



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:37 AM UTC

PDB ID : 3ZGE / pdb_00003zge
Title : Greater efficiency of photosynthetic carbon fixation due to single amino acid substitution
Authors : Paulus, J.K.; Schlieper, D.; Groth, G.
Deposited on : 2012-12-17
Resolution : 2.49 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

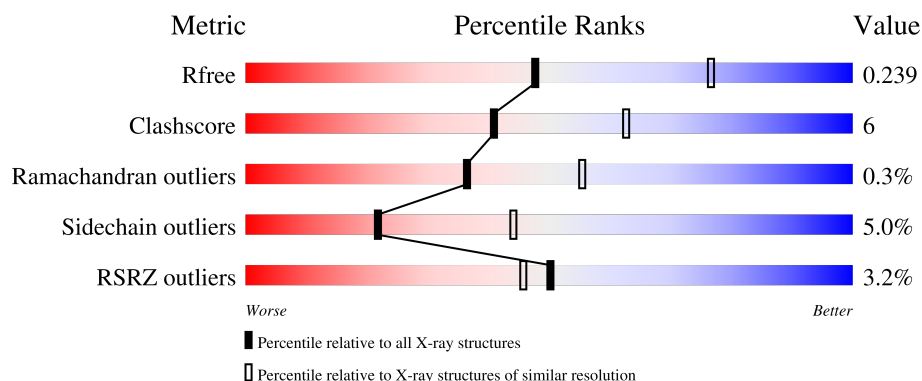
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

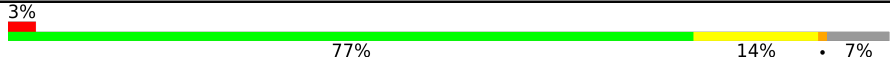
The reported resolution of this entry is 2.49 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	990	 3% 77% 14% • 7%
1	B	990	 3% 77% 13% •• 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14944 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 C4 PHOSPHOENOLPYRUVATE CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	916	Total	C	N	O	S	0	0	0
			7380	4682	1286	1378	34			
1	B	911	Total	C	N	O	S	0	0	0
			7330	4656	1273	1368	33			

There are 48 discrepancies between the modelled and reference sequences:

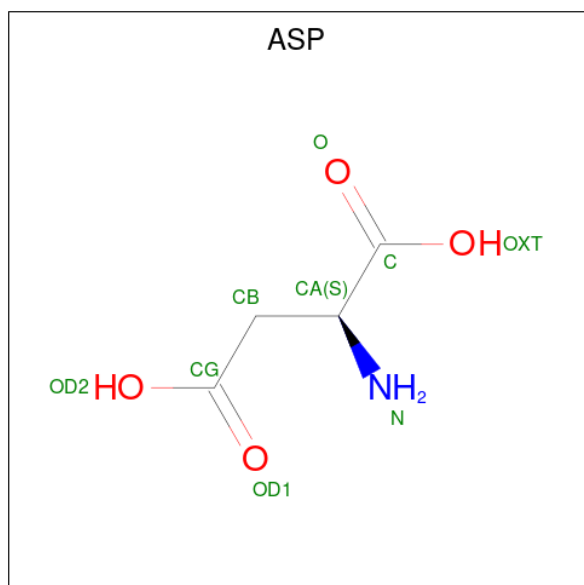
Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP P30694
A	-22	GLY	-	expression tag	UNP P30694
A	-21	HIS	-	expression tag	UNP P30694
A	-20	HIS	-	expression tag	UNP P30694
A	-19	HIS	-	expression tag	UNP P30694
A	-18	HIS	-	expression tag	UNP P30694
A	-17	HIS	-	expression tag	UNP P30694
A	-16	HIS	-	expression tag	UNP P30694
A	-15	HIS	-	expression tag	UNP P30694
A	-14	HIS	-	expression tag	UNP P30694
A	-13	HIS	-	expression tag	UNP P30694
A	-12	HIS	-	expression tag	UNP P30694
A	-11	SER	-	expression tag	UNP P30694
A	-10	SER	-	expression tag	UNP P30694
A	-9	GLY	-	expression tag	UNP P30694
A	-8	HIS	-	expression tag	UNP P30694
A	-7	GLU	-	expression tag	UNP P30694
A	-6	ASN	-	expression tag	UNP P30694
A	-5	LEU	-	expression tag	UNP P30694
A	-4	TYR	-	expression tag	UNP P30694
A	-3	PHE	-	expression tag	UNP P30694
A	-2	GLN	-	expression tag	UNP P30694
A	-1	GLY	-	expression tag	UNP P30694
A	0	HIS	-	expression tag	UNP P30694
B	-23	MET	-	expression tag	UNP P30694

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLY	-	expression tag	UNP P30694
B	-21	HIS	-	expression tag	UNP P30694
B	-20	HIS	-	expression tag	UNP P30694
B	-19	HIS	-	expression tag	UNP P30694
B	-18	HIS	-	expression tag	UNP P30694
B	-17	HIS	-	expression tag	UNP P30694
B	-16	HIS	-	expression tag	UNP P30694
B	-15	HIS	-	expression tag	UNP P30694
B	-14	HIS	-	expression tag	UNP P30694
B	-13	HIS	-	expression tag	UNP P30694
B	-12	HIS	-	expression tag	UNP P30694
B	-11	SER	-	expression tag	UNP P30694
B	-10	SER	-	expression tag	UNP P30694
B	-9	GLY	-	expression tag	UNP P30694
B	-8	HIS	-	expression tag	UNP P30694
B	-7	GLU	-	expression tag	UNP P30694
B	-6	ASN	-	expression tag	UNP P30694
B	-5	LEU	-	expression tag	UNP P30694
B	-4	TYR	-	expression tag	UNP P30694
B	-3	PHE	-	expression tag	UNP P30694
B	-2	GLN	-	expression tag	UNP P30694
B	-1	GLY	-	expression tag	UNP P30694
B	0	HIS	-	expression tag	UNP P30694

- Molecule 2 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	1	4		
2	B	1	Total	C	N	O	0	0
			9	4	1	4		

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



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

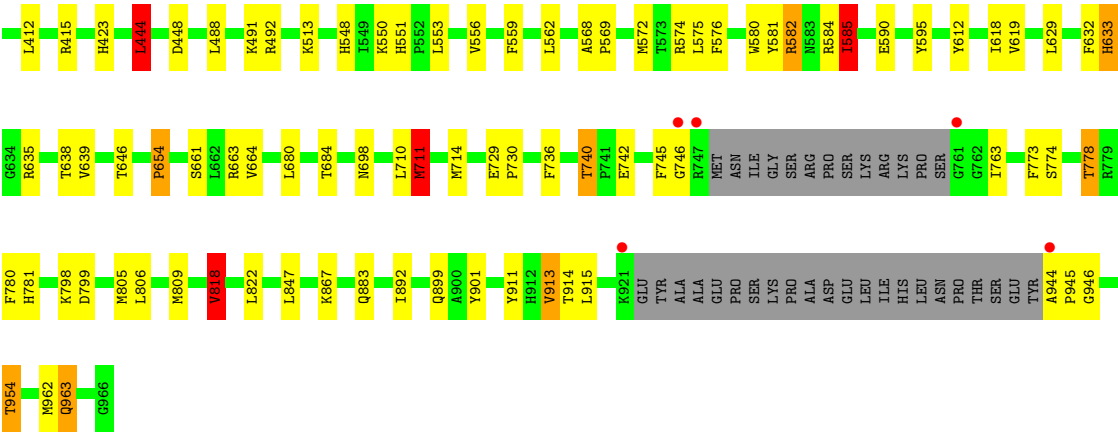
- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	116	Total	O	0	0
			116	116		
5	B	82	Total	O	0	0
			82	82		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	162.52Å 122.11Å 131.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.00 – 2.49 37.00 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.00-2.49) 99.6 (37.00-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.20 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.204 , 0.237 0.207 , 0.239	Depositor DCC
R_{free} test set	1848 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14944	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: EDO, SO4

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	1.17	15/7533 (0.2%)	1.08	12/10182 (0.1%)
1	B	1.24	12/7482 (0.2%)	1.11	20/10112 (0.2%)
All	All	1.20	27/15015 (0.2%)	1.09	32/20294 (0.2%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	548	HIS	CG-CD2	7.03	1.43	1.35
1	A	147	HIS	CG-CD2	6.29	1.42	1.35
1	A	794	HIS	CG-CD2	6.19	1.42	1.35
1	A	351	HIS	CG-CD2	6.18	1.42	1.35
1	B	582	ARG	CA-C	-6.15	1.44	1.52
1	A	492	ARG	CA-C	-5.99	1.46	1.52
1	A	548	HIS	CG-CD2	5.99	1.42	1.35
1	A	200	ILE	CA-CB	5.78	1.60	1.53
1	B	253	LYS	C-O	-5.76	1.17	1.24
1	A	871	HIS	CG-CD2	5.75	1.42	1.35
1	A	71	HIS	CB-CG	5.74	1.58	1.50
1	B	147	HIS	CG-CD2	5.61	1.42	1.35
1	B	633	HIS	CG-CD2	5.53	1.42	1.35
1	B	423	HIS	CG-CD2	5.42	1.41	1.35
1	B	551	HIS	CG-CD2	5.40	1.41	1.35
1	A	71	HIS	CG-CD2	5.38	1.41	1.35
1	A	248	TRP	NE1-CE2	-5.36	1.31	1.37
1	A	147	HIS	CE1-NE2	5.28	1.37	1.32
1	B	698	ASN	C-O	-5.23	1.18	1.24
1	B	185	HIS	CG-CD2	5.21	1.41	1.35
1	A	963	GLN	C-O	-5.21	1.19	1.24
1	A	551	HIS	CG-CD2	5.15	1.41	1.35
1	A	794	HIS	CE1-NE2	5.15	1.37	1.32
1	B	71	HIS	CG-CD2	5.10	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	492	ARG	C-O	-5.05	1.17	1.24
1	B	781	HIS	CG-CD2	5.01	1.41	1.35
1	A	568	ALA	C-O	-5.00	1.19	1.24

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	944	ALA	CA-C-N	8.79	131.04	120.23
1	B	944	ALA	C-N-CA	8.79	131.04	120.23
1	B	711	MET	CG-SD-CE	-8.65	81.88	100.90
1	B	945	PRO	N-CA-C	7.16	121.73	110.50
1	A	908	ASP	CA-C-N	-6.97	111.13	119.84
1	A	908	ASP	C-N-CA	-6.97	111.13	119.84
1	B	584	ARG	CG-CD-NE	-6.57	97.56	112.00
1	B	946	GLY	N-CA-C	6.41	121.65	112.81
1	A	390	GLY	N-CA-C	-6.02	107.13	113.58
1	A	584	ARG	CG-CD-NE	-5.98	98.84	112.00
1	A	711	MET	CG-SD-CE	-5.97	87.76	100.90
1	B	818	VAL	N-CA-CB	-5.94	102.47	110.54
1	B	654	PRO	O-C-N	5.86	124.01	121.31
1	B	684	THR	N-CA-C	-5.83	104.85	111.14
1	B	585	ILE	CA-CB-CG2	5.78	120.33	110.50
1	B	229	PRO	N-CA-C	5.71	117.67	110.70
1	B	664	VAL	CB-CA-C	-5.57	100.74	110.71
1	A	818	VAL	N-CA-CB	-5.55	102.99	110.54
1	B	444	LEU	CB-CG-CD1	-5.51	94.18	110.70
1	A	763	ILE	N-CA-C	5.49	116.22	110.62
1	A	845	GLU	CB-CA-C	-5.44	102.11	110.81
1	B	354	GLU	N-CA-C	5.40	119.52	112.13
1	A	200	ILE	N-CA-C	5.33	115.27	108.12
1	B	763	ILE	N-CA-C	5.29	116.02	110.62
1	A	603	GLY	N-CA-C	-5.25	106.13	112.48
1	B	144	ARG	NE-CZ-NH2	-5.24	114.48	119.20
1	B	359	ILE	CB-CA-C	-5.20	105.90	111.00
1	B	164	THR	CA-CB-CG2	5.17	119.29	110.50
1	B	635	ARG	N-CA-C	5.06	117.21	110.53
1	A	772	ILE	CB-CA-C	-5.06	105.49	111.97
1	B	47	ASP	CB-CA-C	-5.03	102.44	110.79
1	A	144	ARG	NE-CZ-NH2	-5.01	114.69	119.20

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	7380	0	7359	97	0
1	B	7330	0	7310	95	0
2	A	9	0	3	0	0
2	B	9	0	3	0	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	116	0	0	4	0
5	B	82	0	0	3	0
All	All	14944	0	14687	191	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 6.

All (191) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:LEU:HA	1:B:809:MET:HE3	1.41	1.01
1:A:805:MET:HG2	1:A:809:MET:HE2	1.39	0.99
1:B:805:MET:HG2	1:B:809:MET:HE2	1.53	0.91
1:A:319:GLU:HA	1:A:322:MET:HE3	1.53	0.90
1:B:319:GLU:HA	1:B:322:MET:HE3	1.53	0.90
1:B:84:THR:HG21	1:B:911:TYR:OH	1.79	0.82
1:B:806:LEU:CA	1:B:809:MET:HE3	2.10	0.82
1:A:240:MET:HG3	1:A:309:MET:HE1	1.64	0.77
1:A:806:LEU:HA	1:A:809:MET:HE3	1.67	0.76
1:A:20:VAL:CG1	1:A:20:VAL:O	2.33	0.76
1:B:325:MET:HA	1:B:327:MET:HE3	1.70	0.72
1:B:325:MET:HA	1:B:327:MET:CE	2.20	0.72
1:B:20:VAL:CG1	1:B:20:VAL:O	2.37	0.71
1:B:559:PHE:HZ	1:B:572:MET:CE	2.06	0.68
1:B:38:LEU:CD1	1:B:101:MET:HE2	2.24	0.68
1:A:228:THR:HG22	1:A:229:PRO:O	1.94	0.67
1:A:84:THR:HG21	1:A:911:TYR:OH	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:GLN:OE1	1:A:954:THR:CG2	2.44	0.65
1:A:325:MET:HE1	1:A:417:LEU:HD11	1.79	0.65
1:B:638:THR:HG21	1:B:818:VAL:HG13	1.78	0.65
1:A:20:VAL:HG21	1:A:883:GLN:HG3	1.78	0.64
1:B:38:LEU:HD11	1:B:101:MET:HE2	1.78	0.64
1:B:550:LYS:NZ	5:B:2046:HOH:O	2.31	0.64
1:B:559:PHE:CZ	1:B:572:MET:CE	2.80	0.64
1:B:740:THR:HG22	1:B:742:GLU:H	1.61	0.64
1:B:231:THR:HG23	1:B:234:ASP:H	1.63	0.63
1:A:231:THR:HG23	1:A:234:ASP:H	1.63	0.63
1:A:740:THR:HG22	1:A:742:GLU:H	1.65	0.62
1:B:806:LEU:N	1:B:809:MET:HE3	2.14	0.62
1:B:20:VAL:HG21	1:B:883:GLN:HG3	1.82	0.62
1:A:20:VAL:O	1:A:20:VAL:HG13	2.00	0.61
1:A:910:ASN:HB2	5:A:2114:HOH:O	1.99	0.61
1:A:226:ARG:CZ	1:A:226:ARG:HB2	2.30	0.61
1:A:231:THR:HG22	1:A:234:ASP:CG	2.26	0.61
1:B:20:VAL:O	1:B:20:VAL:HG13	2.00	0.61
1:A:909:PRO:HD2	5:A:2115:HOH:O	1.99	0.61
1:B:913:VAL:HG13	1:B:914:THR:N	2.15	0.61
1:B:164:THR:HG22	1:B:661:SER:HA	1.83	0.60
1:B:322:MET:HE1	1:B:373:ARG:HD3	1.82	0.60
1:B:899:GLN:OE1	1:B:954:THR:CG2	2.49	0.60
1:B:581:TYR:CZ	1:B:585:ILE:CD1	2.84	0.60
1:A:909:PRO:CD	5:A:2115:HOH:O	2.48	0.59
1:B:386:LEU:HD23	1:B:391:LYS:HA	1.84	0.59
1:A:806:LEU:CA	1:A:809:MET:HE3	2.32	0.59
1:A:805:MET:CG	1:A:809:MET:HE2	2.26	0.59
1:B:559:PHE:CE2	1:B:572:MET:HE3	2.38	0.59
1:B:231:THR:HG22	1:B:234:ASP:CG	2.28	0.59
1:B:740:THR:HG23	1:B:774:SER:HB3	1.84	0.58
1:A:618:ILE:HG22	1:A:629:LEU:CD2	2.33	0.58
1:A:778:THR:HG22	1:A:780:PHE:HB2	1.85	0.58
1:B:559:PHE:CZ	1:B:572:MET:HE3	2.38	0.58
1:A:559:PHE:HZ	1:A:572:MET:CE	2.15	0.58
1:B:313:MET:HE1	1:B:444:LEU:CD2	2.33	0.58
1:A:805:MET:C	1:A:809:MET:HE3	2.29	0.57
1:B:240:MET:HB3	1:B:309:MET:HE1	1.86	0.57
1:B:913:VAL:CG1	1:B:914:THR:N	2.68	0.57
1:A:740:THR:CG2	1:A:742:GLU:H	2.18	0.56
1:B:581:TYR:CZ	1:B:585:ILE:HD13	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:LEU:C	1:B:822:LEU:HD23	2.31	0.56
1:A:19:LEU:HD11	1:A:890:PRO:HG3	1.88	0.56
1:B:740:THR:CG2	1:B:742:GLU:H	2.18	0.56
1:A:240:MET:CG	1:A:309:MET:HE1	2.32	0.55
1:B:568:ALA:HB3	1:B:569:PRO:HD3	1.86	0.55
1:A:315:PHE:O	1:A:318:ILE:HG22	2.06	0.55
1:A:562:LEU:HD13	1:A:610:GLN:HG2	1.88	0.55
1:A:559:PHE:CZ	1:A:572:MET:CE	2.90	0.55
1:A:806:LEU:N	1:A:809:MET:HE3	2.22	0.55
1:B:740:THR:CG2	1:B:774:SER:HB3	2.36	0.54
1:B:736:PHE:O	1:B:740:THR:HB	2.08	0.54
1:B:333:GLU:OE1	1:B:415:ARG:NH1	2.41	0.54
1:B:805:MET:C	1:B:809:MET:HE3	2.33	0.53
1:A:559:PHE:CE2	1:A:572:MET:HE3	2.44	0.53
1:A:166:GLU:OE1	1:A:663:ARG:HD2	2.09	0.53
1:A:618:ILE:HG22	1:A:629:LEU:HD21	1.91	0.53
1:B:778:THR:HG22	1:B:780:PHE:HB2	1.90	0.52
1:B:8:LYS:HE2	1:B:8:LYS:C	2.35	0.52
1:A:20:VAL:O	1:A:20:VAL:HG12	2.09	0.52
1:A:909:PRO:N	5:A:2115:HOH:O	2.43	0.52
1:A:534:THR:HG23	1:A:575:LEU:HG	1.90	0.52
1:A:556:VAL:HG22	1:A:590:GLU:HB3	1.91	0.52
1:B:166:GLU:CD	1:B:663:ARG:HD2	2.35	0.52
1:A:305:LEU:HG	1:A:387:LEU:HD21	1.91	0.51
1:A:84:THR:HG23	1:A:901:TYR:CG	2.45	0.51
1:A:319:GLU:HA	1:A:322:MET:CE	2.32	0.51
1:A:379:THR:HA	1:A:399:VAL:HG22	1.93	0.51
1:A:559:PHE:CZ	1:A:572:MET:HE3	2.46	0.51
1:A:553:LEU:HD12	1:A:553:LEU:N	2.26	0.51
1:B:379:THR:HA	1:B:399:VAL:HG22	1.93	0.51
1:A:166:GLU:CD	1:A:663:ARG:HD2	2.36	0.50
1:A:799:ASP:OD1	1:A:801:LYS:HE3	2.11	0.50
1:A:822:LEU:C	1:A:822:LEU:HD23	2.36	0.50
1:B:166:GLU:OE1	1:B:663:ARG:HD2	2.12	0.50
1:B:581:TYR:CZ	1:B:585:ILE:HD11	2.46	0.50
1:A:231:THR:CG2	1:A:234:ASP:H	2.25	0.50
1:B:295:THR:HB	1:B:296:PRO:HD2	1.94	0.50
1:A:899:GLN:HB2	1:A:954:THR:CG2	2.43	0.49
1:B:745:PHE:CD2	1:B:773:PHE:CE1	3.01	0.49
1:B:334:LEU:HD12	1:B:412:LEU:HG	1.94	0.49
1:A:740:THR:CG2	1:A:774:SER:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:GLN:OE1	1:A:954:THR:HG23	2.13	0.49
1:B:84:THR:HG23	1:B:901:TYR:CD1	2.47	0.49
1:A:711:MET:HE2	1:A:711:MET:CA	2.33	0.48
1:A:740:THR:HG23	1:A:774:SER:HB3	1.95	0.48
1:A:745:PHE:CD2	1:A:773:PHE:CE1	3.01	0.48
1:A:581:TYR:CZ	1:A:585:ILE:CD1	2.97	0.48
1:A:736:PHE:O	1:A:740:THR:HB	2.13	0.48
1:B:740:THR:CG2	1:B:742:GLU:HB2	2.44	0.48
1:B:107:LEU:HD21	1:B:185:HIS:HB3	1.95	0.48
1:A:120:LYS:HD2	1:B:25:SER:HB3	1.96	0.47
1:B:963:GLN:NE2	5:B:2066:HOH:O	2.46	0.47
1:A:782:LEU:C	1:A:782:LEU:HD23	2.39	0.47
1:B:8:LYS:HE2	1:B:8:LYS:CA	2.45	0.47
1:A:638:THR:HG21	1:A:818:VAL:HG13	1.97	0.47
1:B:318:ILE:HG23	1:B:322:MET:HE2	1.97	0.47
1:B:581:TYR:CE1	1:B:585:ILE:HD13	2.49	0.47
1:B:556:VAL:HG22	1:B:590:GLU:HB3	1.98	0.46
1:B:778:THR:O	1:B:778:THR:CG2	2.64	0.46
1:A:295:THR:HB	1:A:296:PRO:HD2	1.98	0.46
1:A:322:MET:HE1	1:A:373:ARG:HD3	1.97	0.46
1:B:805:MET:C	1:B:809:MET:CE	2.88	0.46
1:A:444:LEU:HD12	1:A:444:LEU:HA	1.59	0.45
1:B:335:ARG:O	1:B:339:GLU:HG2	2.17	0.45
1:A:485:LEU:HD11	1:A:578:MET:HE2	1.97	0.45
1:A:19:LEU:HD21	1:A:68:GLU:HB3	1.97	0.45
1:A:831:ASN:OD1	1:A:831:ASN:C	2.59	0.45
1:B:710:LEU:HG	1:B:714:MET:HE2	1.97	0.45
1:A:701:ILE:HD11	1:A:812:THR:HG22	1.98	0.44
1:A:461:ASP:O	1:A:465:GLN:HG3	2.18	0.44
1:B:231:THR:CG2	1:B:234:ASP:H	2.27	0.44
1:B:612:TYR:CE2	1:B:654:PRO:HG3	2.53	0.44
1:A:137:ASP:OD1	1:A:137:ASP:C	2.61	0.44
1:A:618:ILE:HG22	1:A:629:LEU:HD22	1.98	0.44
1:B:595:TYR:OH	1:B:633:HIS:ND1	2.42	0.44
1:A:84:THR:HG23	1:A:901:TYR:CD1	2.53	0.44
1:B:632:PHE:CD1	1:B:663:ARG:HG2	2.53	0.44
1:A:711:MET:HE2	1:A:711:MET:HB2	1.35	0.43
1:B:892:ILE:HD13	1:B:962:MET:HE3	1.99	0.43
1:A:335:ARG:O	1:A:339:GLU:HG2	2.19	0.43
1:A:799:ASP:OD1	1:A:799:ASP:C	2.60	0.43
1:B:84:THR:HG23	1:B:901:TYR:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:GLN:HB2	1:A:954:THR:HG23	1.99	0.43
1:B:488:LEU:HD22	1:B:580:TRP:CZ2	2.54	0.43
1:A:19:LEU:HD21	1:A:68:GLU:CB	2.48	0.42
1:A:740:THR:CG2	1:A:742:GLU:HB2	2.49	0.42
1:B:19:LEU:HD23	1:B:19:LEU:HA	1.83	0.42
1:B:618:ILE:HG22	1:B:629:LEU:HD22	2.01	0.42
1:A:231:THR:HG23	1:A:233:GLN:HB2	2.02	0.42
1:B:407:LEU:O	1:B:408:GLU:C	2.62	0.42
1:B:553:LEU:HD12	1:B:553:LEU:N	2.35	0.42
1:A:386:LEU:HD23	1:A:391:LYS:HA	2.01	0.42
1:A:199:ASP:OD1	1:A:199:ASP:N	2.53	0.42
1:A:164:THR:O	1:A:164:THR:HG22	2.20	0.41
1:A:576:PHE:O	1:A:582:ARG:HD2	2.20	0.41
1:B:85:SER:O	1:B:915:LEU:HA	2.21	0.41
1:B:576:PHE:O	1:B:582:ARG:HD2	2.20	0.41
1:B:711:MET:HB2	1:B:711:MET:HE2	0.94	0.41
1:B:444:LEU:HA	1:B:444:LEU:HD12	1.19	0.41
1:A:333:GLU:OE1	1:A:415:ARG:NH1	2.53	0.41
1:A:899:GLN:OE1	1:A:954:THR:HG22	2.21	0.41
1:B:805:MET:CG	1:B:809:MET:HE2	2.37	0.41
1:A:84:THR:CG2	1:A:901:TYR:CD1	3.03	0.41
1:A:422:ASP:O	1:A:423:HIS:C	2.62	0.41
1:A:527:ILE:HD13	1:A:556:VAL:HB	2.02	0.41
1:A:557:PRO:HG3	1:A:572:MET:HE1	2.02	0.41
1:A:813:TRP:O	1:A:814:PRO:C	2.62	0.41
1:B:240:MET:CB	1:B:309:MET:HE1	2.48	0.41
1:B:581:TYR:CE1	1:B:585:ILE:CD1	3.03	0.41
1:B:164:THR:HG22	1:B:661:SER:CA	2.50	0.41
1:B:178:ARG:NH2	3:B:1968:SO4:O2	2.39	0.41
1:A:612:TYR:CE2	1:A:654:PRO:HG3	2.56	0.41
1:B:448:ASP:CG	1:B:663:ARG:HH22	2.29	0.41
1:A:609:TRP:CD2	1:A:711:MET:HG2	2.55	0.41
1:B:315:PHE:O	1:B:318:ILE:HG22	2.22	0.41
1:A:568:ALA:HB3	1:A:569:PRO:HD3	2.04	0.40
1:A:581:TYR:CZ	1:A:585:ILE:HD13	2.56	0.40
1:B:200:ILE:O	1:B:200:ILE:CG2	2.69	0.40
1:A:334:LEU:HD23	1:A:334:LEU:O	2.22	0.40
1:B:325:MET:HA	1:B:327:MET:HE2	2.02	0.40
1:B:574:ARG:O	1:B:575:LEU:C	2.64	0.40
1:B:799:ASP:C	1:B:799:ASP:OD1	2.63	0.40
1:A:538:LEU:HD11	1:A:578:MET:SD	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:ILE:HD13	1:A:834:ILE:HA	1.82	0.40
1:B:20:VAL:O	1:B:20:VAL:HG12	2.17	0.40
1:B:313:MET:HE1	1:B:444:LEU:HD22	2.04	0.40
1:B:847:LEU:HD23	1:B:847:LEU:HA	1.91	0.40
1:A:107:LEU:HD21	1:A:185:HIS:HB3	2.04	0.40
1:B:110:GLU:OE1	1:B:189:ARG:NH1	2.53	0.40
1:B:680:LEU:HD12	5:B:2007:HOH:O	2.20	0.40
1:B:729:GLU:HA	1:B:730:PRO:HD3	1.92	0.40
1:B:899:GLN:HB2	1:B:954:THR:CG2	2.51	0.40
1:A:110:GLU:OE1	1:A:189:ARG:NH1	2.53	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	906/990 (92%)	885 (98%)	18 (2%)	3 (0%)	36	55
1	B	897/990 (91%)	876 (98%)	18 (2%)	3 (0%)	36	55
All	All	1803/1980 (91%)	1761 (98%)	36 (2%)	6 (0%)	36	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	746	GLY
1	B	175	GLN
1	B	746	GLY
1	A	24	VAL
1	B	24	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	802/866 (93%)	762 (95%)	40 (5%)	22	44
1	B	796/866 (92%)	756 (95%)	40 (5%)	22	44
All	All	1598/1732 (92%)	1518 (95%)	80 (5%)	22	44

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	20	VAL
1	A	23	LYS
1	A	53	LEU
1	A	54	LYS
1	A	59	GLN
1	A	84	THR
1	A	88	THR
1	A	149	LEU
1	A	164	THR
1	A	180	SER
1	A	199	ASP
1	A	200	ILE
1	A	210	GLU
1	A	225	ILE
1	A	226	ARG
1	A	327	MET
1	A	357	LYS
1	A	358	ARG
1	A	359	ILE
1	A	397	GLU
1	A	399	VAL
1	A	402	ASN
1	A	513	LYS
1	A	562	LEU
1	A	585	ILE
1	A	639	VAL

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Mol	Chain	Res	Type
1	A	646	THR
1	A	711	MET
1	A	740	THR
1	A	778	THR
1	A	798	LYS
1	A	800	SER
1	A	818	VAL
1	A	867	LYS
1	A	913	VAL
1	A	921	LYS
1	A	922	GLU
1	A	948	GLU
1	A	954	THR
1	B	8	LYS
1	B	20	VAL
1	B	23	LYS
1	B	53	LEU
1	B	54	LYS
1	B	59	GLN
1	B	84	THR
1	B	88	THR
1	B	149	LEU
1	B	164	THR
1	B	180	SER
1	B	200	ILE
1	B	210	GLU
1	B	311	SER
1	B	327	MET
1	B	331	ASN
1	B	350	LYS
1	B	357	LYS
1	B	358	ARG
1	B	359	ILE
1	B	397	GLU
1	B	399	VAL
1	B	402	ASN
1	B	444	LEU
1	B	491	LYS
1	B	513	LYS
1	B	562	LEU
1	B	585	ILE
1	B	619	VAL

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Mol	Chain	Res	Type
1	B	639	VAL
1	B	646	THR
1	B	711	MET
1	B	740	THR
1	B	778	THR
1	B	798	LYS
1	B	818	VAL
1	B	867	LYS
1	B	913	VAL
1	B	954	THR
1	B	963	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	466	HIS
1	A	610	GLN
1	A	617	GLN
1	A	802	ASN
1	A	963	GLN
1	B	15	GLN
1	B	100	HIS
1	B	150	ASN
1	B	279	GLN
1	B	610	GLN
1	B	673	GLN
1	B	794	HIS
1	B	802	ASN
1	B	963	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

6 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	$\# Z > 2$
3	SO4	A	1968	-	4,4,4	0.46	0	6,6,6	0.14	0
4	EDO	B	1969	-	3,3,3	0.62	0	2,2,2	0.33	0
2	ASP	A	1967	-	7,8,8	1.42	1 (14%)	6,10,10	0.88	0
4	EDO	A	1969	-	3,3,3	0.53	0	2,2,2	0.09	0
2	ASP	B	1967	-	7,8,8	1.34	2 (28%)	6,10,10	0.71	0
3	SO4	B	1968	-	4,4,4	0.28	0	6,6,6	0.52	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
4	EDO	A	1969	-	-	0/1/1/1	-
2	ASP	B	1967	-	-	1/8/8/8	-
4	EDO	B	1969	-	-	0/1/1/1	-
2	ASP	A	1967	-	-	2/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1967	ASP	OXT-C	-2.38	1.23	1.30
2	B	1967	ASP	OD2-CG	-2.10	1.23	1.30
2	B	1967	ASP	OXT-C	-2.08	1.24	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1967	ASP	O-C-CA-N
2	A	1967	ASP	OXT-C-CA-N
2	B	1967	ASP	OXT-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1968	SO4	1	0

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	916/990 (92%)	0.08	32 (3%) 47 42	27, 44, 80, 123	0
1	B	911/990 (92%)	-0.10	27 (2%) 52 48	21, 38, 71, 134	0
All	All	1827/1980 (92%)	-0.01	59 (3%) 50 46	21, 42, 75, 134	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	VAL	6.1
1	B	944	ALA	5.6
1	B	761	GLY	5.3
1	A	225	ILE	5.2
1	B	228	THR	5.0
1	A	24	VAL	4.8
1	B	23	LYS	4.6
1	A	761	GLY	4.4
1	B	8	LYS	4.4
1	A	229	PRO	4.3
1	A	747	ARG	4.3
1	B	747	ARG	4.2
1	A	23	LYS	4.2
1	A	199	ASP	4.0
1	A	21	PRO	4.0
1	B	175	GLN	4.0
1	B	22	GLY	4.0
1	B	25	SER	4.0
1	B	921	LYS	4.0
1	A	351	HIS	3.8
1	A	200	ILE	3.7
1	A	8	LYS	3.7
1	B	391	LYS	3.5
1	A	205	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	350	LYS	3.4
1	A	922	GLU	3.4
1	B	351	HIS	3.3
1	B	746	GLY	3.3
1	A	909	PRO	3.1
1	A	912	HIS	3.0
1	A	25	SER	3.0
1	A	913	VAL	2.9
1	B	229	PRO	2.9
1	A	22	GLY	2.9
1	A	746	GLY	2.8
1	A	344	THR	2.7
1	A	227	ARG	2.6
1	B	197	ALA	2.6
1	B	268	ASN	2.5
1	A	354	GLU	2.4
1	B	18	LEU	2.4
1	B	117	ARG	2.3
1	A	226	ARG	2.3
1	A	393	ASP	2.3
1	A	355	PHE	2.3
1	A	202	PRO	2.3
1	B	176	SER	2.2
1	B	355	PHE	2.2
1	A	921	LYS	2.2
1	B	26	GLU	2.2
1	A	390	GLY	2.2
1	B	230	PRO	2.1
1	A	946	GLY	2.1
1	A	357	LYS	2.1
1	B	74	LYS	2.1
1	A	231	THR	2.1
1	A	148	LYS	2.1
1	B	122	LYS	2.1
1	B	21	PRO	2.1

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

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
4	EDO	B	1969	4/4	0.94	0.11	30,36,38,42	0
2	ASP	A	1967	9/9	0.95	0.08	24,34,40,45	0
2	ASP	B	1967	9/9	0.96	0.08	25,31,33,34	0
3	SO4	B	1968	5/5	0.97	0.09	38,48,51,52	0
4	EDO	A	1969	4/4	0.97	0.09	34,38,38,44	0
3	SO4	A	1968	5/5	0.97	0.12	47,50,53,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.