



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 09:14 am GMT

PDB ID : 3ZGE  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, 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

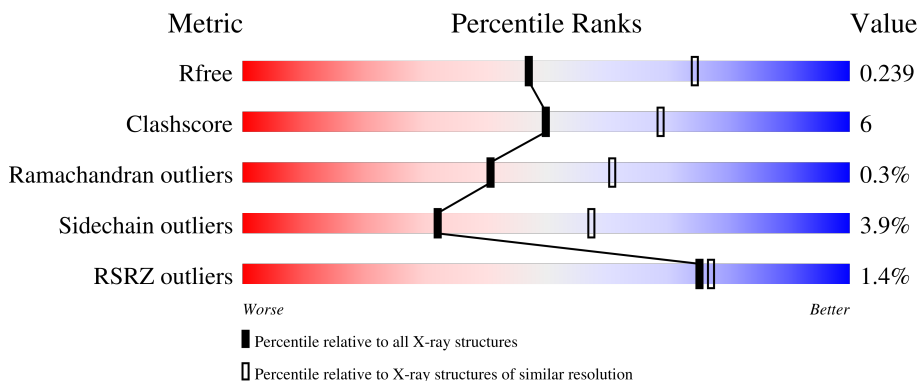
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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  $\geq 3$ , 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	 2% 79% 12% • 7%
1	B	990	 % 80% 11% • 8%

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	916	7380	4682	1286	1378	34	0	0	0
1	B	911	7330	4656	1273	1368	33	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

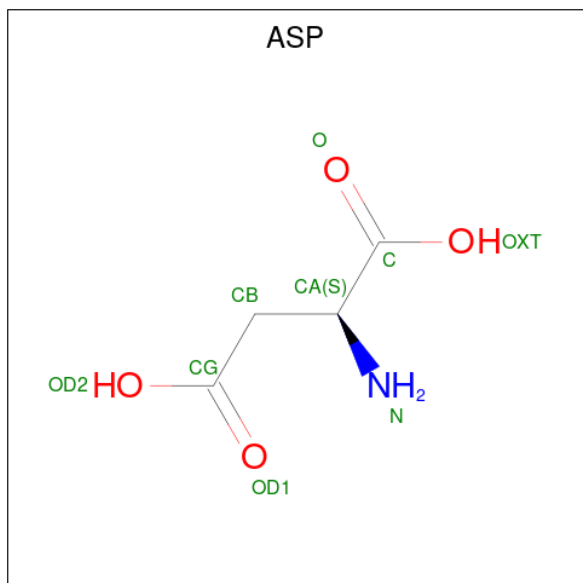
Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP P30694
A	-22	GLY	-	expression tag	UNP P30694
A	-21	HIS	-	expression tag	UNP P30694
A	-20	HIS	-	expression tag	UNP P30694
A	-19	HIS	-	expression tag	UNP P30694
A	-18	HIS	-	expression tag	UNP P30694
A	-17	HIS	-	expression tag	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 (three-letter code: ASP) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>4</sub>).



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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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 (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

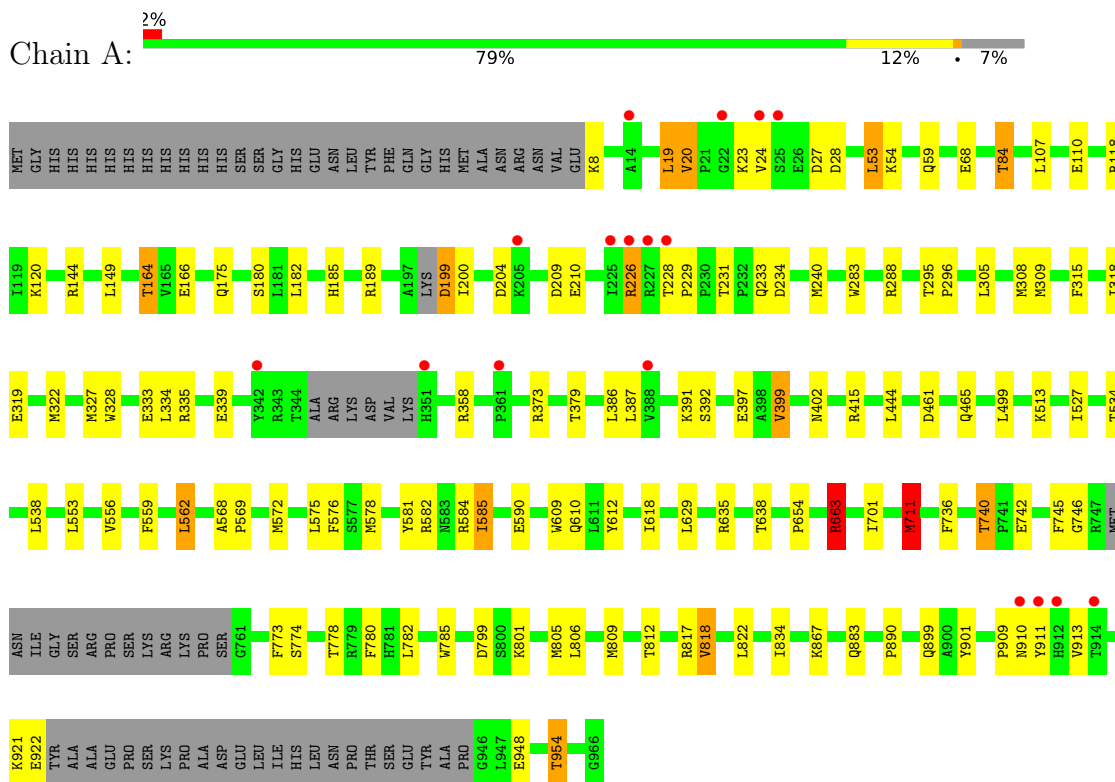
- Molecule 5 is water.

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

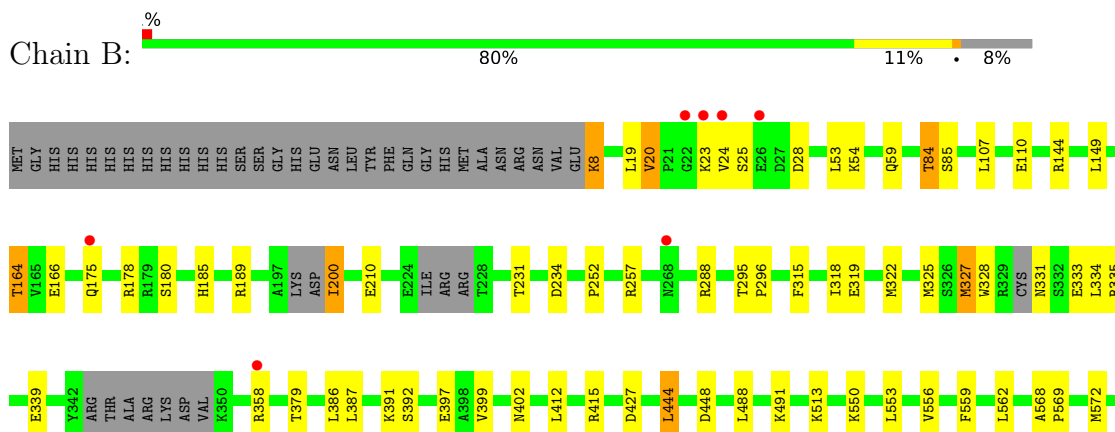
### 3 Residue-property plots [i](#)

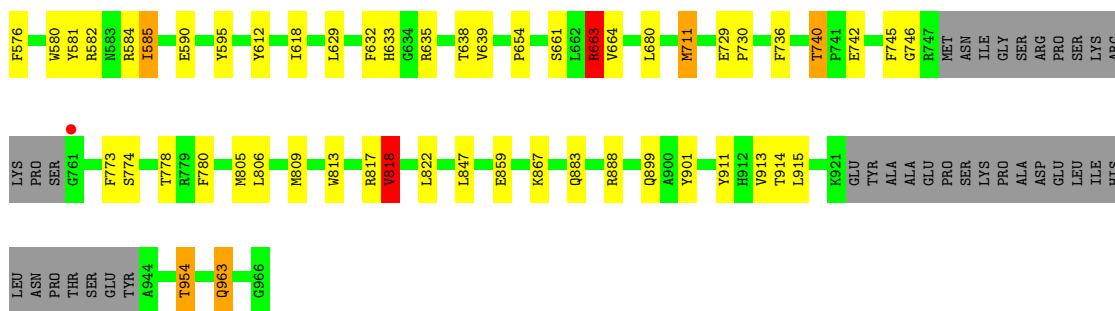
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: C4 PHOSPHOENOLPYRUVATE CARBOXYLASE



- Molecule 1: C4 PHOSPHOENOLPYRUVATE CARBOXYLASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 99.7 (37.00-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.20 (at 2.48Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.204 , 0.237 0.207 , 0.239	Depositor DCC
$R_{free}$ test set	1845 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtrriage
Anisotropy	0.038	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14944	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SO4, EDO

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	0.86	3/7533 (0.0%)	0.94	19/10182 (0.2%)
1	B	0.92	2/7482 (0.0%)	0.97	19/10112 (0.2%)
All	All	0.89	5/15015 (0.0%)	0.96	38/20294 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	859	GLU	CD-OE1	6.59	1.32	1.25
1	A	283	TRP	CD2-CE2	5.90	1.48	1.41
1	A	328	TRP	CD2-CE2	5.65	1.48	1.41
1	A	785	TRP	CD2-CE2	5.26	1.47	1.41
1	B	328	TRP	CD2-CE2	5.06	1.47	1.41

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	ARG	NE-CZ-NH2	-11.64	114.48	120.30
1	B	711	MET	CG-SD-CE	-11.45	81.88	100.20
1	A	144	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	A	663	ARG	NE-CZ-NH1	10.89	125.75	120.30
1	B	663	ARG	NE-CZ-NH1	10.23	125.42	120.30
1	B	288	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	B	444	LEU	CB-CG-CD1	-9.90	94.18	111.00
1	B	288	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	A	144	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	A	663	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	B	144	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	663	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	711	MET	CG-SD-CE	-7.78	87.76	100.20
1	A	817	ARG	NE-CZ-NH2	-7.59	116.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	A	288	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	B	584	ARG	CG-CD-NE	-6.78	97.56	111.80
1	A	635	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	28	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	584	ARG	CG-CD-NE	-6.17	98.84	111.80
1	A	182	LEU	CB-CG-CD2	-5.98	100.84	111.00
1	B	817	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	B	635	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	818	VAL	CG1-CB-CG2	5.83	120.23	110.90
1	A	19	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	28	ASP	CB-CG-OD1	5.76	123.49	118.30
1	B	664	VAL	CB-CA-C	-5.61	100.74	111.40
1	A	204	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	448	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	499	LEU	CB-CG-CD1	5.43	120.23	111.00
1	A	27	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	B	387	LEU	CA-CB-CG	5.42	127.78	115.30
1	B	257	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	308	MET	CG-SD-CE	5.28	108.64	100.20
1	A	209	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	118	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	427	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	888	ARG	NE-CZ-NH1	5.13	122.86	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	7380	0	7359	90	0
1	B	7330	0	7310	81	0
2	A	9	0	3	0	0
2	B	9	0	3	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	170	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 (170) 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:84:THR:HG21	1:B:911:TYR:OH	1.79	0.82
1:B:325:MET:HA	1:B:327:MET:HE3	1.63	0.79
1:A:20:VAL:CG1	1:A:20:VAL:O	2.33	0.76
1:A:319:GLU:HA	1:A:322:MET:HE2	1.68	0.76
1:B:805:MET:C	1:B:809:MET:HE2	2.07	0.74
1:B:20:VAL:CG1	1:B:20:VAL:O	2.37	0.71
1:B:325:MET:HA	1:B:327:MET:CE	2.20	0.70
1:A:805:MET:HG2	1:A:809:MET:HE2	1.73	0.68
1:B:559:PHE:HZ	1:B:572:MET:CE	2.06	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
1:A:240:MET:HG3	1:A:309:MET:HE1	1.78	0.66
1:A:899:GLN:OE1	1:A:954:THR:CG2	2.44	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: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:HA	1:B:809:MET:HE3	1.79	0.62
1:B:805:MET:O	1:B:809:MET:HE2	1.99	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:B:806:LEU:HD23	1:B:809:MET:HE3	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:711:MET:HE1	1:B:813:TRP:HZ3	1.65	0.60
1:B:164:THR:HG22	1:B:661:SER:HA	1.83	0.60
1:B:899:GLN:OE1	1:B:954:THR:CG2	2.49	0.60
1:A:805:MET:HG2	1:A:809:MET:CE	2.31	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:HA	1:A:809:MET:HE3	1.83	0.59
1:B:740:THR:HG23	1:B:774:SER:HB3	1.84	0.58
1:A:319:GLU:HA	1:A:322:MET:CE	2.32	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:A:559:PHE:HZ	1:A:572:MET:CE	2.15	0.58
1:B:806:LEU:HA	1:B:809:MET:CE	2.32	0.58
1:B:913:VAL:CG1	1:B:914:THR:N	2.68	0.57
1:A:231:THR:HG22	1:A:234:ASP:CG	2.26	0.56
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
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: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:B:740:THR:CG2	1:B:774:SER:HB3	2.36	0.54
1:B:231:THR:HG22	1:B:234:ASP:CG	2.28	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: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: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:A:322:MET:HE1	1:A:373:ARG:HD3	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:MET:C	1:A:809:MET:HE2	2.30	0.51
1:B:822:LEU:C	1:B:822:LEU:HD23	2.31	0.51
1:A:379:THR:HA	1:A:399:VAL:HG22	1.93	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:799:ASP:OD1	1:A:801:LYS:HE3	2.11	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
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:B:559:PHE:CZ	1:B:572:MET:HE3	2.48	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:B:8:LYS:HE2	1:B:8:LYS:C	2.35	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:166:GLU:CD	1:B:663:ARG:HD2	2.35	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:595:TYR:OH	1:B:633:HIS:ND1	2.42	0.46
1:B:778:THR:O	1:B:778:THR:CG2	2.64	0.46
1:A:166:GLU:CD	1:A:663:ARG:HD2	2.36	0.46
1:A:295:THR:HB	1:A:296:PRO:HD2	1.98	0.46
1:A:822:LEU:C	1:A:822:LEU:HD23	2.36	0.46
1:A:806:LEU:HD23	1:A:809:MET:HE3	1.98	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:19:LEU:HD21	1:A:68:GLU:HB3	1.97	0.45
1:A:701:ILE:HD11	1:A:812:THR:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:ASP:O	1:A:465:GLN:HG3	2.18	0.44
1:A:711:MET:CA	1:A:711:MET:HE2	2.42	0.44
1:A:805:MET:O	1:A:809:MET:HE2	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:618:ILE:HG22	1:A:629:LEU:HD22	1.98	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:335:ARG:O	1:A:339:GLU:HG2	2.19	0.43
1:B:84:THR:HG23	1:B:901:TYR:CG	2.53	0.43
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:A:782:LEU:C	1:A:782:LEU:HD23	2.39	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:B:319:GLU:HA	1:B:322:MET:CE	2.49	0.42
1:A:231:THR:HG23	1:A:233:GLN:HB2	2.02	0.42
1:B:806:LEU:CA	1:B:809:MET:HE3	2.48	0.42
1:B:711:MET:HB2	1:B:711:MET:HE2	1.25	0.42
1:B:805:MET:HG2	1:B:809:MET:CE	2.50	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:53:LEU:O	1:A:53:LEU:HG	2.20	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:559:PHE:CE2	1:A:572:MET:HE3	2.56	0.41
1:A:576:PHE:O	1:A:582:ARG:HD2	2.20	0.41
1:A:711:MET:HB2	1:A:711:MET:HE3	1.37	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: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:A:84:THR:CG2	1:A:901:TYR:CD1	3.03	0.41
1:A:527:ILE:HD13	1:A:556:VAL:HB	2.02	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:559:PHE:CZ	1:A:572:MET:HE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:TYR:CE2	1:A:654:PRO:HG3	2.56	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:B:559:PHE:CE2	1:B:572:MET:HE3	2.56	0.40
1:A:334:LEU:HD23	1:A:334:LEU:O	2.22	0.40
1:A:538:LEU:HD11	1:A:578:MET:SD	2.62	0.40
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: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:A:806:LEU:CA	1:A:809:MET:HE3	2.51	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%)	41 61
1	B	897/990 (91%)	876 (98%)	18 (2%)	3 (0%)	41 61
All	All	1803/1980 (91%)	1761 (98%)	36 (2%)	6 (0%)	41 61

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 [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	802/866 (93%)	769 (96%)	33 (4%)	30	55
1	B	796/866 (92%)	766 (96%)	30 (4%)	33	58
All	All	1598/1732 (92%)	1535 (96%)	63 (4%)	32	57

All (63) 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	149	LEU
1	A	164	THR
1	A	180	SER
1	A	199	ASP
1	A	200	ILE
1	A	210	GLU
1	A	226	ARG
1	A	327	MET
1	A	358	ARG
1	A	392	SER
1	A	397	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	399	VAL
1	A	402	ASN
1	A	513	LYS
1	A	562	LEU
1	A	585	ILE
1	A	663	ARG
1	A	711	MET
1	A	740	THR
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	149	LEU
1	B	164	THR
1	B	180	SER
1	B	200	ILE
1	B	210	GLU
1	B	252	PRO
1	B	327	MET
1	B	331	ASN
1	B	358	ARG
1	B	392	SER
1	B	397	GLU
1	B	402	ASN
1	B	491	LYS
1	B	513	LYS
1	B	562	LEU
1	B	585	ILE
1	B	639	VAL
1	B	663	ARG
1	B	740	THR
1	B	818	VAL

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Mol	Chain	Res	Type
1	B	867	LYS
1	B	954	THR
1	B	963	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	673	GLN
1	A	802	ASN
1	A	963	GLN
1	B	15	GLN
1	B	673	GLN
1	B	794	HIS
1	B	802	ASN
1	B	963	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 monosaccharides 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	0.38	0	6,6,6	0.18	0
4	EDO	B	1969	-	3,3,3	0.64	0	2,2,2	0.40	0
2	ASP	B	1967	-	6,8,8	1.40	1 (16%)	8,10,10	1.00	0
2	ASP	A	1967	-	6,8,8	1.49	1 (16%)	8,10,10	0.97	0
4	EDO	A	1969	-	3,3,3	0.56	0	2,2,2	0.13	0
3	SO4	B	1968	-	4,4,4	0.20	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
2	ASP	B	1967	-	-	0/8/8/8	-
2	ASP	A	1967	-	-	2/8/8/8	-
4	EDO	A	1969	-	-	0/1/1/1	-
4	EDO	B	1969	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1967	ASP	OXT-C	-2.28	1.23	1.30
2	B	1967	ASP	OD2-CG	-2.04	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (2) 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	916/990 (92%)	-0.25	17 (1%) 66 69	27, 44, 80, 123	0
1	B	911/990 (92%)	-0.39	8 (0%) 84 86	21, 38, 71, 134	0
All	All	1827/1980 (92%)	-0.32	25 (1%) 75 77	21, 42, 75, 134	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	VAL	5.6
1	A	24	VAL	5.2
1	A	227	ARG	4.9
1	B	23	LYS	4.5
1	B	22	GLY	4.3
1	A	388	VAL	4.3
1	A	226	ARG	3.9
1	B	761	GLY	3.7
1	A	228	THR	3.4
1	A	22	GLY	3.2
1	B	26	GLU	2.9
1	A	914	THR	2.6
1	A	361	PRO	2.5
1	B	268	ASN	2.5
1	A	14	ALA	2.5
1	A	351	HIS	2.5
1	A	912	HIS	2.3
1	A	225	ILE	2.3
1	A	910	ASN	2.3
1	B	358	ARG	2.3
1	A	205	LYS	2.1
1	A	911	TYR	2.1
1	B	175	GLN	2.1
1	A	342	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	25	SER	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 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<sup>th</sup> 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	0.95	0.22	30,36,38,42	0
4	EDO	A	1969	4/4	0.96	0.22	34,38,38,44	0
2	ASP	A	1967	9/9	0.97	0.14	24,34,40,45	0
2	ASP	B	1967	9/9	0.98	0.10	25,31,33,34	0
3	SO4	A	1968	5/5	0.99	0.11	47,50,53,57	0
3	SO4	B	1968	5/5	0.99	0.09	38,48,51,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.