Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 02:52 PM JST

PDB ID	:	5WSK
Title	:	Structure of Ribulose-1,5-bisphosphate carboxylase/oxygenase from wheat
Authors	:	Ma, Y.; Liu, C.
Deposited on	:	2016-12-07
Resolution	:	1.78 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:

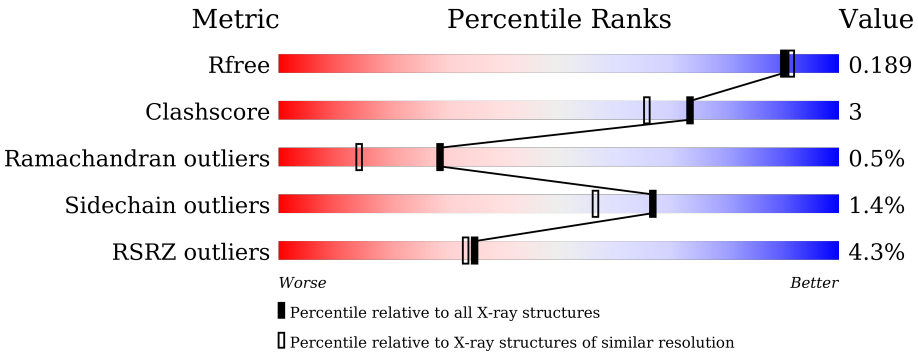
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	477	4% 84% 7% • 8%
1	B	477	5% 84% 7% • 8%
1	C	477	4% 86% 6% • 8%
1	D	477	3% 86% 6% • 8%
2	E	175	2% 64% 5% • 30%
2	F	175	2% 65% 5% 30%

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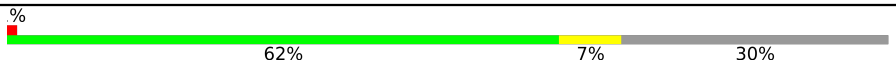
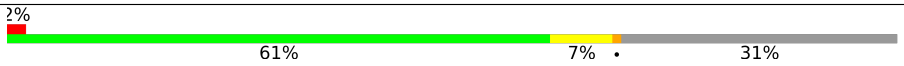
Mol	Chain	Length	Quality of chain
2	G	175	
2	H	175	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 36747 atoms, of which 17215 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 Ribulose bisphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	441	Total	C	H	N	O	S	0	2	0
			6769	2183	3319	610	636	21			
1	B	439	Total	C	H	N	O	S	0	4	0
			6762	2180	3318	609	634	21			
1	C	440	Total	C	H	N	O	S	0	2	0
			6774	2186	3323	610	634	21			
1	D	440	Total	C	H	N	O	S	0	2	0
			6755	2178	3314	609	633	21			

- Molecule 2 is a protein called Ribulose bisphosphate carboxylase small chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	122	Total	C	H	N	O	S	0	0	0
			1984	661	979	160	176	8			
2	F	122	Total	C	H	N	O	S	0	0	0
			1995	661	990	160	176	8			
2	H	120	Total	C	H	N	O	S	0	0	0
			1977	656	982	158	174	7			
2	G	122	Total	C	H	N	O	S	0	0	0
			1995	661	990	160	176	8			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

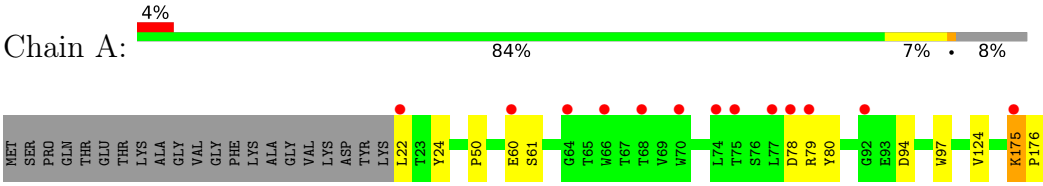
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	285	Total O 285 285	0	0
4	B	277	Total O 277 277	0	0
4	C	375	Total O 375 375	0	0
4	D	373	Total O 373 373	0	0
4	E	99	Total O 99 99	0	0
4	F	102	Total O 102 102	0	0
4	H	110	Total O 110 110	0	0
4	G	111	Total O 111 111	0	0

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.

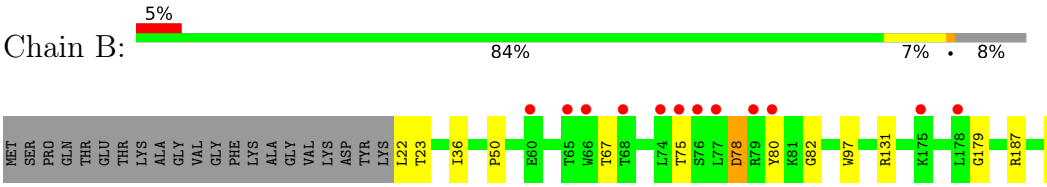
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain A:



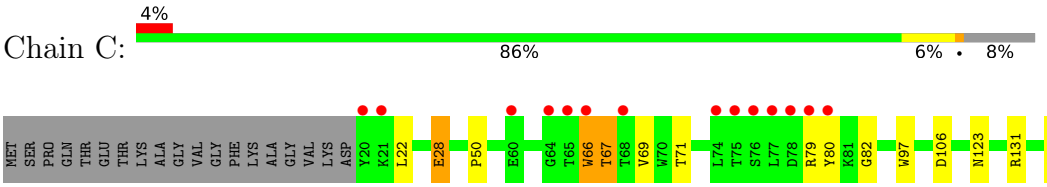
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain B:



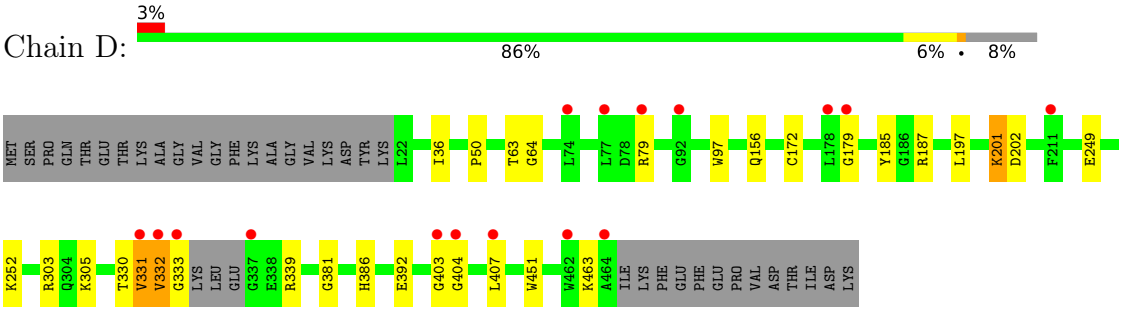
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain C:



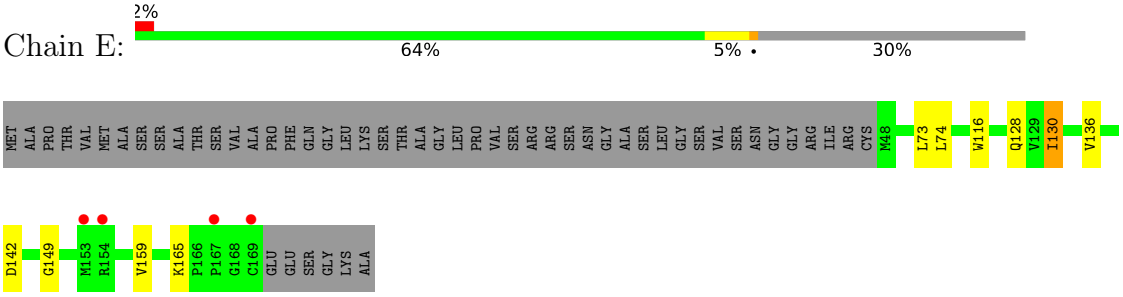
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain D:



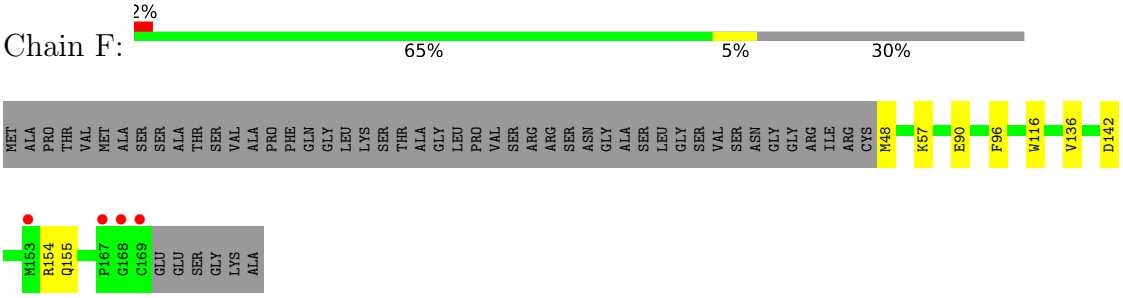
- Molecule 2: Ribulose bisphosphate carboxylase small chain

Chain E:



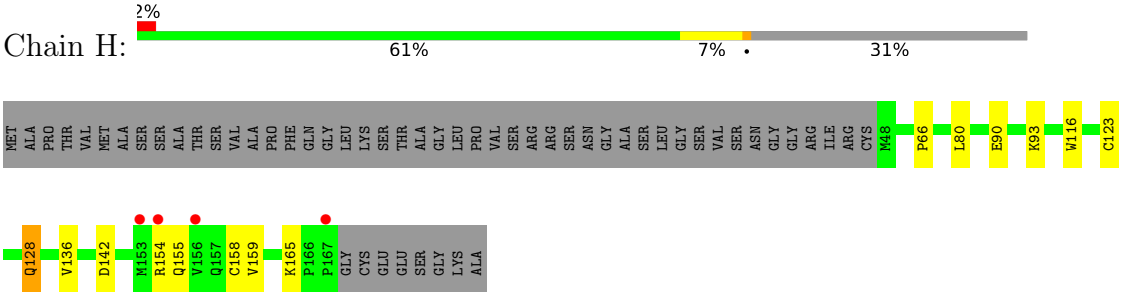
- Molecule 2: Ribulose bisphosphate carboxylase small chain

Chain F:



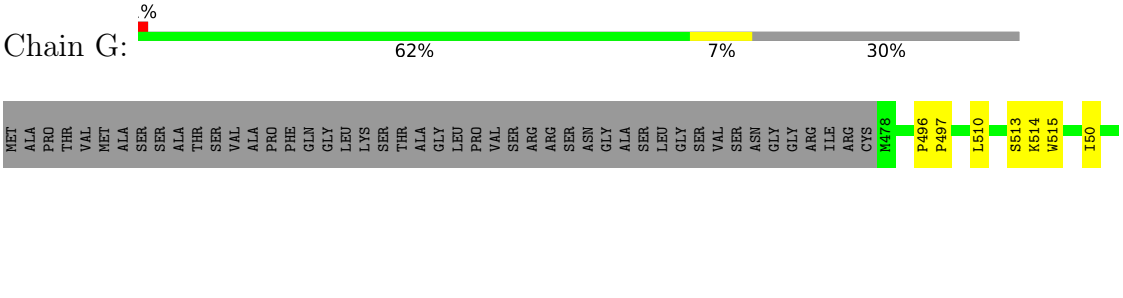
- Molecule 2: Ribulose bisphosphate carboxylase small chain

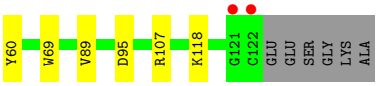
Chain H:



- Molecule 2: Ribulose bisphosphate carboxylase small chain

Chain G:




Y60
W69
V89
D95
R107
K118
G121
C122
GLU
GLU
SER
GLY
LYS
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α, β, γ	110.72Å 110.72Å 200.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.41 – 1.78 44.42 – 1.78	Depositor EDS
% Data completeness (in resolution range)	98.4 (44.41-1.78) 98.4 (44.42-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.154 , 0.187 0.157 , 0.189	Depositor DCC
R_{free} test set	11328 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 29.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.145 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	36747	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.56	0/3532	0.65	1/4787 (0.0%)
1	B	0.56	0/3539	0.65	1/4798 (0.0%)
1	C	0.63	0/3534	0.72	2/4789 (0.0%)
1	D	0.63	0/3523	0.70	1/4775 (0.0%)
2	E	0.50	0/1037	0.61	0/1407
2	F	0.52	0/1037	0.60	0/1407
2	G	0.56	0/1037	0.61	0/1407
2	H	0.60	0/1027	0.63	0/1394
All	All	0.59	0/18266	0.67	5/24764 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	187	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	C	187	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	187	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	B	360	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	303	ARG	NE-CZ-NH1	5.33	122.96	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3450	3319	3334	23	0
1	B	3444	3318	3323	24	2
1	C	3451	3323	3338	25	0
1	D	3441	3314	3328	25	1
2	E	1005	979	991	5	0
2	F	1005	990	991	5	2
2	G	1005	990	991	9	0
2	H	995	982	983	10	1
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	285	0	0	4	1
4	B	277	0	0	7	1
4	C	375	0	0	9	1
4	D	373	0	0	8	1
4	E	99	0	0	0	0
4	F	102	0	0	2	0
4	G	111	0	0	1	0
4	H	110	0	0	5	0
All	All	19532	17215	17279	115	5

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 3.

All (115) 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)
2:H:123:CYS:SG	2:H:128:GLN:NE2	2.33	1.02
1:C:28:GLU:OE1	4:C:601:HOH:O	1.80	0.96
2:F:154:ARG:NH1	4:F:201:HOH:O	1.97	0.96
1:D:252:LYS:NZ	4:D:602:HOH:O	2.05	0.90
1:D:156:GLN:NE2	4:D:601:HOH:O	2.04	0.88
1:B:356:LYS:NZ	4:B:601:HOH:O	2.07	0.86
1:C:402:PHE:O	4:C:602:HOH:O	2.06	0.73
1:B:210:PRO:O	4:B:602:HOH:O	2.07	0.73
1:C:67:THR:OG1	4:C:603:HOH:O	2.08	0.72
1:C:123:ASN:OD1	4:C:604:HOH:O	2.08	0.71
2:H:155:GLN:O	4:H:201:HOH:O	2.12	0.67
1:D:79:ARG:NH1	4:D:606:HOH:O	2.27	0.67
1:C:82:GLY:N	4:C:607:HOH:O	2.26	0.67
2:F:155:GLN:O	4:F:202:HOH:O	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:142:ASP:OD1	4:H:202:HOH:O	2.13	0.65
1:C:69:VAL:HG23	1:D:407:LEU:HB3	1.79	0.63
1:A:356:LYS:NZ	4:A:604:HOH:O	2.31	0.62
1:B:131:ARG:NH2	4:B:606:HOH:O	2.32	0.61
1:A:330:THR:O	1:A:332:VAL:N	2.35	0.60
2:H:154:ARG:NH1	4:H:206:HOH:O	2.35	0.59
1:B:78:ASP:N	1:B:78:ASP:OD1	2.36	0.59
1:C:79:ARG:NH2	4:C:608:HOH:O	2.30	0.58
1:D:332:VAL:HG22	1:D:333:GLY:N	2.20	0.57
1:A:210:PRO:O	4:A:601:HOH:O	2.17	0.56
1:A:204:GLU:O	4:A:602:HOH:O	2.17	0.56
1:C:79:ARG:HH11	1:C:79:ARG:HG3	1.71	0.56
1:A:201:KCX:HB3	1:A:239:TYR:CD2	2.42	0.55
1:B:381:GLY:N	4:B:605:HOH:O	2.31	0.54
1:D:339:ARG:NH1	4:D:612:HOH:O	2.40	0.54
1:B:82:GLY:N	4:B:603:HOH:O	2.42	0.53
1:B:446:ARG:NH2	2:G:497:PRO:O	2.41	0.53
1:A:356:LYS:HG3	1:A:365:THR:N	2.24	0.53
2:G:107:ARG:NH1	4:G:603:HOH:O	2.42	0.52
1:D:339:ARG:NH2	1:D:392:GLU:OE1	2.43	0.52
1:C:172:CYS:HB2	1:C:197:LEU:CD1	2.40	0.51
2:H:128:GLN:NE2	4:H:208:HOH:O	2.39	0.51
1:B:80:TYR:O	4:B:603:HOH:O	2.19	0.51
1:C:340:GLU:OE1	4:C:605:HOH:O	2.19	0.51
1:D:201:KCX:OQ2	4:D:603:HOH:O	2.19	0.50
1:D:50:PRO:HG3	1:D:97:TRP:CZ2	2.46	0.50
1:C:69:VAL:CG2	1:D:407:LEU:HB3	2.41	0.50
2:F:116:TRP:CD2	2:F:136:VAL:HG22	2.46	0.50
1:B:204:GLU:HG2	1:B:205:ASN:N	2.27	0.50
1:A:331:VAL:HA	1:A:336:GLU:N	2.27	0.49
1:B:460:GLU:O	1:B:463:LYS:HE3	2.13	0.49
1:A:50:PRO:HG3	1:A:97:TRP:CZ2	2.47	0.48
1:C:28:GLU:HG2	4:C:770:HOH:O	2.11	0.48
1:B:50:PRO:HG3	1:B:97:TRP:CE2	2.48	0.48
1:C:50:PRO:HG3	1:C:97:TRP:CZ2	2.48	0.48
1:C:69:VAL:HG22	1:C:71:THR:H	1.79	0.48
2:E:74:LEU:HG	2:E:130:ILE:HD12	1.96	0.48
1:A:316:LYS:HE2	1:A:348:LEU:HD22	1.96	0.48
2:H:80:LEU:HD21	2:H:159:VAL:HG11	1.96	0.47
1:A:175:LYS:HA	1:A:176:PRO:C	2.35	0.47
1:A:61:SER:HB3	1:A:124:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ILE:HD12	1:D:36:ILE:N	2.31	0.46
2:E:149:GLY:N	2:E:159:VAL:HG23	2.31	0.46
1:A:78:ASP:OD1	1:A:78:ASP:N	2.48	0.46
2:H:93:LYS:NZ	4:H:202:HOH:O	2.48	0.46
2:G:69:TRP:CD2	2:G:89:VAL:HG22	2.51	0.45
1:D:381:GLY:N	4:D:607:HOH:O	2.29	0.45
2:E:116:TRP:CD2	2:E:136:VAL:HG22	2.52	0.45
2:H:154:ARG:NH2	2:H:158:CYS:HB2	2.32	0.45
1:D:185:TYR:OH	1:D:202:ASP:HA	2.16	0.45
1:D:332:VAL:HG21	1:D:386:HIS:CD2	2.52	0.45
1:B:36:ILE:N	1:B:36:ILE:HD12	2.33	0.44
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.98	0.44
1:B:268:ASP:CB	4:B:672:HOH:O	2.64	0.44
1:D:451:TRP:CZ3	2:H:66:PRO:HD3	2.52	0.44
1:B:331:VAL:CG1	1:B:342:THR:HG21	2.48	0.44
1:D:332:VAL:CG2	1:D:333:GLY:N	2.80	0.44
1:B:450:LYS:N	1:B:450:LYS:HD3	2.33	0.44
1:C:414:ALA:HB3	1:C:415:PRO:HD3	1.99	0.44
2:G:513:SER:O	2:G:514:LYS:HB2	2.18	0.44
1:C:66:TRP:NE1	1:D:404:GLY:HA3	2.33	0.44
2:F:57:LYS:HB3	2:F:96:PHE:CE1	2.53	0.44
1:D:187:ARG:NH2	4:D:618:HOH:O	2.47	0.44
1:A:463:LYS:HD2	1:A:463:LYS:HA	1.81	0.43
2:F:142:ASP:OD1	2:F:142:ASP:N	2.52	0.43
2:G:95:ASP:OD1	2:G:95:ASP:N	2.44	0.43
1:B:201:KCX:HB3	1:B:239:TYR:CD2	2.54	0.43
1:C:80:TYR:CE2	1:D:179:GLY:HA2	2.53	0.43
1:D:330:THR:O	1:D:332:VAL:HG12	2.18	0.43
1:D:305:LYS:NZ	4:D:624:HOH:O	2.51	0.42
1:A:79:ARG:NE	4:A:603:HOH:O	2.27	0.42
1:A:214:TRP:CD2	1:A:253:ARG:HG2	2.55	0.42
1:A:80:TYR:CE2	1:B:179:GLY:HA2	2.54	0.42
1:C:171:GLY:HA2	1:C:199:PHE:O	2.19	0.42
1:D:331:VAL:O	1:D:332:VAL:HB	2.19	0.42
1:A:22:LEU:HD12	1:A:24:TYR:H	1.84	0.42
2:H:116:TRP:CD2	2:H:136:VAL:HG22	2.54	0.42
1:B:197:LEU:HG	1:B:417:ALA:HB1	2.02	0.42
1:C:235:ILE:CD1	2:G:50:ILE:HD13	2.50	0.42
1:C:451:TRP:CH2	2:G:496:PRO:HD3	2.54	0.42
1:C:50:PRO:HG3	1:C:97:TRP:CE2	2.55	0.42
1:C:79:ARG:NH2	1:C:106:ASP:OD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:CYS:HB2	1:D:197:LEU:CD1	2.50	0.42
2:E:73:LEU:HD23	2:E:130:ILE:HD13	2.01	0.42
1:B:22:LEU:HD23	1:B:23:THR:HG22	2.01	0.41
1:C:66:TRP:O	1:C:67:THR:HG22	2.20	0.41
1:D:331:VAL:O	1:D:331:VAL:HG22	2.19	0.41
2:E:142:ASP:OD1	2:E:142:ASP:N	2.48	0.41
1:B:407:LEU:HD23	1:B:413:ASN:OD1	2.20	0.41
1:C:185:TYR:OH	1:C:202:ASP:HA	2.20	0.41
2:G:510:LEU:HD23	2:G:515:TRP:HE3	1.85	0.41
1:A:60:GLU:CB	1:A:124:VAL:HG12	2.51	0.41
1:A:179:GLY:C	1:B:75:THR:HG21	2.41	0.41
1:B:414:ALA:HB3	1:B:415:PRO:HD3	2.02	0.41
1:C:79:ARG:NH1	4:C:631:HOH:O	2.53	0.41
1:A:301:ILE:HD11	1:A:314:LEU:HD21	2.03	0.41
1:D:249:GLU:OE1	1:D:252:LYS:NZ	2.47	0.41
1:A:185:TYR:OH	1:A:202:ASP:HA	2.21	0.41
1:B:225:ILE:HD11	1:B:238:HIS:HB3	2.03	0.40
1:A:404:GLY:HA3	1:B:67:THR:CG2	2.52	0.40
2:G:60:TYR:CD1	2:G:60:TYR:C	2.94	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:691:HOH:O	4:D:649:HOH:O[4_565]	2.06	0.14
1:B:187:ARG:NH1	2:F:90:GLU:OE2[4_555]	2.07	0.13
4:A:839:HOH:O	4:B:842:HOH:O[4_555]	2.08	0.12
1:D:187:ARG:NH2	2:H:90:GLU:OE2[4_565]	2.10	0.10
1:B:187:ARG:HH12	2:F:90:GLU:OE2[4_555]	1.58	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	438/477 (92%)	423 (97%)	13 (3%)	2 (0%)	29 14
1	B	438/477 (92%)	422 (96%)	14 (3%)	2 (0%)	29 14
1	C	437/477 (92%)	421 (96%)	14 (3%)	2 (0%)	29 14
1	D	437/477 (92%)	420 (96%)	12 (3%)	5 (1%)	14 4
2	E	120/175 (69%)	116 (97%)	4 (3%)	0	100 100
2	F	120/175 (69%)	114 (95%)	6 (5%)	0	100 100
2	G	120/175 (69%)	112 (93%)	8 (7%)	0	100 100
2	H	118/175 (67%)	112 (95%)	6 (5%)	0	100 100
All	All	2228/2608 (85%)	2140 (96%)	77 (4%)	11 (0%)	29 14

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	VAL
1	C	67	THR
1	D	64	GLY
1	D	63	THR
1	D	332	VAL
1	B	403	GLY
1	D	403	GLY
1	A	403	GLY
1	C	403	GLY
1	B	331	VAL
1	D	331	VAL

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	355/384 (92%)	348 (98%)	7 (2%)	55 40
1	B	356/384 (93%)	351 (99%)	5 (1%)	67 56
1	C	355/384 (92%)	349 (98%)	6 (2%)	60 48
1	D	354/384 (92%)	353 (100%)	1 (0%)	92 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	110/149 (74%)	107 (97%)	3 (3%)	44 28
2	F	110/149 (74%)	109 (99%)	1 (1%)	78 72
2	G	110/149 (74%)	109 (99%)	1 (1%)	78 72
2	H	109/149 (73%)	107 (98%)	2 (2%)	59 45
All	All	1859/2132 (87%)	1833 (99%)	26 (1%)	67 56

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	A	175	LYS
1	A	210	PRO
1	A	268	ASP
1	A	332	VAL
1	A	439	ARG
1	A	463	LYS
1	B	78	ASP
1	B	303	ARG
1	B	338	GLU
1	B	450	LYS
1	B	460	GLU
1	C	22	LEU
1	C	28	GLU
1	C	66	TRP
1	C	131	ARG
1	C	268	ASP
1	C	338	GLU
1	D	463	LYS
2	E	128	GLN
2	E	130	ILE
2	E	165	LYS
2	F	48	MET
2	H	128	GLN
2	H	165	LYS
2	G	118	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	128	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	KCX	A	201	3,1	9,11,12	1.69	2 (22%)	5,12,14	1.29	1 (20%)
1	KCX	D	201	3,1	9,11,12	1.64	3 (33%)	5,12,14	2.40	2 (40%)
1	KCX	C	201	3,1	9,11,12	1.02	0	5,12,14	0.98	0
1	KCX	B	201	3,1	9,11,12	2.22	1 (11%)	5,12,14	1.20	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	KCX	A	201	3,1	-	1/9/10/12	-
1	KCX	D	201	3,1	-	1/9/10/12	-
1	KCX	C	201	3,1	-	0/9/10/12	-
1	KCX	B	201	3,1	-	0/9/10/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	201	KCX	OQ1-CX	6.36	1.33	1.21
1	A	201	KCX	OQ1-CX	3.64	1.28	1.21
1	D	201	KCX	CE-NZ	-2.82	1.39	1.46
1	D	201	KCX	OQ1-CX	2.75	1.26	1.21
1	A	201	KCX	CX-NZ	-2.53	1.30	1.35
1	D	201	KCX	CX-NZ	-2.41	1.30	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	201	KCX	OQ1-CX-NZ	-4.94	117.30	124.96
1	A	201	KCX	OQ1-CX-NZ	-2.84	120.55	124.96
1	D	201	KCX	CE-NZ-CX	-2.07	118.57	121.89

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	201	KCX	C-CA-CB-CG
1	D	201	KCX	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	201	KCX	1	0
1	D	201	KCX	1	0
1	B	201	KCX	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 (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

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	440/477 (92%)	0.19	21 (4%)	30	29	13, 21, 55, 73	0
1	B	438/477 (91%)	0.22	26 (5%)	22	21	13, 21, 55, 69	0
1	C	439/477 (92%)	0.14	20 (4%)	32	31	9, 15, 46, 75	0
1	D	439/477 (92%)	0.11	16 (3%)	42	41	9, 15, 45, 60	0
2	E	122/175 (69%)	0.14	4 (3%)	46	45	17, 26, 45, 70	0
2	F	122/175 (69%)	0.08	4 (3%)	46	45	16, 26, 46, 65	0
2	G	122/175 (69%)	0.13	2 (1%)	72	72	12, 22, 38, 90	0
2	H	120/175 (68%)	0.08	4 (3%)	46	45	12, 21, 38, 60	0
All	All	2242/2608 (85%)	0.15	97 (4%)	35	33	9, 20, 50, 90	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	TYR	13.0
1	B	407	LEU	10.1
2	G	122	CYS	10.0
1	B	332	VAL	8.9
1	B	331	VAL	8.1
1	B	66	TRP	7.2
1	A	407	LEU	6.9
1	C	77	LEU	6.8
1	A	331	VAL	6.4
1	C	68	THR	6.2
1	D	332	VAL	5.6
1	D	331	VAL	5.4
1	D	178	LEU	5.4
1	A	66	TRP	5.3
1	D	407	LEU	5.2
1	B	178	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	66	TRP	5.1
1	B	74	LEU	5.0
1	A	333	GLY	5.0
1	C	21	LYS	5.0
1	A	178	LEU	5.0
1	A	77	LEU	4.9
1	B	77	LEU	4.9
1	B	462	TRP	4.9
1	B	330	THR	4.7
1	A	68	THR	4.5
1	A	74	LEU	4.5
1	A	464	ALA	4.4
1	D	404	GLY	4.3
1	B	337	GLY	4.3
1	C	331	VAL	4.1
1	A	92	GLY	4.1
1	B	65	THR	4.1
1	A	175	LYS	4.0
1	C	74	LEU	3.9
1	A	462	TRP	3.9
1	A	332	VAL	3.7
2	E	169	CYS	3.7
1	B	68	THR	3.6
1	A	22	LEU	3.6
2	E	154	ARG	3.6
1	B	80	TYR	3.6
1	D	337	GLY	3.5
1	B	461	VAL	3.4
2	E	167	PRO	3.4
1	B	406	THR	3.4
1	C	80	TYR	3.4
1	D	462	TRP	3.3
1	C	79	ARG	3.3
1	B	211[A]	PHE	3.2
2	F	169	CYS	3.0
2	E	153	MET	3.0
1	B	76	SER	3.0
1	C	407	LEU	3.0
2	H	167	PRO	2.9
1	D	211[A]	PHE	2.9
1	A	70	TRP	2.8
1	B	60	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	60	GLU	2.7
1	A	79	ARG	2.7
1	C	76	SER	2.7
1	B	408	GLY	2.7
1	B	403	GLY	2.7
2	F	168	GLY	2.7
1	C	75	THR	2.7
1	A	403	GLY	2.6
1	B	79	ARG	2.6
2	H	153	MET	2.6
1	D	77	LEU	2.6
2	H	154	ARG	2.5
1	D	79	ARG	2.5
2	F	153	MET	2.5
1	C	65	THR	2.5
1	D	333	GLY	2.5
1	B	439	ARG	2.4
1	D	179	GLY	2.4
1	C	462	TRP	2.4
1	C	178	LEU	2.4
1	D	464	ALA	2.4
1	C	211[A]	PHE	2.3
1	C	78	ASP	2.3
1	D	92	GLY	2.3
1	A	64	GLY	2.3
1	C	337	GLY	2.2
1	B	404	GLY	2.2
2	F	167	PRO	2.2
1	D	403	GLY	2.2
1	D	74	LEU	2.2
1	A	78	ASP	2.1
1	B	405	GLY	2.1
2	G	121	GLY	2.1
2	H	156	VAL	2.1
1	A	75	THR	2.1
1	C	64	GLY	2.1
1	C	60	GLU	2.1
1	B	75	THR	2.0
1	B	175	LYS	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, 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	KCX	B	201	12/13	0.76	0.17	20,20,20,20	0
1	KCX	C	201	12/13	0.86	0.14	20,20,20,20	0
1	KCX	D	201	12/13	0.87	0.14	20,20,20,20	0
1	KCX	A	201	12/13	0.91	0.11	20,20,20,20	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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
3	MG	B	501	1/1	0.93	0.08	41,41,41,41	0
3	MG	A	501	1/1	0.96	0.10	42,42,42,42	0
3	MG	C	501	1/1	0.98	0.06	27,27,27,27	0
3	MG	D	501	1/1	0.99	0.04	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.