



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:53 PM UTC

PDB ID : 5WSK / pdb_00005wsk
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

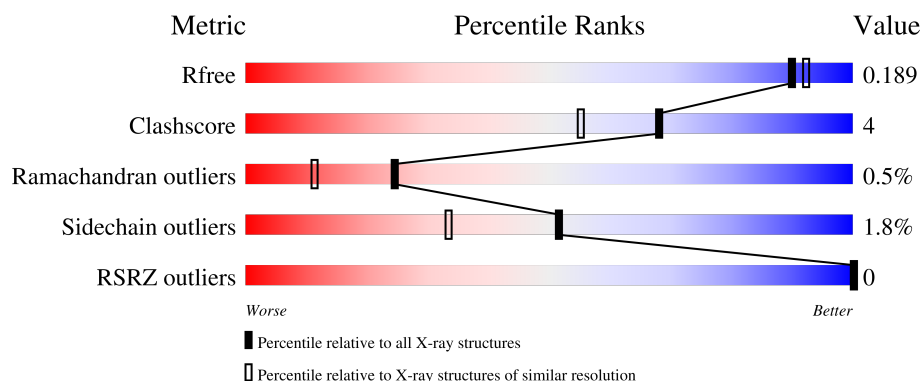
1 Overall quality at a glance

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}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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 $\leq 5\%$. 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	
1	B	477	
1	C	477	
1	D	477	
2	E	175	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	175	 64%6%30%
2	G	175	 62%7%30%
2	H	175	 60%8%31%

2 Entry composition

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 biphosphate 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 biphosphate 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 (CCD ID: 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		

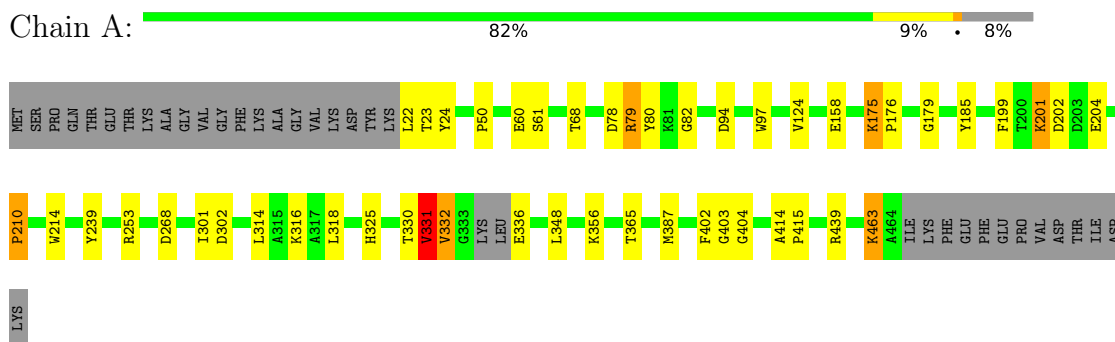
- Molecule 4 is water.

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

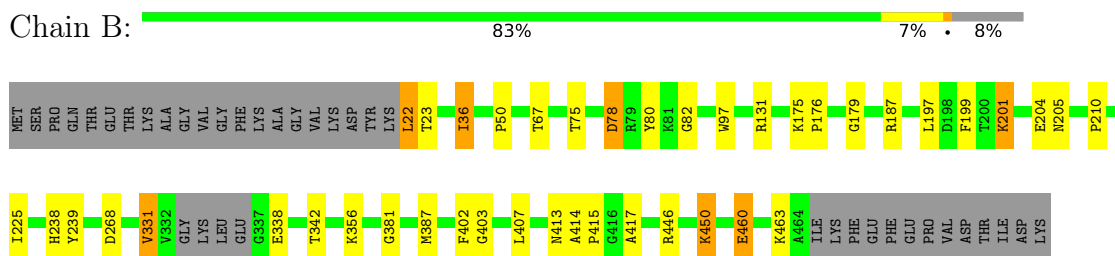
3 Residue-property plots

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.

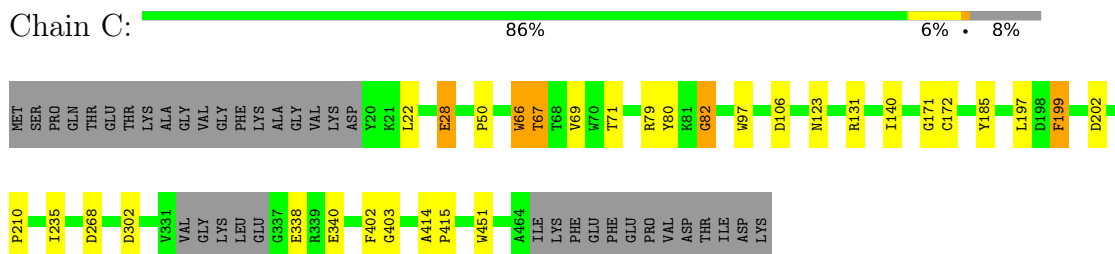
- Molecule 1: Ribulose biphosphate carboxylase large chain



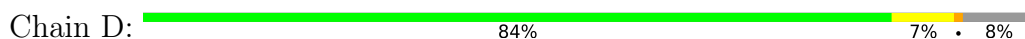
- Molecule 1: Ribulose biphosphate carboxylase large chain

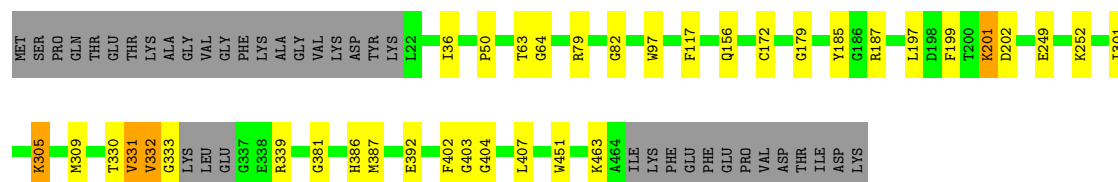


- Molecule 1: Ribulose biphosphate carboxylase large chain



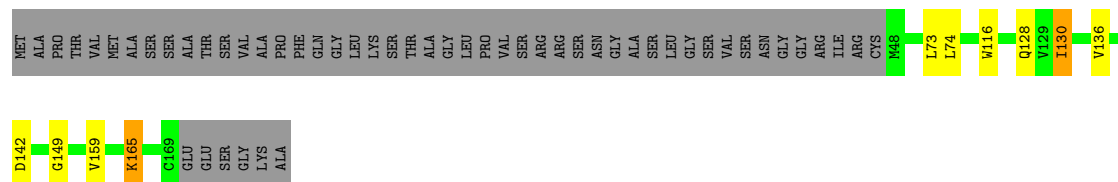
- Molecule 1: Ribulose biphosphate carboxylase large chain





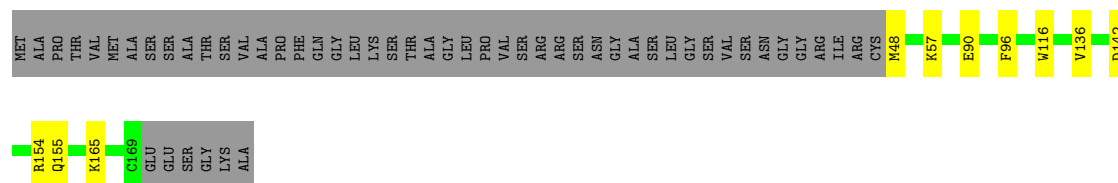
- Molecule 2: Ribulose biphosphate carboxylase small chain

Chain E: 64% 5% 30%



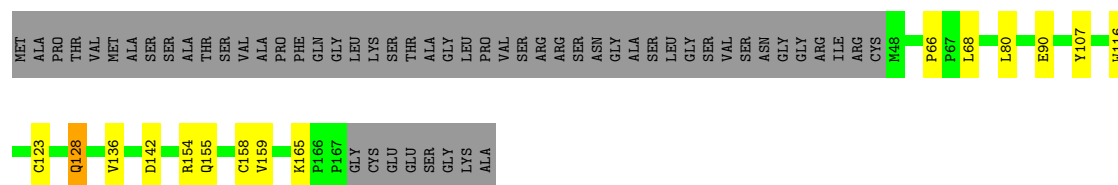
- Molecule 2: Ribulose biphosphate carboxylase small chain

Chain F: 64% 6% 30%



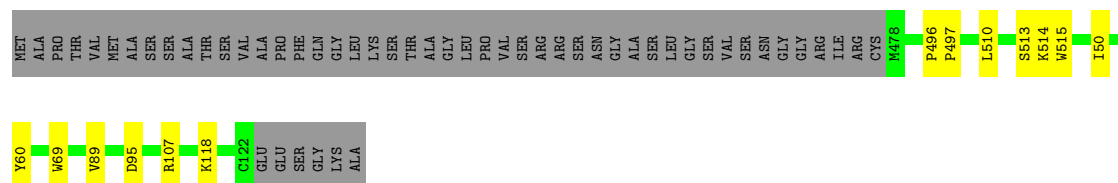
- Molecule 2: Ribulose biphosphate carboxylase small chain

Chain H: 60% 8% 31%



- Molecule 2: Ribulose biphosphate carboxylase small chain

Chain G: 62% 7% 30%



4 Data and refinement statistics

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 44.41 – 1.78	Depositor EDS
% Data completeness (in resolution range)	98.4 (44.41-1.78) 98.4 (44.41-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	11334 reflections (4.93%)	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)	0.37 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.145 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MG, KCX

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	0.71	1/3532 (0.0%)	0.83	2/4787 (0.0%)
1	B	0.71	0/3539	0.83	1/4798 (0.0%)
1	C	0.79	1/3534 (0.0%)	0.87	3/4789 (0.1%)
1	D	0.81	2/3523 (0.1%)	0.85	2/4775 (0.0%)
2	E	0.61	0/1037	0.84	2/1407 (0.1%)
2	F	0.61	0/1037	0.85	2/1407 (0.1%)
2	G	0.69	0/1037	0.77	0/1407
2	H	0.70	0/1027	0.80	0/1394
All	All	0.73	4/18266 (0.0%)	0.84	12/24764 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	199	PHE	C-O	-7.65	1.14	1.23
1	A	199	PHE	C-O	-6.23	1.16	1.23
1	D	199	PHE	C-O	-5.86	1.16	1.23
1	D	301	ILE	CA-CB	5.07	1.60	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	GLY	N-CA-C	-7.79	102.09	112.14
1	B	199	PHE	N-CA-C	6.31	118.77	109.24
1	D	82	GLY	N-CA-C	-6.13	104.23	112.14
1	C	140	ILE	CA-C-N	-6.08	115.28	119.66
1	C	140	ILE	C-N-CA	-6.08	115.28	119.66
1	A	82	GLY	N-CA-C	-5.59	104.92	112.14
1	A	331	VAL	N-CA-C	5.40	120.57	109.34
1	D	199	PHE	N-CA-C	5.27	117.40	109.23
2	F	165	LYS	CA-C-N	-5.18	115.05	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	165	LYS	C-N-CA	-5.18	115.05	120.38
2	E	165	LYS	CA-C-N	-5.17	115.05	120.38
2	E	165	LYS	C-N-CA	-5.17	115.05	120.38

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	27	0
1	B	3444	3318	3323	26	2
1	C	3451	3323	3338	27	0
1	D	3441	3314	3328	27	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	10	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	4	0
All	All	19532	17215	17279	125	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 4.

All (125) 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
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
1:A:175:LYS:HA	1:A:176:PRO:C	2.35	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:D:117:PHE:CE1	1:D:309:MET:HE1	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:61:SER:HB3	1:A:124:VAL:HG11	1.97	0.46
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
1:A:179:GLY:C	1:B:75:THR:HG21	2.41	0.46
2:G:69:TRP:CD2	2:G:89:VAL:HG22	2.51	0.45
1:D:387:MET:HE1	1:D:402:PHE:CZ	2.52	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
1:B:387:MET:HE1	1:B:402:PHE:CZ	2.51	0.45
2:H:154:ARG:NH2	2:H:158:CYS:HB2	2.32	0.45
2:G:60:TYR:CD1	2:G:60:TYR:C	2.94	0.45
1:B:175:LYS:HA	1:B:176:PRO:C	2.42	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:387:MET:HE1	1:A:402:PHE:CZ	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
1:D:305:LYS:NZ	4:D:624:HOH:O	2.51	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
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
1:C:28:GLU:CD	4:C:601:HOH:O	2.49	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
2:H:107:TYR:CD1	2:H:107:TYR:C	2.99	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:A:318:LEU:C	1:A:318:LEU:HD13	2.45	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:C:302:ASP:OD1	1:C:302:ASP:C	2.64	0.40
1:A:158:GLU:CD	1:A:325:HIS:HE2	2.23	0.40
1:A:302:ASP:C	1:A:302:ASP:OD1	2.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:GLY:HA3	1:B:67:THR:CG2	2.52	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 ⓘ

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	438/477 (92%)	423 (97%)	13 (3%)	2 (0%)	24	11
1	B	438/477 (92%)	422 (96%)	14 (3%)	2 (0%)	24	11
1	C	437/477 (92%)	421 (96%)	14 (3%)	2 (0%)	24	11
1	D	437/477 (92%)	420 (96%)	12 (3%)	5 (1%)	11	3
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%)	24	11

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 ⓘ

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%)	345 (97%)	10 (3%)	38	17
1	B	356/384 (93%)	350 (98%)	6 (2%)	53	36
1	C	355/384 (92%)	348 (98%)	7 (2%)	48	29
1	D	354/384 (92%)	352 (99%)	2 (1%)	78	70
2	E	110/149 (74%)	107 (97%)	3 (3%)	39	19
2	F	110/149 (74%)	109 (99%)	1 (1%)	70	59
2	G	110/149 (74%)	109 (99%)	1 (1%)	70	59
2	H	109/149 (73%)	106 (97%)	3 (3%)	38	17
All	All	1859/2132 (87%)	1826 (98%)	33 (2%)	51	33

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	68	THR
1	A	79	ARG
1	A	94	ASP
1	A	175	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	210	PRO
1	A	268	ASP
1	A	332	VAL
1	A	439	ARG
1	A	463	LYS
1	B	22	LEU
1	B	36	ILE
1	B	78	ASP
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	210	PRO
1	C	268	ASP
1	C	338	GLU
1	D	305	LYS
1	D	463	LYS
2	E	128	GLN
2	E	130	ILE
2	E	165	LYS
2	F	48	MET
2	H	68	LEU
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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	D	156	GLN
2	F	128	GLN
2	H	128	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	10,11,12	1.73	2 (20%)	6,12,14	1.25	1 (16%)
1	KCX	D	201	3,1	10,11,12	1.66	3 (30%)	6,12,14	2.24	2 (33%)
1	KCX	B	201	3,1	10,11,12	2.18	1 (10%)	6,12,14	1.16	0
1	KCX	C	201	3,1	10,11,12	1.02	0	6,12,14	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	KCX	A	201	3,1	-	1/9/10/12	-
1	KCX	D	201	3,1	-	1/9/10/12	-
1	KCX	B	201	3,1	-	1/9/10/12	-
1	KCX	C	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	6.42	1.33	1.21
1	A	201	KCX	OQ1-CX	3.68	1.28	1.21
1	D	201	KCX	CE-NZ	-2.87	1.39	1.46
1	D	201	KCX	OQ1-CX	2.77	1.26	1.21
1	A	201	KCX	CX-NZ	-2.55	1.30	1.35
1	D	201	KCX	CX-NZ	-2.44	1.30	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	201	KCX	OQ1-CX-NZ	-5.02	117.30	124.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	KCX	OQ1-CX-NZ	-2.87	120.55	124.92
1	D	201	KCX	CE-NZ-CX	-2.01	118.57	121.98

There are no chirality outliers.

All (3) 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
1	B	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 oligosaccharides 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 ⓘ

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	440/477 (92%)	-1.23	0 100 100	14, 24, 61, 80	1 (0%)
1	B	438/477 (91%)	-1.21	0 100 100	11, 23, 60, 76	2 (0%)
1	C	439/477 (92%)	-1.32	0 100 100	9, 17, 50, 82	1 (0%)
1	D	439/477 (92%)	-1.31	0 100 100	10, 17, 50, 69	1 (0%)
2	E	122/175 (69%)	-1.24	0 100 100	18, 29, 55, 79	0
2	F	122/175 (69%)	-1.28	0 100 100	17, 29, 53, 72	0
2	G	122/175 (69%)	-1.28	0 100 100	13, 24, 46, 96	0
2	H	120/175 (68%)	-1.30	0 100 100	13, 23, 42, 64	0
All	All	2242/2608 (85%)	-1.27	0 100 100	9, 22, 55, 96	5 (0%)

There are no RSRZ outliers to report.

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	KCX	B	201	12/13	0.97	0.06	20,20,20,20	0
1	KCX	A	201	12/13	0.98	0.04	20,20,20,20	0
1	KCX	C	201	12/13	0.99	0.03	20,20,20,20	0
1	KCX	D	201	12/13	0.99	0.04	20,20,20,20	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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
3	MG	B	501	1/1	0.99	0.07	41,41,41,41	0
3	MG	A	501	1/1	1.00	0.07	42,42,42,42	0
3	MG	C	501	1/1	1.00	0.04	27,27,27,27	0
3	MG	D	501	1/1	1.00	0.05	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.