



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:51 AM UTC

PDB ID : 1WA3 / pdb_00001wa3
Title : Mechanism of the Class I KDPG aldolase
Authors : Fullerton, S.W.B.; Griffiths, J.S.; Merkel, A.B.; Wymer, N.J.; Hutchins, M.J.; Fierke, C.A.; Toone, E.J.; Naismith, J.H.
Deposited on : 2004-10-22
Resolution : 1.90 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

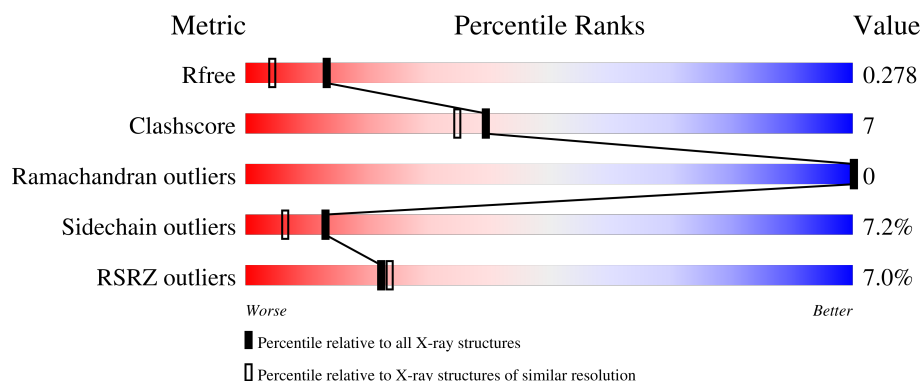
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	205	 81% 15% ..
1	B	205	 82% 13% ..
1	C	205	 7% 79% 16% ..
1	D	205	 23% 86% 11% ..
1	E	205	 % 84% 13% ..

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Mol	Chain	Length	Quality of chain
1	F	205	8% 74% 21%

2 Entry composition [i](#)

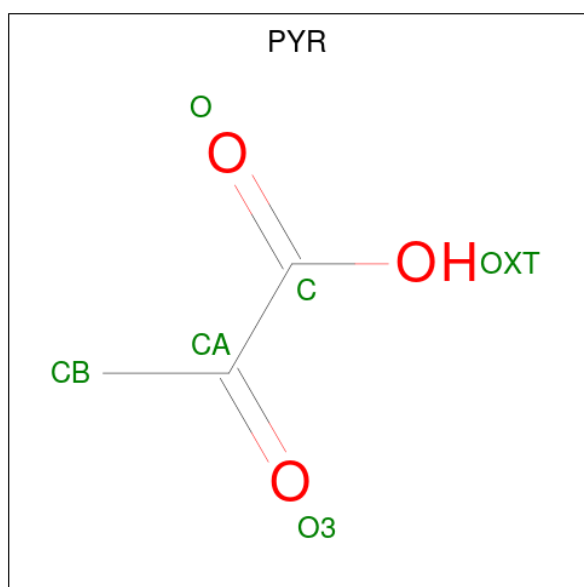
There are 4 unique types of molecules in this entry. The entry contains 9569 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-KETO-3-DEOXY-6-PHOSPHOGLUCONATE ALDOLASE.

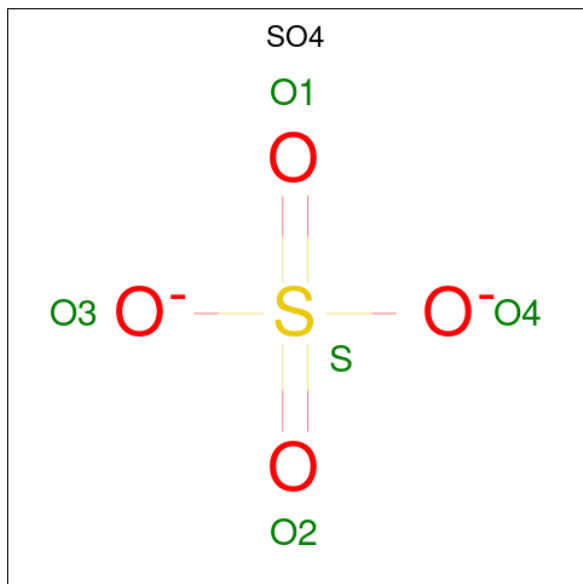
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1536	995	253	279	9			
1	B	202	Total	C	N	O	S	0	0	0
			1536	995	253	279	9			
1	C	201	Total	C	N	O	S	0	0	0
			1527	989	251	278	9			
1	D	203	Total	C	N	O	S	0	0	0
			1541	998	254	280	9			
1	E	202	Total	C	N	O	S	0	0	0
			1536	995	253	279	9			
1	F	201	Total	C	N	O	S	0	0	0
			1527	989	251	278	9			

- Molecule 2 is PYRUVIC ACID (CCD ID: PYR) (formula: C₃H₄O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 5 3 2	0	0
2	B	1	Total C O 5 3 2	0	0
2	C	1	Total C O 5 3 2	0	0
2	D	1	Total C O 5 3 2	0	0
2	E	1	Total C O 5 3 2	0	0
2	F	1	Total C O 5 3 2	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

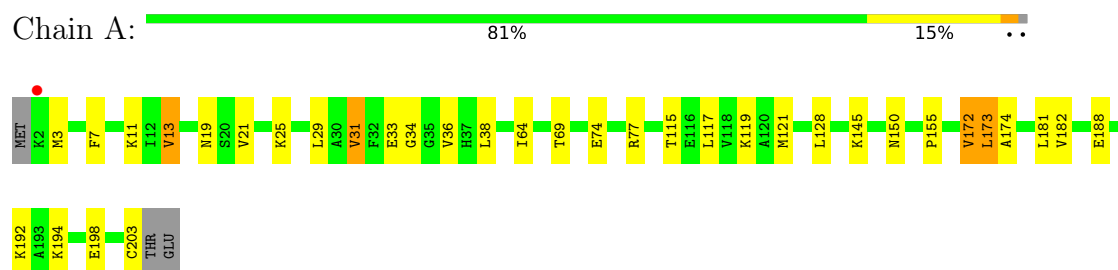
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total 74	O 74	0	0
4	B	73	Total 73	O 73	0	0
4	C	41	Total 41	O 41	0	0
4	D	49	Total 49	O 49	0	0
4	E	46	Total 46	O 46	0	0
4	F	23	Total 23	O 23	0	0

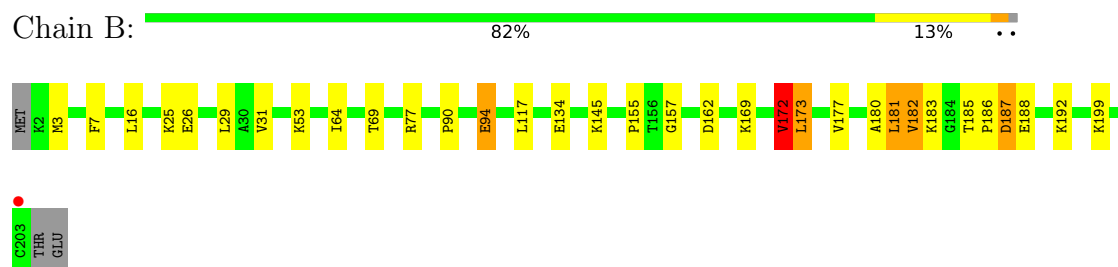
3 Residue-property plots

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.

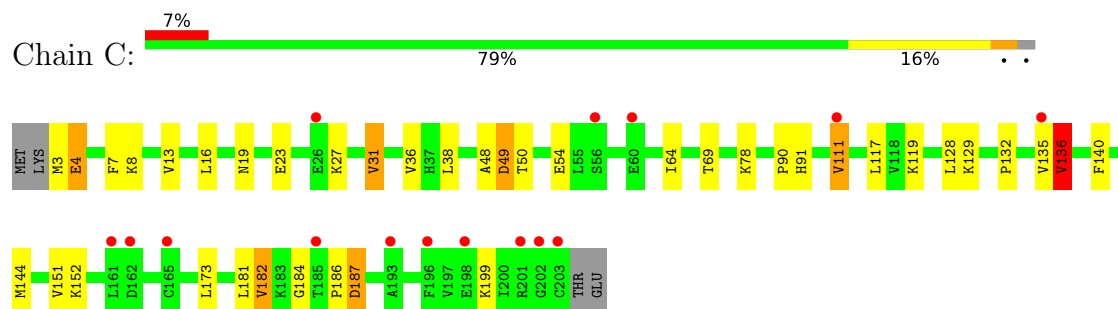
• Molecule 1: 2-KETO-3-DEOXY-6-PHOSPHOGLUCONATE ALDOLASE



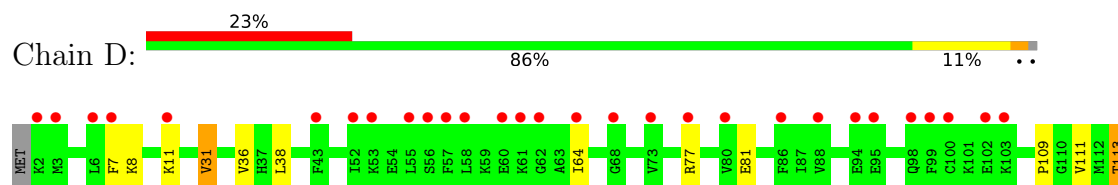
• Molecule 1: 2-KETO-3-DEOXY-6-PHOSPHOGLUCONATE ALDOLASE

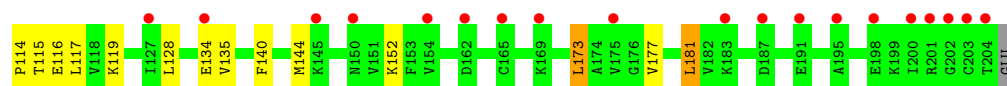


• Molecule 1: 2-KETO-3-DEOXY-6-PHOSPHOGLUCONATE ALDOLASE

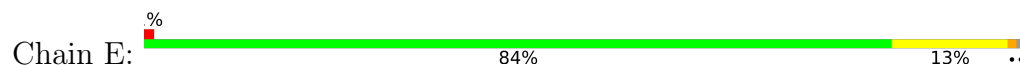


• Molecule 1: 2-KETO-3-DEOXY-6-PHOSPHOGLUCONATE ALDOLASE

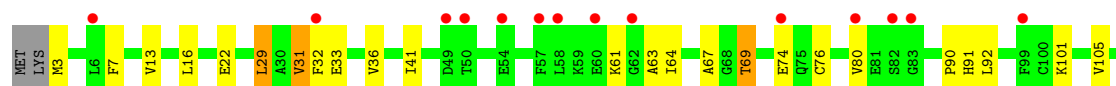
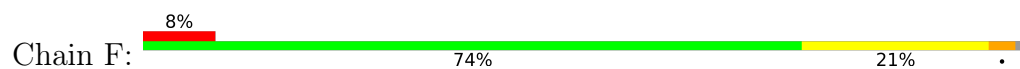




- Molecule 1: 2-KETO-3-DEOXY-6-PHOSPHOGLUCONATE ALDOLASE



- Molecule 1: 2-KETO-3-DEOXY-6-PHOSPHOGLUCONATE ALDOLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.60Å 101.10Å 124.60Å 90.00° 97.20° 90.00°	Depositor
Resolution (Å)	32.44 – 1.90 32.44 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.0 (32.44-1.90) 94.0 (32.44-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, R_{free}	0.193 , 0.239 (Not available) , 0.278	Depositor DCC
R_{free} test set	3900 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9569	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PYR

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	0.99	0/1565	1.02	2/2108 (0.1%)
1	B	0.97	0/1565	1.00	1/2108 (0.0%)
1	C	0.84	0/1556	1.00	6/2097 (0.3%)
1	D	0.77	0/1570	0.91	0/2115
1	E	0.80	0/1565	0.93	0/2108
1	F	0.77	0/1556	0.98	2/2097 (0.1%)
All	All	0.86	0/9377	0.98	11/12633 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	VAL	CB-CA-C	-7.35	99.75	110.63
1	B	172	VAL	CG1-CB-CG2	6.28	124.63	110.80
1	C	111	VAL	N-CA-CB	-6.27	100.75	112.36
1	C	111	VAL	CG1-CB-CG2	6.04	124.08	110.80
1	A	172	VAL	CG1-CB-CG2	5.71	123.36	110.80
1	C	136	VAL	CB-CA-C	5.58	120.44	111.29
1	C	136	VAL	N-CA-CB	-5.33	102.44	111.23
1	C	48	ALA	CA-C-N	5.08	129.27	121.19
1	C	48	ALA	C-N-CA	5.08	129.27	121.19
1	F	137	GLY	CA-C-N	5.07	124.85	119.28
1	F	137	GLY	C-N-CA	5.07	124.85	119.28

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	1536	0	1593	18	2
1	B	1536	0	1592	17	1
1	C	1527	0	1579	25	1
1	D	1541	0	1594	22	0
1	E	1536	0	1592	24	0
1	F	1527	0	1579	29	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	74	0	0	2	0
4	B	73	0	0	1	0
4	C	41	0	0	1	0
4	D	49	0	0	0	0
4	E	46	0	0	0	0
4	F	23	0	0	1	0
All	All	9569	0	9529	126	3

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 7.

All (126) 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:C:117:LEU:HD13	1:C:144:MET:HE3	1.22	1.19
1:C:117:LEU:HD13	1:C:144:MET:CE	1.80	1.09
1:E:136:VAL:HG22	1:E:140:PHE:HB2	1.33	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ASP:OD2	4:B:2066:HOH:O	1.78	1.01
1:C:117:LEU:CD1	1:C:144:MET:HE3	1.90	1.01
1:F:113:THR:HG22	1:F:116:GLU:H	1.26	0.98
1:B:3:MET:HE1	1:B:64:ILE:HG21	1.46	0.94
1:E:128:LEU:HD23	1:E:151:VAL:HG13	1.49	0.94
1:F:117:LEU:HD13	1:F:144:MET:HE3	1.50	0.94
1:F:140:PHE:CZ	1:F:144:MET:HE2	2.04	0.93
1:D:140:PHE:CZ	1:D:144:MET:HE2	2.05	0.91
1:F:29:LEU:O	1:F:33:GLU:HG3	1.73	0.88
1:D:113:THR:HG22	1:D:116:GLU:H	1.40	0.86
1:D:135:VAL:HG11	1:E:136:VAL:HG23	1.58	0.86
1:D:77:ARG:O	1:D:81:GLU:HG3	1.76	0.85
1:F:3:MET:HE1	1:F:64:ILE:HG21	1.58	0.85
1:B:94:GLU:H	1:B:94:GLU:CD	1.84	0.84
1:C:117:LEU:CD1	1:C:144:MET:CE	2.54	0.83
1:E:136:VAL:HG21	1:E:140:PHE:CD1	2.15	0.82
1:C:31:VAL:HG13	1:C:36:VAL:HB	1.62	0.82
1:D:117:LEU:HD13	1:D:144:MET:HE3	1.63	0.78
1:E:116:GLU:OE2	1:F:113:THR:HG21	1.84	0.77
1:B:3:MET:HE1	1:B:64:ILE:CG2	2.14	0.76
1:D:113:THR:HG21	1:F:116:GLU:OE2	1.85	0.76
1:C:7:PHE:HE2	1:C:13:VAL:HG21	1.50	0.75
1:C:199:LYS:NZ	4:C:2039:HOH:O	2.20	0.75
1:F:76:CYS:O	1:F:80:VAL:HG23	1.86	0.75
1:B:16:LEU:HD23	1:B:182:VAL:HG21	1.69	0.73
1:D:117:LEU:CD1	1:D:144:MET:HE3	2.18	0.73
1:F:117:LEU:CD1	1:F:144:MET:HE3	2.20	0.71
1:F:134:GLU:HG2	4:F:2017:HOH:O	1.93	0.69
1:E:136:VAL:HG22	1:E:140:PHE:CB	2.18	0.67
1:F:32:PHE:CE1	1:F:63:ALA:HB2	2.29	0.67
1:A:119:LYS:HG3	4:A:2042:HOH:O	1.94	0.67
1:E:136:VAL:CG2	1:E:140:PHE:CD1	2.78	0.66
1:D:140:PHE:CE2	1:D:144:MET:HE2	2.33	0.64
1:A:3:MET:HE1	1:A:64:ILE:HG21	1.80	0.64
1:C:49:ASP:OD1	1:C:78:LYS:HB3	1.97	0.64
1:C:7:PHE:HE2	1:C:13:VAL:CG2	2.12	0.61
1:A:38:LEU:HD23	1:A:64:ILE:HB	1.83	0.61
1:E:128:LEU:HD23	1:E:151:VAL:CG1	2.28	0.61
1:E:38:LEU:HD23	1:E:64:ILE:HB	1.83	0.60
1:F:114:PRO:HG3	1:F:144:MET:HE1	1.82	0.60
1:E:7:PHE:HE2	1:E:13:VAL:HG21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:VAL:HG13	1:F:36:VAL:HB	1.85	0.58
1:C:128:LEU:HD23	1:C:151:VAL:HG13	1.85	0.58
1:E:182:VAL:O	1:E:182:VAL:HG12	2.04	0.58
1:A:3:MET:HE1	1:A:64:ILE:CG2	2.34	0.57
1:D:117:LEU:C	1:D:117:LEU:HD23	2.30	0.56
1:E:179:SER:HB2	1:E:183:LYS:HD2	1.86	0.56
1:A:31:VAL:HG13	1:A:36:VAL:HB	1.87	0.56
1:A:121:MET:HE3	1:A:150:ASN:HD21	1.72	0.55
1:D:135:VAL:CG1	1:E:136:VAL:HG23	2.32	0.54
1:F:190:ARG:HG2	1:F:194:LYS:HE3	1.91	0.53
1:F:140:PHE:CE2	1:F:144:MET:HE2	2.44	0.52
1:E:136:VAL:CG2	1:E:140:PHE:HB2	2.23	0.52
1:E:94:GLU:HG2	1:E:123:LEU:HD11	1.93	0.51
1:C:27:LYS:HD3	1:C:182:VAL:HG13	1.93	0.51
1:A:29:LEU:O	1:A:33:GLU:HG3	2.12	0.50
1:F:7:PHE:HE2	1:F:13:VAL:CG2	2.25	0.49
1:F:136:VAL:HG13	1:F:140:PHE:CB	2.43	0.49
1:B:7:PHE:HB3	1:B:173:LEU:HD13	1.95	0.49
1:D:134:GLU:OE1	1:E:139:GLN:HG2	2.12	0.49
1:C:90:PRO:HA	1:C:129:LYS:HE2	1.95	0.49
1:E:27:LYS:HD3	1:E:182:VAL:HG12	1.95	0.49
1:C:50:THR:O	1:C:54:GLU:HG3	2.12	0.49
1:A:7:PHE:HE2	1:A:13:VAL:CG2	2.26	0.48
1:F:128:LEU:HD23	1:F:151:VAL:HG13	1.94	0.48
1:B:185:THR:OG1	1:B:188:GLU:HG3	2.12	0.48
1:B:16:LEU:CD2	1:B:182:VAL:HG21	2.40	0.48
1:D:177:VAL:HG12	1:D:181:LEU:HB2	1.95	0.48
1:A:21:VAL:HG12	1:A:25:LYS:HE2	1.95	0.48
1:F:92:LEU:HD21	1:F:119:LYS:HD2	1.95	0.48
1:B:117:LEU:C	1:B:117:LEU:HD23	2.39	0.47
1:A:117:LEU:C	1:A:117:LEU:HD23	2.39	0.47
1:F:41:ILE:O	1:F:67:ALA:HA	2.14	0.47
1:B:177:VAL:HG12	1:B:181:LEU:HB2	1.97	0.47
1:F:111:VAL:HG22	1:F:116:GLU:HB3	1.97	0.47
1:A:115:THR:HG22	1:A:119:LYS:HE2	1.96	0.46
1:C:3:MET:O	1:C:4:GLU:C	2.57	0.46
1:E:7:PHE:HE2	1:E:13:VAL:CG2	2.29	0.46
1:C:117:LEU:C	1:C:117:LEU:HD23	2.41	0.45
1:E:31:VAL:HG13	1:E:36:VAL:HB	1.98	0.45
1:C:117:LEU:CD1	1:C:144:MET:HE2	2.45	0.45
1:B:26:GLU:CG	1:B:186:PRO:HG3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLU:HG2	1:A:192:LYS:HE2	1.98	0.45
1:B:134:GLU:OE1	1:B:157:GLY:HA3	2.17	0.45
1:B:155:PRO:HD3	1:B:172:VAL:HG22	1.98	0.44
1:D:31:VAL:HG13	1:D:36:VAL:HB	1.99	0.44
1:A:7:PHE:HB3	1:A:173:LEU:CD1	2.48	0.44
1:A:34:GLY:HA2	1:A:194:LYS:HE3	2.00	0.44
1:F:155:PRO:HD2	1:F:174:ALA:O	2.18	0.44
1:A:155:PRO:HD2	1:A:174:ALA:O	2.18	0.43
1:B:180:ALA:O	1:B:192:LYS:HD2	2.17	0.43
1:C:27:LYS:NZ	1:C:184:GLY:O	2.51	0.43
1:B:25:LYS:O	1:B:29:LEU:HG	2.19	0.43
1:B:69:THR:HA	1:B:90:PRO:HD3	2.01	0.43
1:D:177:VAL:CG1	1:D:181:LEU:HB2	2.48	0.43
1:C:132:PRO:HG2	1:C:135:VAL:CG2	2.49	0.43
1:D:140:PHE:O	1:D:144:MET:HG2	2.19	0.43
1:C:23:GLU:HG2	1:C:27:LYS:HE2	2.01	0.43
1:D:115:THR:HA	1:F:91:HIS:HB2	2.01	0.42
1:E:27:LYS:HD3	1:E:182:VAL:CG1	2.49	0.42
1:A:11:LYS:NZ	4:A:2005:HOH:O	2.51	0.42
1:C:136:VAL:HG13	1:C:140:PHE:CB	2.50	0.42
1:F:92:LEU:CD2	1:F:119:LYS:HD2	2.50	0.42
1:D:7:PHE:HB3	1:D:173:LEU:HD13	2.01	0.42
1:E:182:VAL:O	1:E:182:VAL:CG1	2.67	0.42
1:E:27:LYS:NZ	1:E:184:GLY:O	2.52	0.42
1:A:7:PHE:CE2	1:A:13:VAL:HG22	2.55	0.41
1:E:116:GLU:OE2	1:F:113:THR:CG2	2.63	0.41
1:D:8:LYS:O	1:D:11:LYS:NZ	2.45	0.41
1:C:119:LYS:HB2	1:C:119:LYS:HE2	1.89	0.41
1:C:19:ASN:N	1:C:23:GLU:OE2	2.38	0.41
1:D:109:PRO:HG2	1:D:128:LEU:CD1	2.50	0.41
1:E:91:HIS:HB2	1:F:115:THR:HA	2.02	0.41
1:D:114:PRO:HG3	1:D:144:MET:HE1	2.02	0.41
1:A:115:THR:HA	1:C:91:HIS:HB2	2.03	0.41
1:C:69:THR:HA	1:C:90:PRO:HD3	2.01	0.41
1:C:38:LEU:HD23	1:C:64:ILE:HB	2.03	0.41
1:B:16:LEU:CD2	1:B:182:VAL:CG2	2.98	0.40
1:D:115:THR:HG22	1:D:119:LYS:HE3	2.02	0.40
1:D:38:LEU:HD23	1:D:64:ILE:HB	2.04	0.40
1:F:3:MET:HE1	1:F:64:ILE:CG2	2.41	0.40
1:F:32:PHE:CD1	1:F:63:ALA:HB2	2.57	0.40
1:F:69:THR:HA	1:F:90:PRO:HD3	2.02	0.40

All (3) 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)
1:A:77:ARG:NH1	1:A:198:GLU:OE2[1_455]	1.82	0.38
1:B:77:ARG:NH1	1:B:162:ASP:OD2[1_455]	2.08	0.12
1:A:19:ASN:OD1	1:C:187:ASP:OD1[2_655]	2.16	0.04

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	200/205 (98%)	200 (100%)	0	0	100	100
1	B	200/205 (98%)	197 (98%)	3 (2%)	0	100	100
1	C	199/205 (97%)	194 (98%)	5 (2%)	0	100	100
1	D	201/205 (98%)	199 (99%)	2 (1%)	0	100	100
1	E	200/205 (98%)	198 (99%)	2 (1%)	0	100	100
1	F	199/205 (97%)	196 (98%)	3 (2%)	0	100	100
All	All	1199/1230 (98%)	1184 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	166/169 (98%)	156 (94%)	10 (6%)	17	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	166/169 (98%)	154 (93%)	12 (7%)	13	6
1	C	165/169 (98%)	152 (92%)	13 (8%)	11	5
1	D	166/169 (98%)	160 (96%)	6 (4%)	31	23
1	E	166/169 (98%)	155 (93%)	11 (7%)	15	8
1	F	165/169 (98%)	145 (88%)	20 (12%)	5	2
All	All	994/1014 (98%)	922 (93%)	72 (7%)	13	6

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	69	THR
1	A	74	GLU
1	A	128	LEU
1	A	145	LYS
1	A	172	VAL
1	A	173	LEU
1	A	181	LEU
1	A	182	VAL
1	A	203	CYS
1	B	31	VAL
1	B	53	LYS
1	B	94	GLU
1	B	145	LYS
1	B	169	LYS
1	B	172	VAL
1	B	173	LEU
1	B	181	LEU
1	B	182	VAL
1	B	183	LYS
1	B	187	ASP
1	B	199	LYS
1	C	4	GLU
1	C	8	LYS
1	C	16	LEU
1	C	31	VAL
1	C	49	ASP
1	C	111	VAL
1	C	136	VAL
1	C	152	LYS

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Mol	Chain	Res	Type
1	C	173	LEU
1	C	181	LEU
1	C	182	VAL
1	C	186	PRO
1	C	187	ASP
1	D	31	VAL
1	D	111	VAL
1	D	113	THR
1	D	152	LYS
1	D	173	LEU
1	D	181	LEU
1	E	8	LYS
1	E	31	VAL
1	E	60	GLU
1	E	94	GLU
1	E	98	GLN
1	E	102	GLU
1	E	166	GLU
1	E	172	VAL
1	E	173	LEU
1	E	181	LEU
1	E	201	ARG
1	F	16	LEU
1	F	22	GLU
1	F	29	LEU
1	F	31	VAL
1	F	61	LYS
1	F	69	THR
1	F	74	GLU
1	F	101	LYS
1	F	105	VAL
1	F	111	VAL
1	F	113	THR
1	F	136	VAL
1	F	145	LYS
1	F	166	GLU
1	F	172	VAL
1	F	173	LEU
1	F	181	LEU
1	F	182	VAL
1	F	183	LYS
1	F	199	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	C	98	GLN
1	E	98	GLN
1	F	37	HIS
1	F	139	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands 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	$\# Z > 2$
2	PYR	D	1205	1	4,4,5	1.94	1 (25%)	4,4,6	1.44	0
2	PYR	E	1204	1	4,4,5	1.79	2 (50%)	4,4,6	1.47	1 (25%)
2	PYR	F	1204	1	4,4,5	1.82	2 (50%)	4,4,6	1.21	0
3	SO4	B	1205	-	4,4,4	0.55	0	6,6,6	0.88	0
3	SO4	D	1206	-	4,4,4	0.33	0	6,6,6	0.60	0
3	SO4	E	1205	-	4,4,4	0.22	0	6,6,6	0.70	0
2	PYR	C	1204	1	4,4,5	1.43	1 (25%)	4,4,6	1.77	2 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PYR	A	1204	1	4,4,5	2.10	2 (50%)	4,4,6	1.26	0
3	SO4	A	1205	-	4,4,4	0.20	0	6,6,6	0.73	0
3	SO4	C	1205	-	4,4,4	0.20	0	6,6,6	0.67	0
2	PYR	B	1204	1	4,4,5	1.77	1 (25%)	4,4,6	1.16	0
3	SO4	F	1205	-	4,4,4	0.20	0	6,6,6	0.43	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
2	PYR	D	1205	1	-	1/2/2/4	-
2	PYR	E	1204	1	-	0/2/2/4	-
2	PYR	F	1204	1	-	1/2/2/4	-
2	PYR	C	1204	1	-	0/2/2/4	-
2	PYR	A	1204	1	-	1/2/2/4	-
2	PYR	B	1204	1	-	0/2/2/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1204	PYR	O-C	3.67	1.34	1.22
2	D	1205	PYR	O-C	3.30	1.32	1.22
2	B	1204	PYR	O-C	2.99	1.31	1.22
2	F	1204	PYR	O-C	2.94	1.31	1.22
2	E	1204	PYR	O-C	2.74	1.31	1.22
2	C	1204	PYR	O-C	2.27	1.29	1.22
2	E	1204	PYR	CA-C	-2.17	1.39	1.50
2	F	1204	PYR	CA-C	-2.14	1.40	1.50
2	A	1204	PYR	CA-C	-2.02	1.40	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1204	PYR	OXT-C-O	-2.54	116.81	123.33
2	C	1204	PYR	OXT-C-CA	2.13	122.43	113.49
2	E	1204	PYR	OXT-C-CA	2.12	122.39	113.49

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1204	PYR	O-C-CA-CB
2	D	1205	PYR	O-C-CA-CB
2	F	1204	PYR	O-C-CA-CB

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, 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	202/205 (98%)	-0.07	1 (0%) 87 89	2, 9, 20, 24	1 (0%)
1	B	202/205 (98%)	-0.18	1 (0%) 87 89	3, 9, 19, 25	0
1	C	201/205 (98%)	0.80	15 (7%) 20 21	2, 10, 22, 32	0
1	D	203/205 (99%)	1.48	48 (23%) 2 1	5, 12, 24, 30	0
1	E	202/205 (98%)	0.24	3 (1%) 72 75	3, 14, 25, 29	1 (0%)
1	F	201/205 (98%)	1.00	17 (8%) 16 17	7, 23, 38, 48	0
All	All	1211/1230 (98%)	0.55	85 (7%) 22 24	2, 12, 29, 48	2 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	LYS	7.7
1	E	2	LYS	5.8
1	D	202	GLY	4.5
1	C	165	CYS	4.4
1	D	2	LYS	4.3
1	D	60	GLU	3.9
1	D	201	ARG	3.9
1	D	58	LEU	3.8
1	D	98	GLN	3.8
1	D	203	CYS	3.7
1	C	56	SER	3.7
1	D	7	PHE	3.6
1	D	204	THR	3.5
1	C	203	CYS	3.4
1	D	187	ASP	3.3
1	D	95	GLU	3.2
1	D	11	LYS	3.1
1	D	145	LYS	3.1
1	D	64	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	57	PHE	3.0
1	D	191	GLU	3.0
1	F	57	PHE	3.0
1	E	203	CYS	3.0
1	D	169	LYS	2.9
1	D	62	GLY	2.9
1	F	187	ASP	2.9
1	F	58	LEU	2.8
1	D	61	LYS	2.8
1	D	102	GLU	2.8
1	D	165	CYS	2.8
1	D	77	ARG	2.7
1	F	82	SER	2.7
1	C	161	LEU	2.7
1	D	6	LEU	2.7
1	F	62	GLY	2.6
1	F	60	GLU	2.6
1	D	198	GLU	2.6
1	D	56	SER	2.6
1	C	202	GLY	2.6
1	C	201	ARG	2.5
1	D	55	LEU	2.5
1	D	183	LYS	2.5
1	F	203	CYS	2.5
1	F	83	GLY	2.5
1	F	54	GLU	2.5
1	D	80	VAL	2.5
1	D	154	VAL	2.5
1	C	135	VAL	2.4
1	D	73	VAL	2.4
1	F	74	GLU	2.4
1	F	99	PHE	2.4
1	D	53	LYS	2.4
1	C	185	THR	2.4
1	D	195	ALA	2.4
1	C	198	GLU	2.4
1	D	94	GLU	2.4
1	B	203	CYS	2.4
1	D	150	ASN	2.4
1	D	103	LYS	2.4
1	F	49	ASP	2.3
1	D	43	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	3	MET	2.3
1	F	50	THR	2.3
1	D	68	GLY	2.3
1	C	60	GLU	2.3
1	D	99	PHE	2.2
1	D	175	VAL	2.2
1	F	200	ILE	2.2
1	F	80	VAL	2.2
1	D	162	ASP	2.2
1	F	6	LEU	2.2
1	D	86	PHE	2.1
1	D	127	ILE	2.1
1	D	200	ILE	2.1
1	C	162	ASP	2.1
1	D	88	VAL	2.1
1	C	111	VAL	2.1
1	C	196	PHE	2.1
1	F	32	PHE	2.1
1	D	100	CYS	2.1
1	C	193	ALA	2.1
1	C	26	GLU	2.0
1	D	134	GLU	2.0
1	D	52	ILE	2.0
1	E	182	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
2	PYR	F	1204	5/6	0.92	0.11	17,19,20,20	0
3	SO4	D	1206	5/5	0.93	0.10	28,30,32,33	0
3	SO4	A	1205	5/5	0.94	0.09	24,25,29,29	0
2	PYR	E	1204	5/6	0.94	0.08	15,15,17,17	0
3	SO4	F	1205	5/5	0.94	0.09	29,31,32,32	0
3	SO4	E	1205	5/5	0.95	0.08	24,25,28,28	0
2	PYR	C	1204	5/6	0.95	0.08	10,13,13,15	0
2	PYR	D	1205	5/6	0.96	0.07	12,12,14,14	0
2	PYR	A	1204	5/6	0.96	0.08	7,7,9,9	0
3	SO4	C	1205	5/5	0.96	0.12	22,23,24,25	0
2	PYR	B	1204	5/6	0.97	0.06	9,10,12,12	0
3	SO4	B	1205	5/5	0.97	0.10	13,13,17,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.