Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2021 – 09:41 PM EDT

PDB ID	:	3KOM
Title	:	Crystal structure of apo transketolase from Francisella tularensis
Authors	:	Anderson, S.M.; Wawrzak, Z.; Skarina, T.; Gordon, E.; Kwon, K.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2009-11-13
Resolution	:	1.60 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 following versions of software and data (see references (i)) were used in the production of this report:

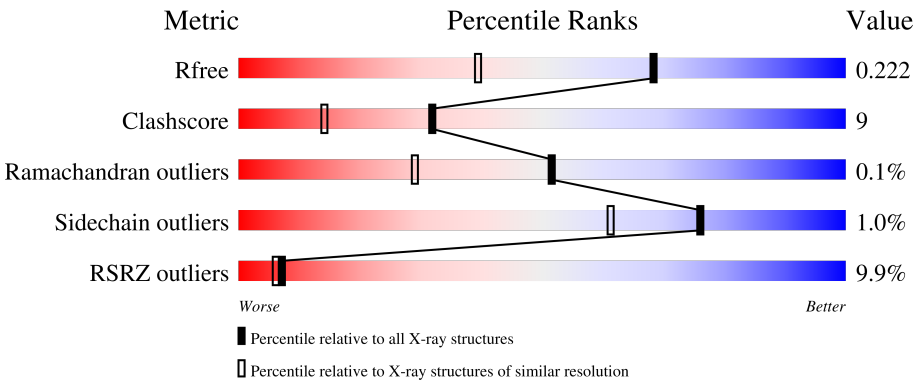
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	663	7% 85% 13% ••
1	B	663	12% 83% 14% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11675 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 Transketolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	654	5209	3315	886	981	6	21	0	21	0
1	B	648	5130	3268	871	962	6	23	0	13	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	313	ARG	TRP	engineered mutation	UNP Q5NF74
B	313	ARG	TRP	engineered mutation	UNP Q5NF74

- Molecule 2 is water.

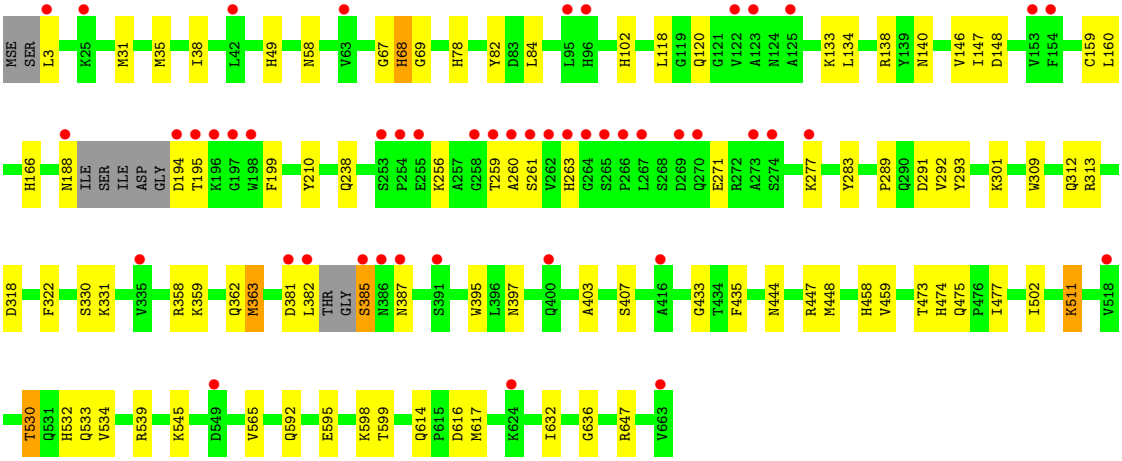
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	698	723	723	0	25
2	B	597	613	613	0	16

3 Residue-property plots (i)

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

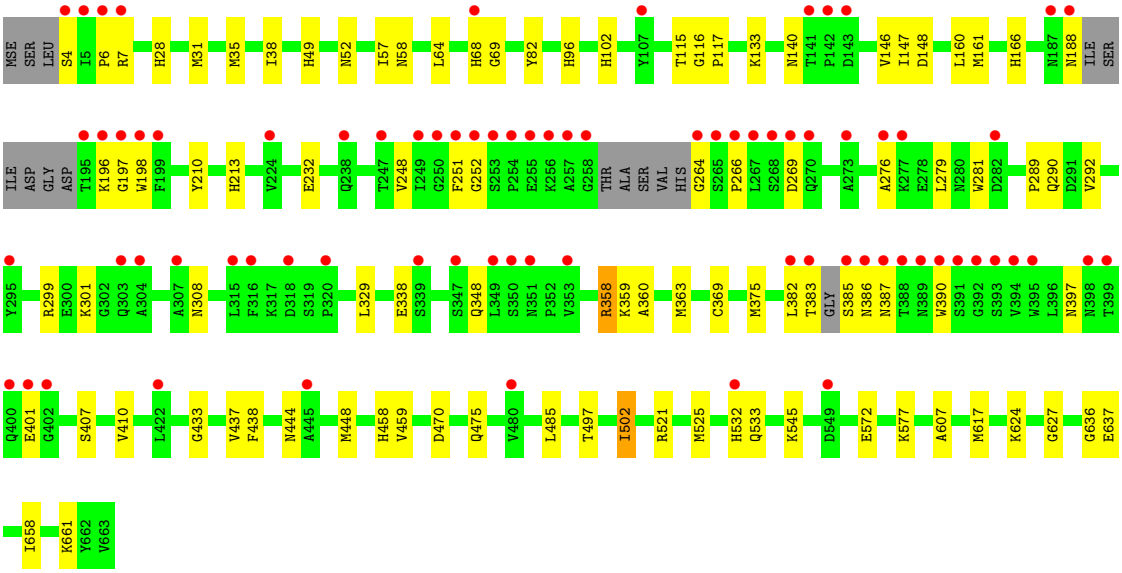
- Molecule 1: Transketolase

Chain A:



- Molecule 1: Transketolase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.49Å 109.29Å 128.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.04 – 1.60 29.04 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.04-1.60) 98.3 (29.04-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.163 , 0.199 0.193 , 0.222	Depositor DCC
R_{free} test set	7930 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	15.1	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11675	wwPDB-VP
Average B, all atoms (Å^2)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.61	0/5358	0.70	2/7226 (0.0%)
1	B	0.56	0/5263	0.64	0/7097
All	All	0.59	0/10621	0.67	2/14323 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	363	MSE	CG-SE-CE	-8.98	79.15	98.90
1	A	447	ARG	NE-CZ-NH2	-5.64	117.48	120.30

There are no chirality outliers.

There are no planarity outliers.

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	5209	0	5144	99	0
1	B	5130	0	5056	104	0
2	A	723	0	0	22	0
2	B	613	0	0	27	0
All	All	11675	0	10200	183	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 (183) 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:A:616:ASP:HB2	1:B:617[B]:MSE:CE	1.66	1.25
1:A:617:MSE:HG3	1:B:617[B]:MSE:SE	1.88	1.21
1:A:138[B]:ARG:HH11	1:A:138[B]:ARG:HG2	1.16	1.10
1:A:616:ASP:CB	1:B:617[B]:MSE:HE1	1.80	1.10
1:A:138[B]:ARG:HH11	1:A:138[B]:ARG:CG	1.63	1.09
1:B:358:ARG:HD3	1:B:385:SER:O	1.54	1.08
1:A:616:ASP:CB	1:B:617[B]:MSE:CE	2.36	1.02
1:A:617:MSE:CG	1:B:617[B]:MSE:SE	2.62	0.98
1:B:497:THR:HG23	2:B:961:HOH:O	1.62	0.97
1:A:58:ASN:HD21	1:A:148:ASP:H	1.11	0.96
1:B:502:ILE:HD13	2:B:1113:HOH:O	1.68	0.94
1:B:58:ASN:HD21	1:B:148:ASP:H	1.16	0.91
1:B:290[B]:GLN:HG3	2:B:785:HOH:O	1.71	0.90
1:A:530:THR:HG21	2:A:850:HOH:O	1.72	0.89
1:A:616:ASP:HB2	1:B:617[B]:MSE:HE1	0.89	0.88
1:A:511:LYS:HE3	2:A:1015:HOH:O	1.73	0.87
1:B:397:ASN:HD21	1:B:407:SER:H	1.25	0.85
1:B:382:LEU:O	1:B:383:THR:HB	1.76	0.85
1:A:291[A]:ASP:OD1	1:A:292:VAL:N	2.11	0.84
1:A:120:GLN:HE22	1:A:444:ASN:HD22	1.22	0.84
1:A:138[B]:ARG:CG	1:A:138[B]:ARG:NH1	2.35	0.83
1:A:256:LYS:HE2	1:A:271:GLU:OE2	1.79	0.82
1:B:133:LYS:HE2	2:B:832:HOH:O	1.78	0.82
1:A:301:LYS:HD3	2:A:1011:HOH:O	1.78	0.81
1:B:369:CYS:SG	1:B:375[B]:MSE:HE2	2.20	0.81
1:A:435:PHE:CE2	2:A:913:HOH:O	2.37	0.78
1:B:525:MSE:SE	2:B:994:HOH:O	2.51	0.77
1:A:309:TRP:CH2	1:A:313:ARG:HD2	2.20	0.77
1:A:435:PHE:HE2	2:A:913:HOH:O	1.69	0.75
1:A:397:ASN:HD21	1:A:407:SER:H	1.33	0.75
1:B:624:LYS:HD3	2:B:1296:HOH:O	1.85	0.75
1:A:138[B]:ARG:HG2	1:A:138[B]:ARG:NH1	1.92	0.74
1:A:382:LEU:HD21	1:B:161:MSE:HE1	1.70	0.74
1:B:31:MSE:HE3	1:B:69:GLY:HA3	1.70	0.74
1:A:138[B]:ARG:HH11	1:A:138[B]:ARG:HG3	1.54	0.73
1:B:140:ASN:HD21	1:B:147:ILE:H	1.36	0.73
1:A:166:HIS:HD2	1:A:210:TYR:OH	1.72	0.72
1:A:616:ASP:CB	1:B:617[B]:MSE:HE3	2.17	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:CYS:SG	1:B:375[B]:MSE:CE	2.77	0.72
1:A:502:ILE:HD12	2:A:1108:HOH:O	1.89	0.71
1:A:138[B]:ARG:NH2	1:A:403:ALA:O	2.23	0.71
1:B:358:ARG:NH2	1:B:521:ARG:O	2.24	0.70
1:B:624:LYS:CD	2:B:1296:HOH:O	2.39	0.70
1:B:266:PRO:HB2	2:B:1183:HOH:O	1.91	0.70
1:B:166:HIS:HD2	1:B:210:TYR:OH	1.74	0.70
1:B:658:ILE:HA	1:B:661:LYS:HD3	1.74	0.69
1:A:140:ASN:HD21	1:A:147:ILE:H	1.40	0.69
1:A:530:THR:HG22	1:A:533:GLN:H	1.56	0.69
1:B:57:ILE:HD13	1:B:329:LEU:HD13	1.75	0.69
1:A:647:ARG:NH1	1:B:96:HIS:NE2	2.42	0.68
1:B:358:ARG:HD2	1:B:387:ASN:ND2	2.09	0.67
1:A:58:ASN:ND2	1:A:148:ASP:H	1.90	0.67
1:A:358:ARG:HD3	2:A:1292:HOH:O	1.93	0.67
1:B:338:GLU:HG2	2:B:805:HOH:O	1.95	0.67
1:A:78:HIS:HE1	1:A:293:TYR:OH	1.76	0.67
1:A:381:ASP:OD2	1:A:385:SER:N	2.27	0.66
1:B:49:HIS:HD2	1:B:82:TYR:OH	1.79	0.66
1:A:322:PHE:HE1	2:A:1288:HOH:O	1.78	0.65
1:A:530:THR:HG23	2:A:989:HOH:O	1.96	0.65
1:A:616:ASP:HB3	1:B:617[B]:MSE:CE	2.25	0.64
1:A:49:HIS:HD2	1:A:82:TYR:OH	1.79	0.64
1:A:616:ASP:HB3	1:B:617[B]:MSE:HE3	1.79	0.64
1:B:386:ASN:ND2	2:B:849:HOH:O	2.31	0.63
1:B:545:LYS:HE3	2:B:912:HOH:O	1.98	0.63
1:B:213:HIS:HD2	2:B:702:HOH:O	1.82	0.62
1:B:52:ASN:HB2	2:B:841:HOH:O	1.99	0.61
1:B:197:GLY:HA3	2:B:917:HOH:O	2.01	0.60
1:B:31:MSE:CE	1:B:69:GLY:HA3	2.31	0.60
1:A:359:LYS:HE3	2:A:1225:HOH:O	2.01	0.60
1:A:359:LYS:O	1:A:363:MSE:HG3	2.02	0.60
1:A:395:TRP:CZ3	1:A:407:SER:OG	2.54	0.59
1:B:385:SER:CB	2:B:1299:HOH:O	2.52	0.58
1:A:382:LEU:HD23	1:B:198:TRP:HE1	1.67	0.58
1:A:473:THR:HB	1:B:117:PRO:HD3	1.85	0.58
1:A:312:GLN:NE2	2:A:1085:HOH:O	2.37	0.57
1:A:133[B]:LYS:HE3	2:A:1165:HOH:O	2.03	0.57
1:B:58:ASN:ND2	1:B:148:ASP:H	1.96	0.57
1:A:382:LEU:CD2	1:B:198:TRP:HE1	2.18	0.57
1:A:138[B]:ARG:NH1	1:A:138[B]:ARG:HG3	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ASN:HD22	1:B:146:VAL:HG12	1.67	0.57
1:A:362:GLN:HB2	1:A:387:ASN:HB3	1.86	0.56
1:B:28:HIS:ND1	1:B:264:GLY:HA3	2.20	0.56
1:B:252:GLY:HA3	1:B:279:LEU:HD11	1.87	0.56
1:A:195:THR:HB	1:A:199:PHE:HB3	1.87	0.56
1:B:358:ARG:HH11	1:B:385:SER:CB	2.18	0.56
1:B:290[B]:GLN:CG	2:B:785:HOH:O	2.42	0.56
1:A:49:HIS:HE1	2:A:968:HOH:O	1.89	0.56
1:B:213:HIS:HE1	1:B:232:GLU:OE2	1.89	0.55
1:B:401:GLU:HA	1:B:401:GLU:OE1	2.07	0.54
1:A:35[B]:MSE:SE	1:A:38:ILE:HD12	2.57	0.54
1:A:134:LEU:O	1:A:138[B]:ARG:HG3	2.07	0.54
1:A:78:HIS:HD2	1:A:84:LEU:O	1.91	0.54
1:B:35[B]:MSE:SE	1:B:38:ILE:HD12	2.57	0.54
1:B:433:GLY:HA2	1:B:459:VAL:O	2.08	0.53
1:A:617:MSE:HG2	1:B:617[B]:MSE:SE	2.53	0.53
1:B:382:LEU:O	1:B:383:THR:CB	2.53	0.52
1:B:437[A]:VAL:HG13	1:B:438:PHE:CD1	2.45	0.52
1:A:359:LYS:HE2	2:A:1224:HOH:O	2.08	0.52
1:B:49:HIS:HE1	2:B:788:HOH:O	1.92	0.51
1:B:358:ARG:NH2	1:B:521:ARG:HA	2.25	0.51
1:B:7[B]:ARG:NE	1:B:7[B]:ARG:H	2.07	0.51
1:A:530:THR:CG2	1:A:532:HIS:HB3	2.40	0.51
1:A:140:ASN:ND2	1:A:146[B]:VAL:H	2.09	0.51
1:A:289:PRO:HG2	1:A:291[A]:ASP:OD1	2.11	0.51
1:A:140:ASN:ND2	1:A:146[A]:VAL:H	2.09	0.50
1:A:259:THR:O	1:A:260:ALA:HB3	2.12	0.50
1:B:369:CYS:HB3	1:B:390:TRP:CE2	2.47	0.50
1:B:577:LYS:HE3	2:B:972:HOH:O	2.12	0.50
1:A:67[A]:GLY:C	1:A:68[A]:HIS:O	2.47	0.50
1:A:433:GLY:HA2	1:A:459:VAL:O	2.12	0.49
1:B:497:THR:CG2	2:B:961:HOH:O	2.38	0.49
1:A:475:GLN:NE2	1:A:636:GLY:HA3	2.28	0.49
1:B:252:GLY:HA2	1:B:279:LEU:HD21	1.94	0.49
1:B:348:GLN:NE2	2:B:1144:HOH:O	2.45	0.49
1:A:102:HIS:HE1	2:A:928[B]:HOH:O	1.95	0.49
1:A:133[A]:LYS:HE3	2:A:1171:HOH:O	2.13	0.49
1:A:166:HIS:HE1	1:B:160:LEU:O	1.95	0.49
1:A:458:HIS:HD2	2:A:1110:HOH:O	1.94	0.49
1:A:31:MSE:HE3	1:A:69[B]:GLY:HA3	1.94	0.49
1:A:291[A]:ASP:OD1	1:A:292:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532[B]:HIS:CE1	1:B:533:GLN:HG3	2.48	0.49
1:A:120:GLN:NE2	1:A:444:ASN:HD22	2.00	0.48
1:A:595:GLU:O	1:A:599:THR:HG23	2.12	0.48
1:B:358:ARG:CD	1:B:385:SER:O	2.44	0.48
1:B:31:MSE:HE1	1:B:64:LEU:HD11	1.95	0.48
1:A:301:LYS:CD	2:A:1011:HOH:O	2.51	0.48
1:B:166:HIS:CD2	1:B:210:TYR:OH	2.62	0.48
1:B:624:LYS:HD2	2:B:1296:HOH:O	2.12	0.48
1:B:140:ASN:ND2	1:B:146:VAL:HG12	2.29	0.48
1:B:308:ASN:OD1	1:B:308:ASN:C	2.53	0.47
1:B:248:VAL:O	1:B:251:PHE:HB2	2.14	0.47
1:A:477:ILE:HG23	1:A:632[B]:ILE:HG23	1.97	0.47
1:A:102:HIS:HD2	1:B:470:ASP:O	1.96	0.47
1:B:475:GLN:OE1	1:B:636:GLY:HA3	2.15	0.47
1:B:502:ILE:CD1	2:B:1113:HOH:O	2.45	0.47
1:A:188:ASN:OD1	1:A:194:ASP:N	2.48	0.47
1:A:539:ARG:HE	1:A:592:GLN:NE2	2.13	0.47
1:B:301:LYS:HE2	2:B:749:HOH:O	2.15	0.47
1:B:196:LYS:NZ	1:B:196:LYS:HB3	2.30	0.46
1:A:277:LYS:HD2	2:A:1026:HOH:O	2.15	0.46
1:B:358:ARG:NH1	1:B:385:SER:CB	2.78	0.46
1:B:532[B]:HIS:NE2	2:B:953:HOH:O	2.36	0.46
1:A:166:HIS:CD2	1:A:210:TYR:OH	2.60	0.46
1:B:485:LEU:CD2	1:B:617[B]:MSE:HE2	2.45	0.46
1:B:276:ALA:HB1	1:B:281:TRP:O	2.16	0.46
1:A:539:ARG:NH2	2:A:759:HOH:O	2.34	0.45
1:B:444:ASN:O	1:B:448:MSE:HG2	2.17	0.45
1:A:160:LEU:O	1:B:166:HIS:HE1	1.99	0.44
1:A:530:THR:HG23	1:A:532:HIS:H	1.82	0.44
1:B:485:LEU:HD21	1:B:617[B]:MSE:HE2	1.99	0.44
1:A:363:MSE:HB3	1:A:363:MSE:HE2	1.82	0.44
1:A:238:GLN:NE2	2:A:786:HOH:O	2.43	0.44
1:B:28:HIS:HD2	1:B:68:HIS:HA	1.82	0.44
1:B:133:LYS:CE	2:B:832:HOH:O	2.50	0.44
1:A:397:ASN:ND2	1:A:397:ASN:H	2.16	0.44
1:B:458:HIS:HD2	2:B:1112:HOH:O	2.01	0.44
1:A:330:SER:O	1:A:331:LYS:HB2	2.18	0.43
1:B:299:ARG:HD2	2:B:843:HOH:O	2.18	0.43
1:A:545:LYS:HE2	1:A:565:VAL:HG13	2.01	0.43
1:B:401:GLU:OE1	1:B:401:GLU:CA	2.67	0.43
1:B:572[B]:GLU:HG2	1:B:577:LYS:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ASN:O	1:A:448:MSE:HG2	2.19	0.43
1:B:607:ALA:O	1:B:627:GLY:HA3	2.19	0.43
1:B:102:HIS:HB3	1:B:115:THR:O	2.19	0.42
1:B:369:CYS:SG	1:B:375[B]:MSE:HE1	2.55	0.42
1:A:318:ASP:HA	2:A:1197:HOH:O	2.19	0.42
1:A:382:LEU:HD23	1:B:198:TRP:NE1	2.34	0.42
1:B:359:LYS:HG3	1:B:363:MSE:HE2	2.02	0.42
1:B:360:ALA:HA	1:B:363:MSE:HE3	2.01	0.42
1:B:140:ASN:ND2	1:B:146:VAL:H	2.17	0.42
1:B:397:ASN:ND2	1:B:397:ASN:H	2.18	0.42
1:A:331:LYS:HE2	1:A:331:LYS:HB3	1.83	0.41
1:B:6:PRO:HA	1:B:7[B]:ARG:NH2	2.35	0.41
1:B:636:GLY:C	1:B:637:GLU:HG3	2.41	0.41
1:A:283:TYR:CZ	1:A:289:PRO:HG3	2.54	0.41
1:A:598:LYS:HA	1:A:598:LYS:HD3	1.84	0.41
1:A:502:ILE:HD11	1:A:534:VAL:HG13	2.02	0.41
1:A:473:THR:OG1	1:A:474:HIS:HD2	2.04	0.41
1:A:259:THR:C	1:A:261:SER:H	2.24	0.41
1:A:118:LEU:HD12	1:B:410:VAL:HG11	2.03	0.40
1:B:289:PRO:HG2	1:B:292:VAL:HG23	2.03	0.40
1:A:166:HIS:HD2	1:A:210:TYR:HH	1.68	0.40
1:A:260:ALA:HA	1:A:263:HIS:HB2	2.02	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	668/663 (101%)	648 (97%)	20 (3%)	0	100	100
1	B	652/663 (98%)	640 (98%)	11 (2%)	1 (0%)	47	26
All	All	1320/1326 (100%)	1288 (98%)	31 (2%)	1 (0%)	51	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	116	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	567/535 (106%)	560 (99%)	7 (1%)	71	54
1	B	555/535 (104%)	550 (99%)	5 (1%)	78	65
All	All	1122/1070 (105%)	1110 (99%)	12 (1%)	76	57

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	68[A]	HIS
1	A	68[B]	HIS
1	A	385	SER
1	A	511	LYS
1	A	530	THR
1	A	614	GLN
1	B	4	SER
1	B	188	ASN
1	B	269	ASP
1	B	358	ARG
1	B	502	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	49	HIS
1	A	58	ASN
1	A	78	HIS

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Mol	Chain	Res	Type
1	A	102	HIS
1	A	124	ASN
1	A	140	ASN
1	A	166	HIS
1	A	178	ASN
1	A	238	GLN
1	A	263	HIS
1	A	312	GLN
1	A	397	ASN
1	A	444	ASN
1	A	454	GLN
1	A	474	HIS
1	A	475	GLN
1	A	488	ASN
1	A	523	ASN
1	A	536	ASN
1	A	569	ASN
1	A	592	GLN
1	A	654	ASN
1	B	49	HIS
1	B	52	ASN
1	B	58	ASN
1	B	68	HIS
1	B	102	HIS
1	B	120	GLN
1	B	140	ASN
1	B	166	HIS
1	B	178	ASN
1	B	213	HIS
1	B	236	GLN
1	B	348	GLN
1	B	371	ASN
1	B	397	ASN
1	B	523	ASN
1	B	536	ASN
1	B	569	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 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	OCS	A	159	1	7,8,9	1.14	0	6,11,13	1.63	2 (33%)
1	OCS	B	159	1	7,8,9	1.10	0	6,11,13	0.93	0

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	OCS	A	159	1	-	0/4/7/9	-
1	OCS	B	159	1	-	0/4/7/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	159	OCS	OD1-SG-CB	2.72	110.17	106.94
1	A	159	OCS	OD3-SG-CB	2.38	109.76	106.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	633/663 (95%)	0.43	48 (7%)	13	12	2, 3, 18, 45	0
1	B	627/663 (94%)	0.65	77 (12%)	4	3	2, 5, 26, 44	0
All	All	1260/1326 (95%)	0.54	125 (9%)	7	6	2, 4, 23, 45	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	257	ALA	9.4
1	B	265	SER	8.3
1	A	260	ALA	7.2
1	B	198	TRP	7.0
1	B	382	LEU	6.6
1	B	383	THR	6.6
1	B	142	PRO	6.4
1	A	265	SER	6.3
1	A	198	TRP	6.0
1	B	4	SER	5.9
1	B	249	ILE	5.9
1	B	390	TRP	5.8
1	B	254	PRO	5.8
1	A	262	VAL	5.8
1	A	261	SER	5.5
1	A	194	ASP	5.5
1	A	385	SER	5.1
1	B	255	GLU	5.0
1	B	387	ASN	5.0
1	A	264	GLY	5.0
1	B	350	SER	5.0
1	B	251	PHE	4.9
1	B	197	GLY	4.9
1	B	188	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	382	LEU	4.7
1	B	267	LEU	4.5
1	B	258	GLY	4.5
1	A	386	ASN	4.5
1	B	315	LEU	4.5
1	B	395	TRP	4.3
1	A	263	HIS	4.3
1	B	264	GLY	4.3
1	A	196	LYS	4.2
1	B	252	GLY	4.2
1	B	318	ASP	4.2
1	B	385	SER	4.1
1	A	387	ASN	4.1
1	B	276	ALA	4.0
1	B	386	ASN	4.0
1	B	250	GLY	3.9
1	A	195	THR	3.8
1	B	68	HIS	3.8
1	B	253	SER	3.8
1	B	392	GLY	3.8
1	B	143	ASP	3.7
1	B	256	LYS	3.7
1	B	5	ILE	3.6
1	B	351	ASN	3.6
1	B	270	GLN	3.6
1	B	399	THR	3.6
1	B	187	ASN	3.4
1	B	393	SER	3.3
1	A	254	PRO	3.3
1	A	270	GLN	3.3
1	B	402	GLY	3.3
1	B	391	SER	3.2
1	A	255	GLU	3.2
1	B	196	LYS	3.2
1	B	107	TYR	3.2
1	A	259	THR	3.2
1	A	400	GLN	3.1
1	B	273	ALA	3.1
1	A	335	VAL	3.0
1	B	277	LYS	3.0
1	B	282	ASP	3.0
1	B	316	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	381	ASP	2.9
1	B	401	GLU	2.9
1	A	274	SER	2.9
1	B	320	PRO	2.9
1	A	188	ASN	2.9
1	B	141	THR	2.9
1	B	398	ASN	2.9
1	A	96	HIS	2.9
1	A	95	LEU	2.9
1	A	258	GLY	2.9
1	A	391	SER	2.8
1	B	195	THR	2.8
1	B	532[A]	HIS	2.8
1	A	197	GLY	2.7
1	B	389	ASN	2.7
1	A	153	VAL	2.7
1	A	266	PRO	2.7
1	A	3	LEU	2.7
1	B	266	PRO	2.6
1	B	394	VAL	2.6
1	B	7[A]	ARG	2.6
1	A	277	LYS	2.6
1	B	6	PRO	2.6
1	B	347	SER	2.5
1	B	269	ASP	2.5
1	B	422	LEU	2.5
1	B	400	GLN	2.5
1	B	295	TYR	2.5
1	B	307	ALA	2.5
1	B	199	PHE	2.4
1	A	267	LEU	2.4
1	A	273	ALA	2.4
1	B	224	VAL	2.4
1	B	304	ALA	2.3
1	A	269	ASP	2.3
1	B	480	VAL	2.3
1	B	388	THR	2.3
1	A	42	LEU	2.3
1	A	25	LYS	2.3
1	A	125	ALA	2.2
1	B	549	ASP	2.2
1	A	253	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	122	VAL	2.2
1	A	154	PHE	2.2
1	B	353	VAL	2.2
1	B	238	GLN	2.1
1	B	247	THR	2.1
1	A	416	ALA	2.1
1	A	549	ASP	2.1
1	B	303	GLN	2.1
1	B	268	SER	2.1
1	A	63	VAL	2.1
1	A	123	ALA	2.1
1	B	445	ALA	2.1
1	B	349	LEU	2.1
1	A	663	VAL	2.0
1	B	339	SER	2.0
1	A	624	LYS	2.0
1	A	518	VAL	2.0

6.2 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, 95th 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	OCS	A	159	9/10	0.98	0.09	2,2,8,8	0
1	OCS	B	159	9/10	0.99	0.06	2,3,7,10	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.