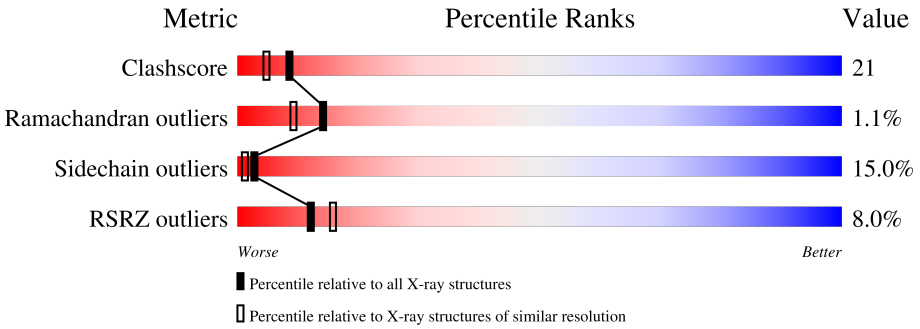
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6673 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 PYRONE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	7	0
			2955	1876	511	549	19			
1	B	376	Total	C	N	O	S	0	7	0
			2943	1869	511	544	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	259	MET	VAL	cloning artifact	UNP P48391
A	169	CSD	CYS	modified residue	UNP P48391
B	259	MET	VAL	cloning artifact	UNP P48391
B	169	CSD	CYS	modified residue	UNP P48391

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	366	Total	O	0	0
			366	366		
2	B	409	Total	O	0	0
			409	409		

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	82.14Å 82.14Å 241.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.10 41.07 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.5 (10.00-2.10) 92.2 (41.07-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.10Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.185 , 0.269 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 134.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6673	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.6793e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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.

4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CSD

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	0.33	0/2998	1.05	13/4057 (0.3%)
1	B	0.36	0/2986	1.25	20/4041 (0.5%)
All	All	0.35	0/5984	1.15	33/8098 (0.4%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	355	ARG	CD-NE-CZ	36.05	174.08	123.60
1	B	264	ARG	CD-NE-CZ	12.57	141.20	123.60
1	B	47	ARG	NE-CZ-NH2	-12.12	114.24	120.30
1	B	375	LEU	CA-CB-CG	11.85	142.55	115.30
1	B	47	ARG	NE-CZ-NH1	11.03	125.81	120.30
1	A	375	LEU	CA-CB-CG	10.12	138.57	115.30
1	B	202	LEU	CA-CB-CG	9.49	137.12	115.30
1	A	330	ARG	CD-NE-CZ	8.89	136.05	123.60
1	A	330	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	B	47	ARG	CD-NE-CZ	8.54	135.55	123.60
1	A	73	ARG	CD-NE-CZ	8.48	135.48	123.60
1	A	73	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	B	239	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	A	73	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	B	239	ARG	CD-NE-CZ	7.63	134.28	123.60
1	B	73	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	357	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	B	73	ARG	CD-NE-CZ	6.83	133.17	123.60
1	B	320	ARG	NE-CZ-NH1	-6.75	116.93	120.30
1	B	343[A]	ILE	CA-CB-CG1	6.32	123.01	111.00
1	B	343[B]	ILE	CA-CB-CG1	6.32	123.01	111.00
1	A	330	ARG	NE-CZ-NH2	-6.26	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	320	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	A	322	LEU	C-N-CA	5.96	136.61	121.70
1	A	161	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	92	MET	C-N-CA	5.69	135.91	121.70
1	B	343[A]	ILE	CA-C-N	5.61	129.53	117.20
1	B	343[B]	ILE	CA-C-N	5.61	129.53	117.20
1	A	202	LEU	CA-CB-CG	5.50	127.94	115.30
1	B	333	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	73	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	132	LEU	CA-CB-CG	5.26	127.40	115.30
1	B	235	LEU	C-N-CA	5.20	134.71	121.70

There are no chirality outliers.

There are no planarity outliers.

4.2 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	2955	0	3021	109	0
1	B	2943	0	3011	144	0
2	A	366	0	0	22	0
2	B	409	0	0	25	0
All	All	6673	0	6032	247	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 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:169:CSD:SG	1:B:169:CSD:OD2	1.94	1.25
1:B:211:LEU:HD12	1:B:211:LEU:O	1.10	1.24
1:B:211:LEU:O	1:B:211:LEU:CD1	2.02	1.07
1:B:211:LEU:HD12	1:B:211:LEU:C	1.73	1.07
1:B:262:HIS:H	1:B:269:THR:HG22	1.22	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LYS:HD2	1:B:244[A]:ILE:HG12	1.46	0.97
1:A:142:MET:HE3	1:B:261:LEU:HD22	1.53	0.89
1:B:24[A]:ILE:HD13	1:B:227:LEU:HD23	1.56	0.88
1:B:292:LEU:HD11	1:B:374:VAL:HG21	1.62	0.82
1:B:274[B]:ARG:H	1:B:274[B]:ARG:HD2	1.46	0.81
1:A:306:MET:HG3	1:A:375:LEU:HB2	1.64	0.80
1:A:73:ARG:HD3	2:A:2018:HOH:O	1.83	0.78
1:A:286:ASN:HB3	2:A:2287:HOH:O	1.85	0.77
1:A:241:ILE:O	1:A:366:THR:HG21	1.85	0.75
1:A:276:VAL:HG13	1:A:382:MET:HE1	1.67	0.75
1:A:316:ASP:O	1:A:320:ARG:HG3	1.87	0.74
1:A:366:THR:HG22	1:A:392:VAL:H	1.53	0.74
1:B:355:ARG:HD3	1:B:356:LYS:HG3	1.68	0.74
1:B:60:LYS:HG2	1:B:63:ARG:NH2	2.02	0.73
1:A:79:GLU:O	1:A:83:GLN:HG2	1.88	0.73
1:B:87:THR:HG23	1:B:95:SER:HB3	1.71	0.73
1:A:47:ARG:HG3	1:A:52:GLU:OE2	1.89	0.72
1:B:241:ILE:O	1:B:366:THR:HG21	1.88	0.72
1:B:285:GLU:O	1:B:289:GLU:HG3	1.89	0.72
1:B:137:THR:OG1	1:B:343[A]:ILE:HD11	1.89	0.72
1:B:271:GLN:HG2	2:B:2292:HOH:O	1.90	0.72
1:B:73:ARG:HD3	2:B:2028:HOH:O	1.90	0.71
1:B:50:LYS:HE3	2:B:2055:HOH:O	1.90	0.71
1:B:250:THR:HB	2:B:2275:HOH:O	1.90	0.70
1:A:71:LYS:HG3	1:A:337:SER:OG	1.91	0.70
1:A:292:LEU:HB3	1:A:297[A]:ILE:HG13	1.74	0.69
1:A:292:LEU:HD22	1:A:297[A]:ILE:HG12	1.73	0.69
1:A:150:VAL:HB	1:A:155:LEU:HB2	1.74	0.69
1:A:19:GLN:HE21	1:A:231:SER:HB2	1.58	0.68
1:B:115:ALA:O	1:B:119:ILE:HG13	1.93	0.68
1:A:168:GLY:HA2	1:A:343[A]:ILE:HD11	1.74	0.68
1:B:201:ILE:HG13	1:B:268:LEU:HB2	1.75	0.67
1:B:78:THR:HG22	2:B:2102:HOH:O	1.94	0.67
1:A:19:GLN:NE2	1:A:231:SER:HB2	2.10	0.66
1:A:34:ASN:HB3	2:A:2073:HOH:O	1.93	0.66
1:A:330:ARG:HG3	1:A:330:ARG:HH11	1.59	0.66
1:A:18:ALA:HB1	1:A:19:GLN:NE2	2.11	0.66
1:A:273:HIS:HD2	1:A:275:ASP:H	1.42	0.66
1:A:19:GLN:HE21	1:A:231:SER:CB	2.09	0.66
1:A:248:ASP:HB2	2:A:2241:HOH:O	1.95	0.65
1:A:258:ALA:HB1	1:A:382:MET:HE2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:HIS:O	1:B:276:VAL:HG23	1.97	0.64
1:A:138:ALA:HA	1:A:201:ILE:HG12	1.80	0.64
1:A:219:LEU:HD22	2:A:2222:HOH:O	1.97	0.64
1:B:177:ARG:HA	1:B:247:THR:HG21	1.79	0.64
1:B:146:ASP:O	1:B:150:VAL:HG12	1.99	0.63
1:A:71:LYS:HE3	1:A:337:SER:OG	2.00	0.61
1:B:91:PHE:CE2	1:B:207:ASN:HB2	2.35	0.61
1:B:55:VAL:O	1:B:59:GLU:HG2	2.00	0.61
1:B:328:LYS:HE2	2:B:2390:HOH:O	2.00	0.61
1:A:273:HIS:CD2	1:A:275:ASP:H	2.18	0.61
1:B:343[A]:ILE:HG13	1:B:344:SER:N	2.16	0.60
1:B:392:VAL:O	1:B:393:ARG:HB2	2.01	0.60
1:B:72:LYS:HE3	1:B:338:GLU:OE1	2.02	0.59
1:B:81:TYR:HB2	2:B:2101:HOH:O	2.03	0.59
1:A:285[B]:GLU:HG2	1:A:322:LEU:HD23	1.85	0.59
1:B:274[A]:ARG:HD3	2:B:2317:HOH:O	2.02	0.58
1:A:366:THR:CG2	1:A:392:VAL:H	2.15	0.58
1:A:306:MET:HG3	1:A:375:LEU:CB	2.33	0.58
1:B:75:LEU:HG	2:B:2095:HOH:O	2.03	0.58
1:B:168:GLY:HA2	1:B:343[A]:ILE:HD12	1.86	0.58
1:B:393:ARG:HD2	2:B:2408:HOH:O	2.02	0.58
1:A:93:ALA:HA	2:A:2091:HOH:O	2.03	0.58
1:B:91:PHE:CD2	1:B:207:ASN:HB2	2.38	0.58
1:B:60:LYS:NZ	1:B:211:LEU:HD22	2.18	0.58
1:A:216:ALA:HB2	1:A:270:PHE:CD2	2.37	0.57
1:B:211:LEU:HD13	1:B:214:LEU:HB3	1.84	0.57
1:B:269:THR:HG23	2:B:2292:HOH:O	2.04	0.57
1:B:147:TYR:O	1:B:150:VAL:HG13	2.04	0.57
1:B:168:GLY:HA3	2:B:2217:HOH:O	2.03	0.57
1:B:306:MET:O	1:B:375:LEU:HA	2.04	0.57
1:A:247:THR:HG22	1:B:160:LYS:NZ	2.19	0.57
1:A:306:MET:CE	1:A:389:LEU:HD12	2.35	0.57
1:A:56:ASP:OD1	1:A:60:LYS:HE3	2.05	0.56
1:B:137:THR:CB	1:B:343[A]:ILE:HD11	2.35	0.56
1:A:242:PHE:CE1	1:A:366:THR:HG23	2.40	0.56
1:A:366:THR:HG22	1:A:391:SER:HB2	1.86	0.56
1:A:285[A]:GLU:HB2	2:A:2284:HOH:O	2.05	0.56
1:A:142:MET:HE3	1:B:261:LEU:CD2	2.33	0.56
1:B:84:GLU:HG3	2:B:2113:HOH:O	2.06	0.55
1:B:244[A]:ILE:HD11	1:B:247:THR:CG2	2.37	0.55
1:B:258:ALA:HB1	1:B:382:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:THR:HG22	1:B:391[A]:SER:HB2	1.89	0.55
1:A:63:ARG:HG2	1:A:63:ARG:HH11	1.72	0.55
1:A:84:GLU:HG3	2:A:2085:HOH:O	2.07	0.54
1:B:24[A]:ILE:HD11	1:B:27:ILE:HG13	1.89	0.54
1:A:61:PHE:CE1	1:A:218:ALA:HB2	2.43	0.54
1:B:24[A]:ILE:HD11	1:B:27:ILE:CG1	2.38	0.54
1:B:24[A]:ILE:HG23	1:B:242:PHE:O	2.07	0.54
1:A:177:ARG:HD3	1:A:247:THR:HG23	1.90	0.53
1:A:247:THR:HG22	1:B:160:LYS:HZ1	1.72	0.53
1:A:60:LYS:HD3	1:A:60:LYS:N	2.23	0.53
1:B:292:LEU:HD11	1:B:374:VAL:CG2	2.36	0.53
1:B:323:ASN:ND2	2:B:2368:HOH:O	2.41	0.53
1:A:247:THR:HG21	2:A:2200:HOH:O	2.08	0.53
1:B:258:ALA:CB	1:B:382:MET:HE2	2.39	0.53
1:A:80:ASP:O	1:A:84:GLU:HB2	2.09	0.52
1:B:131:HIS:HB2	1:B:191:VAL:HG22	1.90	0.52
1:A:158[B]:SER:OG	1:B:250:THR:HG23	2.10	0.52
1:B:199:THR:HG21	1:B:220:PHE:HB3	1.92	0.52
1:A:91:PHE:HB3	1:A:207:ASN:HB2	1.89	0.52
1:B:242:PHE:CE1	1:B:366:THR:HG23	2.45	0.52
1:B:284:ILE:HD11	1:B:376:PHE:CE2	2.44	0.52
1:A:42:ALA:CB	1:A:62:LYS:HG2	2.39	0.52
1:A:193:ILE:O	1:A:226:ALA:HA	2.10	0.52
1:B:34:ASN:HB3	1:B:75:LEU:O	2.09	0.52
1:B:211:LEU:CD1	1:B:211:LEU:C	2.46	0.52
1:A:264[A]:ARG:HD3	2:A:2265:HOH:O	2.10	0.51
1:A:19:GLN:HB2	1:A:231:SER:HB3	1.92	0.51
1:A:64:ILE:O	1:A:68:THR:HG23	2.10	0.51
1:A:306:MET:HE1	1:A:389:LEU:HD12	1.93	0.51
1:B:70:ILE:HG21	1:B:73:ARG:HD2	1.93	0.51
1:B:288:ALA:O	1:B:292:LEU:HD13	2.11	0.51
1:B:43:ASP:O	1:B:47:ARG:HB2	2.11	0.51
1:B:60:LYS:HA	1:B:63:ARG:CZ	2.40	0.50
1:A:208:GLU:OE1	1:A:209:ASN:ND2	2.45	0.50
1:B:252[B]:LEU:HD22	1:B:283:ASN:CB	2.41	0.50
1:A:142:MET:CE	1:B:166:GLN:HE21	2.25	0.50
1:A:55:VAL:HG23	2:A:2048:HOH:O	2.10	0.50
1:B:264:ARG:HG3	1:B:264:ARG:HH11	1.77	0.50
1:A:357:ARG:NH2	2:A:2337:HOH:O	2.44	0.50
1:A:323:ASN:HB2	2:A:2151:HOH:O	2.12	0.50
1:B:60:LYS:HA	1:B:63:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LYS:HE3	2:B:2075:HOH:O	2.12	0.49
1:B:209:ASN:OD1	1:B:210:HIS:N	2.45	0.49
1:A:304:PHE:CE2	1:A:373:GLY:HA3	2.47	0.49
1:B:18:ALA:N	1:B:184:GLU:O	2.45	0.49
1:A:219:LEU:HB3	2:A:2222:HOH:O	2.12	0.49
1:B:91:PHE:HE1	2:B:2306:HOH:O	1.95	0.49
1:A:384[A]:VAL:HG23	2:A:2243:HOH:O	2.12	0.49
1:B:24[A]:ILE:HD13	1:B:227:LEU:CD2	2.36	0.48
1:B:66:GLU:OE1	1:B:66:GLU:HA	2.12	0.48
1:B:347:VAL:HB	1:B:375:LEU:HD22	1.95	0.48
1:A:257:LYS:HA	1:A:260[A]:LYS:HE2	1.95	0.47
1:A:394:VAL:HG11	2:A:2343:HOH:O	2.13	0.47
1:B:207:ASN:ND2	1:B:209:ASN:O	2.48	0.47
1:B:248:ASP:HB3	2:B:2277:HOH:O	2.13	0.47
1:A:384[B]:VAL:HG13	1:A:384[B]:VAL:O	2.15	0.47
1:B:306:MET:HG2	1:B:350:ILE:HG22	1.95	0.47
1:B:350:ILE:O	1:B:354:VAL:HG13	2.15	0.47
1:A:19:GLN:HG2	1:A:232:GLY:HA3	1.97	0.46
1:B:34:ASN:O	1:B:74:TYR:HA	2.15	0.46
1:A:149:LEU:HD13	1:A:153:LEU:HD12	1.97	0.46
1:B:24[A]:ILE:O	1:B:24[A]:ILE:HG13	2.15	0.46
1:A:235:LEU:HB2	2:A:2231:HOH:O	2.14	0.46
1:B:168:GLY:HA2	1:B:343[A]:ILE:CD1	2.46	0.46
1:B:236:ALA:N	2:B:2259:HOH:O	2.49	0.46
1:B:347:VAL:O	1:B:351:ILE:HG13	2.15	0.46
1:B:211:LEU:CD1	1:B:214:LEU:HB3	2.45	0.46
1:B:252[A]:LEU:HD22	1:B:382:MET:HG2	1.97	0.46
1:A:361:GLU:OE1	1:A:363:LYS:NZ	2.49	0.46
1:A:292:LEU:HB3	1:A:297[A]:ILE:CG1	2.43	0.46
1:A:64:ILE:HD13	1:A:215:VAL:HG22	1.97	0.46
1:B:274[B]:ARG:NH2	2:B:2314:HOH:O	2.48	0.46
1:B:363:LYS:HA	1:B:363:LYS:HD3	1.68	0.46
1:B:47:ARG:NH2	1:B:79:GLU:OE2	2.49	0.46
1:A:70:ILE:HG21	1:A:73:ARG:HD2	1.98	0.45
1:A:93:ALA:N	2:A:2093:HOH:O	2.50	0.45
1:B:209:ASN:O	1:B:210:HIS:HB3	2.17	0.45
1:A:63:ARG:HG2	1:A:63:ARG:NH1	2.31	0.45
1:B:60:LYS:HG2	1:B:63:ARG:HH22	1.81	0.45
1:A:68:THR:O	1:A:69:ALA:HB3	2.16	0.45
1:B:274[A]:ARG:NH1	1:B:275:ASP:OD2	2.49	0.45
1:B:289:GLU:O	1:B:293:SER:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:VAL:O	1:B:328:LYS:NZ	2.49	0.45
1:B:60:LYS:HZ1	1:B:211:LEU:HD22	1.81	0.45
1:A:167:GLN:HB3	1:A:171:ALA:HB2	1.98	0.45
1:B:164:LEU:HB3	1:B:167:GLN:HG3	1.98	0.45
1:B:274[B]:ARG:HD3	2:B:2318:HOH:O	2.16	0.45
1:A:236:ALA:N	2:A:2232:HOH:O	2.49	0.45
1:B:356:LYS:NZ	2:B:2384:HOH:O	2.49	0.45
1:A:276:VAL:HG13	1:A:382:MET:CE	2.41	0.45
1:A:381:GLY:N	1:A:382:MET:HA	2.31	0.45
1:B:69:ALA:HB2	1:B:312:ARG:CZ	2.47	0.45
1:B:44:TYR:O	1:B:48:VAL:HB	2.16	0.45
1:B:272:LEU:CD2	1:B:276:VAL:HG21	2.47	0.45
1:A:264[A]:ARG:NH1	2:A:2265:HOH:O	2.50	0.44
1:B:252[A]:LEU:HG	1:B:283:ASN:CG	2.38	0.44
1:B:252[B]:LEU:HD22	1:B:283:ASN:HB3	1.98	0.44
1:B:347:VAL:HB	1:B:375:LEU:CD2	2.48	0.44
1:A:86:PRO:O	1:A:89:CYS:HB2	2.18	0.44
1:B:326:GLU:CB	2:B:2371:HOH:O	2.66	0.44
1:A:93:ALA:HB1	1:A:94:PRO:HD2	2.00	0.44
1:A:52:GLU:HB2	2:A:2044:HOH:O	2.17	0.43
1:B:22:ALA:O	1:B:244[A]:ILE:HG22	2.18	0.43
1:B:306:MET:HB2	1:B:375:LEU:HB2	1.99	0.43
1:A:213:SER:HB2	2:A:2274:HOH:O	2.18	0.43
1:B:64:ILE:O	1:B:68:THR:HG23	2.19	0.43
1:B:75:LEU:N	1:B:75:LEU:HD12	2.32	0.43
1:B:74:TYR:O	1:B:222:ASP:HB2	2.19	0.43
1:A:357:ARG:HD3	1:A:357:ARG:HA	1.85	0.43
1:A:393:ARG:HE	1:A:393:ARG:HB3	1.44	0.43
1:B:83:GLN:NE2	1:B:83:GLN:HA	2.26	0.43
1:A:47:ARG:HG3	1:A:52:GLU:CD	2.39	0.42
1:A:256:GLU:HA	1:A:381:GLY:O	2.20	0.42
1:A:285[B]:GLU:CD	1:A:300:TRP:HE1	2.22	0.42
1:B:60:LYS:HZ2	1:B:211:LEU:HD22	1.84	0.42
1:A:64:ILE:O	1:A:67:LYS:HG3	2.19	0.42
1:A:91:PHE:O	1:A:92:MET:HB2	2.20	0.42
1:B:261:LEU:HD23	1:B:268:LEU:HD11	2.01	0.42
1:A:55:VAL:HG13	1:A:56:ASP:N	2.35	0.42
1:A:297[A]:ILE:HG13	1:A:297[A]:ILE:O	2.20	0.42
1:B:253:PRO:O	1:B:254:ASP:HB2	2.20	0.42
1:A:273:HIS:CD2	1:A:275:ASP:HB2	2.55	0.42
1:B:292:LEU:HD12	1:B:292:LEU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LEU:HD13	1:A:384[A]:VAL:HG13	2.02	0.42
1:B:62:LYS:HE2	1:B:62:LYS:HB3	1.89	0.41
1:A:44:TYR:O	1:A:48:VAL:HG22	2.20	0.41
1:A:330:ARG:HH11	1:A:330:ARG:CG	2.31	0.41
1:B:87:THR:OG1	1:B:93:ALA:HB1	2.21	0.41
1:B:91:PHE:HZ	2:B:2246:HOH:O	2.03	0.41
1:A:328:LYS:HA	1:A:328:LYS:HD2	1.88	0.41
1:A:43:ASP:O	1:A:47:ARG:HD2	2.21	0.41
1:A:64:ILE:HG23	1:A:67:LYS:HE3	2.03	0.41
1:A:330:ARG:HG3	1:A:330:ARG:NH1	2.29	0.41
1:A:273:HIS:HD2	1:A:275:ASP:HB2	1.84	0.41
1:A:330:ARG:NH2	1:A:353:GLU:OE2	2.50	0.41
1:B:87:THR:HG21	1:B:94:PRO:O	2.21	0.41
1:B:44:TYR:CE1	1:B:48:VAL:HG21	2.55	0.41
1:B:57:LEU:HD11	1:B:214:LEU:HD22	2.03	0.41
1:B:291:ALA:HB3	1:B:292:LEU:HD12	2.03	0.41
1:B:152:LEU:HD12	1:B:152:LEU:HA	1.89	0.41
1:B:208:GLU:HB2	2:B:2244:HOH:O	2.21	0.41
1:B:226:ALA:C	1:B:227:LEU:HD12	2.42	0.41
1:A:135:CYS:O	1:A:195:CYS:HA	2.20	0.40
1:B:304:PHE:O	1:B:373:GLY:HA2	2.20	0.40
1:A:343[A]:ILE:HG12	1:A:344:SER:N	2.36	0.40
1:A:272:LEU:CD2	1:A:276:VAL:HG21	2.52	0.40
1:A:330:ARG:HG3	1:A:331:ALA:N	2.37	0.40
1:B:167:GLN:HB3	1:B:171:ALA:HB2	2.03	0.40
1:B:300:TRP:O	1:B:303:VAL:HG22	2.21	0.40
1:B:250:THR:HG22	2:B:2279:HOH:O	2.21	0.40
1:B:381:GLY:N	1:B:382:MET:HA	2.36	0.40

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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	382/402 (95%)	369 (97%)	7 (2%)	6 (2%)	9 5
1	B	380/402 (94%)	365 (96%)	11 (3%)	4 (1%)	14 9
All	All	762/804 (95%)	734 (96%)	18 (2%)	10 (1%)	14 7

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	MET
1	A	208	GLU
1	A	236	ALA
1	B	236	ALA
1	A	343[A]	ILE
1	A	343[B]	ILE
1	B	212	ASP
1	B	343[A]	ILE
1	B	343[B]	ILE
1	A	235	LEU

4.3.2 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	318/328 (97%)	274 (86%)	44 (14%)	3 2
1	B	316/328 (96%)	260 (82%)	56 (18%)	2 1
All	All	634/656 (97%)	534 (84%)	100 (16%)	3 1

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	27	ILE
1	A	56	ASP
1	A	60	LYS
1	A	62	LYS
1	A	63	ARG

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Mol	Chain	Res	Type
1	A	66	GLU
1	A	67	LYS
1	A	71	LYS
1	A	77	LEU
1	A	84	GLU
1	A	90	GLU
1	A	132	LEU
1	A	149	LEU
1	A	151	LYS
1	A	152	LEU
1	A	187	LYS
1	A	201	ILE
1	A	202	LEU
1	A	208	GLU
1	A	209	ASN
1	A	212	ASP
1	A	235	LEU
1	A	247	THR
1	A	250	THR
1	A	251	ILE
1	A	252	LEU
1	A	259	MET
1	A	272	LEU
1	A	278	LEU
1	A	285[A]	GLU
1	A	285[B]	GLU
1	A	295	LEU
1	A	297[A]	ILE
1	A	297[B]	ILE
1	A	306	MET
1	A	325	LYS
1	A	326	GLU
1	A	327	ASP
1	A	330	ARG
1	A	355	ARG
1	A	370	LEU
1	A	375	LEU
1	A	393	ARG
1	B	24[A]	ILE
1	B	24[B]	ILE
1	B	52	GLU
1	B	57	LEU

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Mol	Chain	Res	Type
1	B	60	LYS
1	B	62	LYS
1	B	67	LYS
1	B	71	LYS
1	B	75	LEU
1	B	77	LEU
1	B	78	THR
1	B	83	GLN
1	B	87	THR
1	B	90	GLU
1	B	91	PHE
1	B	92	MET
1	B	102	LEU
1	B	105	THR
1	B	112	LYS
1	B	132	LEU
1	B	149	LEU
1	B	150	VAL
1	B	152	LEU
1	B	164	LEU
1	B	187	LYS
1	B	202	LEU
1	B	211	LEU
1	B	239	ARG
1	B	244[A]	ILE
1	B	244[B]	ILE
1	B	252[A]	LEU
1	B	252[B]	LEU
1	B	257	LYS
1	B	259	MET
1	B	264	ARG
1	B	268	LEU
1	B	269	THR
1	B	271	GLN
1	B	272	LEU
1	B	295	LEU
1	B	312	ARG
1	B	323	ASN
1	B	324	LEU
1	B	326	GLU
1	B	328	LYS
1	B	343[A]	ILE

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Mol	Chain	Res	Type
1	B	343[B]	ILE
1	B	354	VAL
1	B	355	ARG
1	B	357[A]	ARG
1	B	357[B]	ARG
1	B	366	THR
1	B	370	LEU
1	B	375	LEU
1	B	382	MET
1	B	389	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	207	ASN
1	A	209	ASN
1	A	273	HIS
1	A	317	GLN
1	B	34	ASN
1	B	83	GLN
1	B	166	GLN
1	B	273	HIS
1	B	286	ASN

4.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\|>2$
1	CSD	A	169	1	3,7,8	3.02	1 (33%)	1,8,10	2.43	1 (100%)
1	CSD	B	169	1	3,7,8	3.48	2 (66%)	1,8,10	2.42	1 (100%)

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
1	CSD	A	169	1	-	0/2/6/8	-
1	CSD	B	169	1	-	0/2/6/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	169	CSD	CA-N	-5.43	1.31	1.48
1	A	169	CSD	CA-N	-4.85	1.33	1.48
1	B	169	CSD	O-C	2.35	1.29	1.19

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	169	CSD	OD1-SG-CB	2.43	110.17	105.54
1	B	169	CSD	OD1-SG-CB	2.42	110.15	105.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	169	CSD	1	0

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

There are no ligands in this entry.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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	377/402 (93%)	0.40	34 (9%)	9	12	13, 25, 67, 126	0
1	B	375/402 (93%)	0.25	26 (6%)	16	21	11, 23, 59, 135	0
All	All	752/804 (93%)	0.32	60 (7%)	12	16	11, 24, 64, 135	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	91	PHE	11.2
1	B	18	ALA	11.1
1	A	209	ASN	9.9
1	A	18	ALA	9.3
1	A	19	GLN	7.7
1	B	91	PHE	7.4
1	B	19	GLN	6.9
1	B	209	ASN	6.3
1	B	210	HIS	5.1
1	A	92	MET	4.9
1	A	326	GLU	4.8
1	A	210	HIS	4.5
1	A	370	LEU	4.5
1	A	395	THR	4.4
1	B	211	LEU	4.2
1	A	207	ASN	4.2
1	A	93	ALA	4.1
1	A	57	LEU	4.0
1	A	54	MET	4.0
1	B	53	HIS	3.9
1	A	208	GLU	3.8
1	A	51	SER	3.8
1	A	53	HIS	3.6
1	A	87	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	207	ASN	3.5
1	A	56	ASP	3.4
1	B	208	GLU	3.4
1	A	394	VAL	3.3
1	A	47	ARG	3.3
1	A	206	PRO	3.2
1	A	297[A]	ILE	3.1
1	A	327	ASP	3.1
1	B	359	MET	2.9
1	B	206	PRO	2.9
1	B	92	MET	2.8
1	A	164	LEU	2.8
1	B	93	ALA	2.8
1	B	164	LEU	2.7
1	A	55	VAL	2.7
1	B	295	LEU	2.6
1	A	369	GLY	2.6
1	A	90	GLU	2.6
1	B	66	GLU	2.6
1	B	86	PRO	2.5
1	A	211	LEU	2.5
1	A	360	ALA	2.4
1	B	55	VAL	2.3
1	B	294	PRO	2.2
1	B	326	GLU	2.2
1	A	295	LEU	2.2
1	B	165	TYR	2.2
1	A	49	THR	2.2
1	A	235	LEU	2.2
1	B	59	GLU	2.2
1	A	86	PRO	2.2
1	B	63	ARG	2.2
1	A	212	ASP	2.1
1	B	212	ASP	2.0
1	B	343[A]	ILE	2.0
1	B	87	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSD	A	169	8/9	0.98	0.12	14,20,27,34	0
1	CSD	B	169	8/9	0.98	0.12	14,15,23,37	0

5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

5.4 Ligands (i)

There are no ligands in this entry.

5.5 Other polymers (i)

There are no such residues in this entry.