



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:19 PM UTC

PDB ID : 6JL5 / pdb_00006jl5
Title : Crystal structure of aspartate transcarbamoylase from *Trypanosoma cruzi* in complex with aspartate (Asp) and phosphate (Pi).
Authors : Matoba, K.; Shiba, T.; Nara, T.; Aoki, T.; Nagasaki, S.; Hayamizu, R.; Honma, T.; Tanaka, A.; Inoue, M.; Matsuoka, S.; Balogun, E.O.; Inaoka, D.K.; Kita, K.; Harada, S.
Deposited on : 2019-03-04
Resolution : 2.05 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:

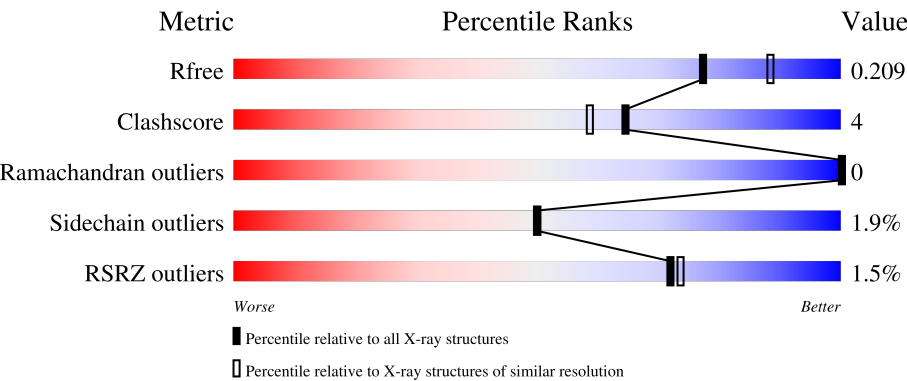
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	330	2% 83% 12% ..
1	B	330	% 93% 5% ..
1	C	330	2% 86% 6% 7%
1	D	330	% 84% 9% 6%

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Mol	Chain	Length	Quality of chain
1	E	330	2% 85% 10% 5%
1	F	330	% 88% 9% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15348 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 Aspartate carbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	1	0
			2447	1545	431	454	17			
1	B	327	Total	C	N	O	S	0	0	0
			2523	1590	442	473	18			
1	C	306	Total	C	N	O	S	0	1	0
			2386	1508	419	443	16			
1	D	311	Total	C	N	O	S	0	0	0
			2409	1519	425	448	17			
1	E	314	Total	C	N	O	S	0	0	0
			2438	1539	431	451	17			
1	F	324	Total	C	N	O	S	0	0	0
			2501	1576	439	469	17			

There are 24 discrepancies between the modelled and reference sequences:

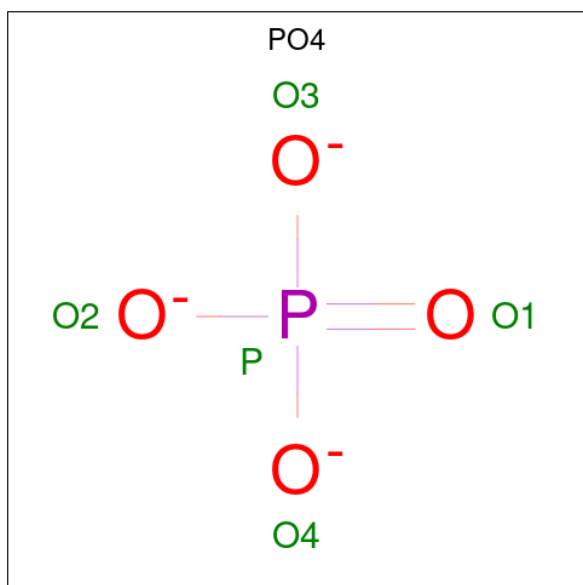
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PRO	-	expression tag	UNP O15636
A	-2	ARG	-	expression tag	UNP O15636
A	-1	GLY	-	expression tag	UNP O15636
A	0	SER	-	expression tag	UNP O15636
B	-3	PRO	-	expression tag	UNP O15636
B	-2	ARG	-	expression tag	UNP O15636
B	-1	GLY	-	expression tag	UNP O15636
B	0	SER	-	expression tag	UNP O15636
C	-3	PRO	-	expression tag	UNP O15636
C	-2	ARG	-	expression tag	UNP O15636
C	-1	GLY	-	expression tag	UNP O15636
C	0	SER	-	expression tag	UNP O15636
D	-3	PRO	-	expression tag	UNP O15636
D	-2	ARG	-	expression tag	UNP O15636
D	-1	GLY	-	expression tag	UNP O15636
D	0	SER	-	expression tag	UNP O15636
E	-3	PRO	-	expression tag	UNP O15636

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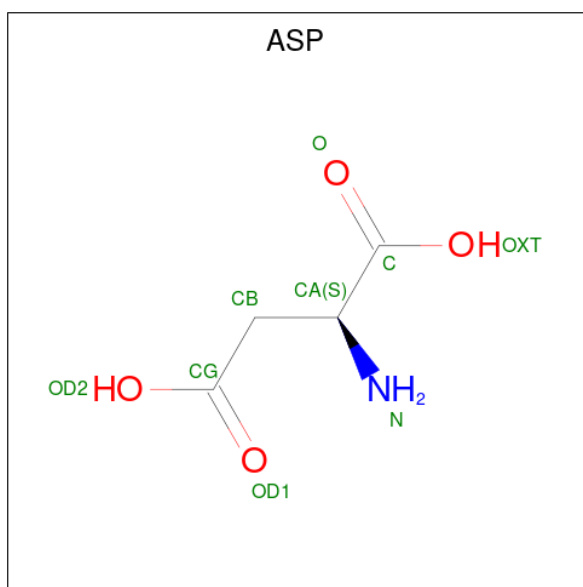
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	ARG	-	expression tag	UNP O15636
E	-1	GLY	-	expression tag	UNP O15636
E	0	SER	-	expression tag	UNP O15636
F	-3	PRO	-	expression tag	UNP O15636
F	-2	ARG	-	expression tag	UNP O15636
F	-1	GLY	-	expression tag	UNP O15636
F	0	SER	-	expression tag	UNP O15636

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



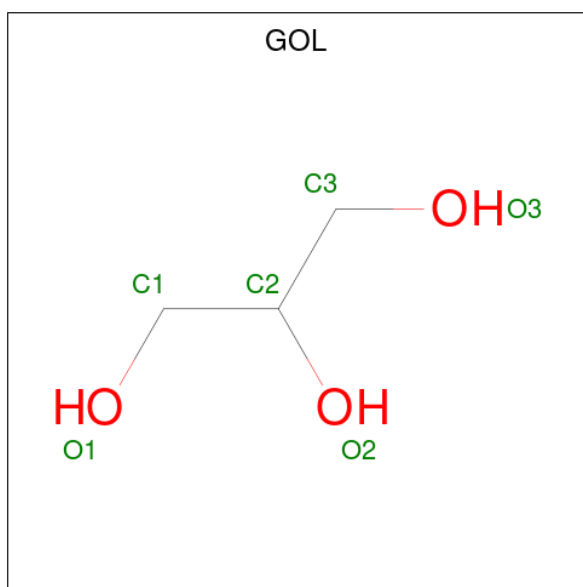
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	4	1	4		
3	B	1	Total	C	N	O	0	0
			9	4	1	4		
3	C	1	Total	C	N	O	0	0
			9	4	1	4		
3	D	1	Total	C	N	O	0	0
			9	4	1	4		
3	E	1	Total	C	N	O	0	0
			9	4	1	4		
3	F	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

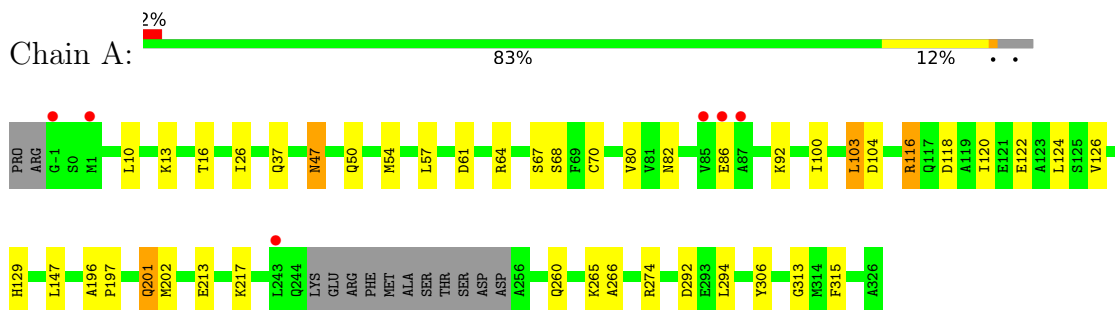
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	91	Total	O	0	0
			91	91		
5	B	77	Total	O	0	0
			77	77		
5	C	72	Total	O	0	0
			72	72		
5	D	110	Total	O	0	0
			110	110		
5	E	62	Total	O	0	0
			62	62		
5	F	112	Total	O	0	0
			112	112		

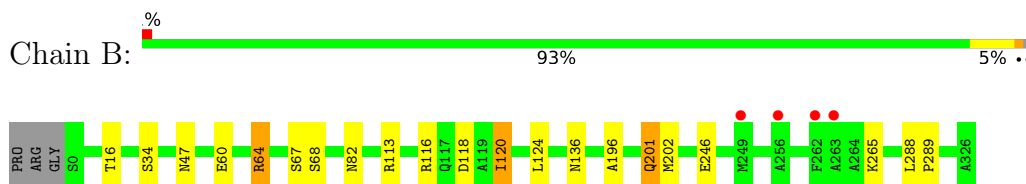
3 Residue-property plots [i](#)

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.

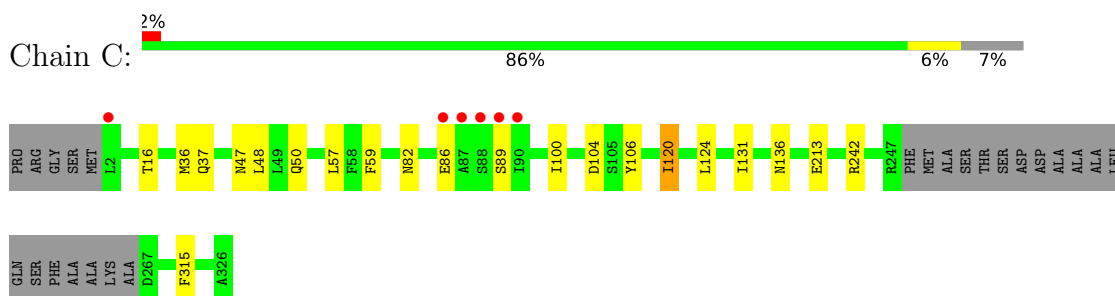
- Molecule 1: Aspartate carbamoyltransferase



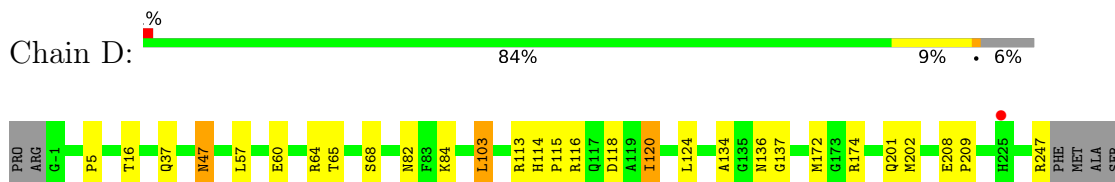
- Molecule 1: Aspartate carbamoyltransferase

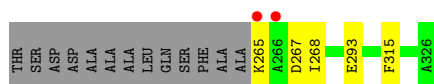


- Molecule 1: Aspartate carbamoyltransferase

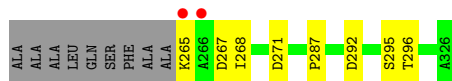
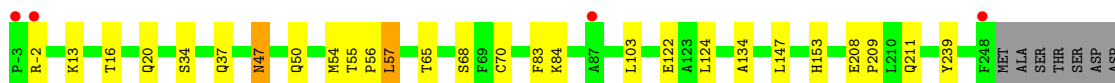
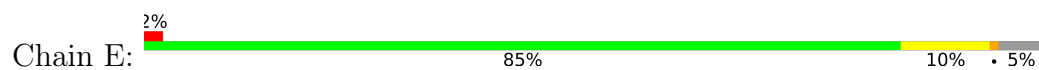


- Molecule 1: Aspartate carbamoyltransferase

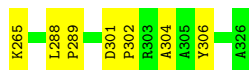
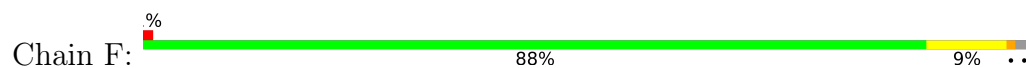




● Molecule 1: Aspartate carbamoyltransferase



● Molecule 1: Aspartate carbamoyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.70Å 158.02Å 88.90Å 90.00° 119.82° 90.00°	Depositor
Resolution (Å)	29.55 – 2.05 29.55 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.55-2.05) 97.5 (29.55-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.175 , 0.216 (Not available) , 0.209	Depositor DCC
R_{free} test set	6539 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for -h-l,k,h 0.015 for l,k,-h-l 0.187 for h,-k,-h-l 0.028 for -h-l,-k,l 0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15348	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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: PO4, GOL

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	0.94	0/2488	1.00	5/3362 (0.1%)
1	B	0.87	0/2563	0.93	2/3464 (0.1%)
1	C	0.89	0/2427	0.94	1/3280 (0.0%)
1	D	0.95	1/2446 (0.0%)	0.95	0/3303
1	E	0.92	0/2477	0.95	2/3344 (0.1%)
1	F	1.00	3/2541 (0.1%)	0.98	1/3435 (0.0%)
All	All	0.93	4/14942 (0.0%)	0.96	11/20188 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	141	HIS	CG-ND1	-7.52	1.29	1.38
1	D	5	PRO	CA-C	6.02	1.57	1.52
1	F	244	GLN	C-O	-5.99	1.17	1.23
1	F	141	HIS	CD2-NE2	-5.76	1.31	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ALA	CA-C-N	-6.70	113.40	120.03
1	A	196	ALA	C-N-CA	-6.70	113.40	120.03
1	E	268	ILE	N-CA-C	6.01	118.97	113.20
1	C	48	LEU	N-CA-C	6.01	118.60	111.33
1	F	103	LEU	CA-CB-CG	-5.59	96.74	116.30
1	A	26	ILE	N-CA-C	5.47	115.67	110.42
1	A	67	SER	CA-C-N	5.09	127.06	120.44
1	A	67	SER	C-N-CA	5.09	127.06	120.44
1	E	13	LYS	N-CA-C	5.08	118.10	109.76
1	B	196	ALA	CA-C-N	-5.05	114.75	119.85
1	B	196	ALA	C-N-CA	-5.05	114.75	119.85

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	2447	0	2516	30	0
1	B	2523	0	2581	16	0
1	C	2386	0	2448	16	0
1	D	2409	0	2477	23	0
1	E	2438	0	2506	26	0
1	F	2501	0	2553	22	0
2	A	5	0	0	0	0
2	B	5	0	0	1	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	9	0	3	0	0
3	B	9	0	3	1	0
3	C	9	0	3	0	0
3	D	9	0	3	0	0
3	E	9	0	3	0	0
3	F	9	0	3	0	0
4	A	6	0	8	2	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
4	E	6	0	8	2	0
4	F	6	0	8	1	0
5	A	91	0	0	1	0
5	B	77	0	0	1	0
5	C	72	0	0	1	0
5	D	110	0	0	2	0
5	E	62	0	0	2	0
5	F	112	0	0	0	0
All	All	15348	0	15147	117	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 4.

All (117) 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:E:265:LYS:NZ	1:E:292:ASP:HB2	1.58	1.17
1:E:265:LYS:HZ1	1:E:292:ASP:HB2	1.25	0.94
1:C:120:ILE:HD13	1:C:136:ASN:HB3	1.53	0.91
1:E:265:LYS:HZ3	1:E:292:ASP:HB2	1.34	0.88
1:A:64:ARG:O	1:A:68:SER:HB2	1.77	0.84
1:A:54:MET:HE2	1:A:80:VAL:HG22	1.58	0.83
1:E:20:GLN:HB3	4:E:403:GOL:H32	1.63	0.80
1:F:120:ILE:HD13	1:F:136:ASN:HB3	1.68	0.75
1:A:57:LEU:HD13	1:A:103:LEU:HD21	1.69	0.75
1:C:16:THR:HG21	1:C:124:LEU:HD11	1.69	0.74
1:F:55:THR:HG21	1:F:103:LEU:HD22	1.68	0.74
1:A:86:GLU:HG2	1:F:264:ALA:HB1	1.70	0.72
1:B:47:ASN:HD21	1:C:50:GLN:HE22	1.38	0.72
1:F:116:ARG:NH1	1:F:118:ASP:OD1	2.24	0.71
1:D:64:ARG:O	1:D:68:SER:HB2	1.91	0.70
1:B:120:ILE:HD13	1:B:136:ASN:HB3	1.75	0.69
1:E:153:HIS:HD2	5:E:512:HOH:O	1.75	0.68
1:D:120:ILE:HD13	1:D:136:ASN:HB3	1.77	0.67
1:B:47:ASN:HD21	1:C:50:GLN:NE2	1.95	0.63
1:D:172:MET:CE	1:D:247:ARG:HB3	2.29	0.62
1:D:267:ASP:HA	5:D:582:HOH:O	1.99	0.61
1:B:16:THR:HG21	1:B:124:LEU:HD11	1.81	0.61
1:D:137:GLY:O	1:D:174:ARG:HD3	2.01	0.60
1:E:55:THR:HG21	1:E:103:LEU:HD22	1.82	0.60
1:F:64:ARG:O	1:F:68:SER:HB2	2.01	0.60
1:B:47:ASN:ND2	1:C:50:GLN:HE22	2.00	0.60
1:A:54:MET:HE1	1:A:70:CYS:HA	1.83	0.59
1:B:288:LEU:HB3	1:B:289:PRO:HA	1.85	0.59
1:F:57:LEU:HD11	1:F:103:LEU:HD13	1.85	0.58
1:B:289:PRO:HG3	1:C:89:SER:HB3	1.84	0.57
1:D:16:THR:HG21	1:D:124:LEU:HD11	1.85	0.57
1:C:213:GLU:HG2	5:C:536:HOH:O	2.04	0.56
1:D:84:LYS:HE3	1:E:84:LYS:HE3	1.87	0.56
1:B:116:ARG:NH1	1:B:118:ASP:OD1	2.40	0.55
1:B:201:GLN:HE21	1:B:202:MET:H	1.54	0.55
1:E:54:MET:HE3	1:E:56:PRO:HG3	1.89	0.54
1:B:67:SER:HB3	1:C:106[B]:TYR:CE1	2.43	0.54
1:D:172:MET:HE2	1:D:247:ARG:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ASN:ND2	1:A:50:GLN:HB2	2.24	0.53
1:A:92:LYS:HD3	1:C:242:ARG:NH2	2.24	0.53
1:D:208:GLU:HB3	1:D:209:PRO:HD3	1.91	0.52
1:A:16:THR:HG21	1:A:124:LEU:HD11	1.92	0.52
1:F:16:THR:HG21	1:F:124:LEU:HD11	1.89	0.52
1:E:16:THR:HG21	1:E:124:LEU:HD11	1.90	0.52
2:B:401:PO4:O1	3:B:402:ASP:N	2.44	0.51
1:A:201:GLN:HE21	1:A:202:MET:H	1.59	0.51
1:F:64:ARG:O	1:F:68:SER:CB	2.58	0.51
1:F:3:GLU:OE1	1:F:39:LYS:HE2	2.11	0.51
1:A:37:GLN:HG3	1:A:315:PHE:CE2	2.45	0.51
1:A:82:ASN:ND2	1:B:82:ASN:HD22	2.09	0.51
1:D:47:ASN:HD21	1:E:50:GLN:HE22	1.58	0.51
1:D:37:GLN:HG3	1:D:315:PHE:CE2	2.47	0.50
1:D:60:GLU:HG3	1:D:113:ARG:HG2	1.93	0.50
1:B:64:ARG:O	1:B:68:SER:HB2	2.12	0.49
1:C:124:LEU:HD23	1:C:131:ILE:HD12	1.94	0.49
1:B:120:ILE:HD12	5:B:523:HOH:O	2.12	0.49
1:C:37:GLN:HG3	1:C:315:PHE:CE2	2.47	0.49
1:D:247:ARG:NE	5:D:503:HOH:O	2.43	0.49
1:D:172:MET:HE3	1:D:247:ARG:HB3	1.95	0.49
1:E:57:LEU:HD21	1:E:103:LEU:HD12	1.95	0.48
1:A:213:GLU:OE1	1:A:217:LYS:HE3	2.13	0.48
1:D:116:ARG:NH1	1:D:118:ASP:OD1	2.46	0.48
1:A:197:PRO:HB2	1:A:260:GLN:HB3	1.96	0.48
1:A:10:LEU:HA	4:A:403:GOL:H11	1.96	0.48
1:A:265:LYS:NZ	1:A:292:ASP:HB2	2.28	0.47
1:F:230:GLU:CG	1:F:234:LYS:HE2	2.44	0.47
1:C:57:LEU:HG	1:C:59:PHE:CE2	2.50	0.47
1:D:265:LYS:HD3	1:D:268:ILE:HD11	1.96	0.47
1:F:86:GLU:H	1:F:86:GLU:CD	2.23	0.47
1:F:288:LEU:HB3	1:F:289:PRO:HA	1.96	0.47
1:D:265:LYS:HD2	1:D:293:GLU:HB3	1.97	0.47
1:E:20:GLN:HB3	4:E:403:GOL:C3	2.40	0.47
1:D:103:LEU:HD13	1:D:103:LEU:HA	1.83	0.46
1:A:116:ARG:NH1	1:A:118:ASP:OD1	2.48	0.46
1:A:57:LEU:HD13	1:A:103:LEU:CD2	2.43	0.46
1:C:57:LEU:HG	1:C:59:PHE:HE2	1.80	0.46
1:E:271:ASP:HA	1:E:295:SER:HB3	1.97	0.46
1:F:47:ASN:HD22	1:F:47:ASN:HA	1.54	0.46
1:E:54:MET:HE1	1:E:70:CYS:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:GLU:HB2	1:F:250:ALA:HA	1.97	0.46
1:E:68:SER:HB3	1:F:106:TYR:CZ	2.51	0.45
1:D:47:ASN:ND2	1:E:50:GLN:HE22	2.15	0.45
1:A:120:ILE:HD11	5:A:553:HOH:O	2.16	0.45
1:E:83:PHE:CG	1:E:103:LEU:HD11	2.52	0.45
1:A:54:MET:CE	1:A:80:VAL:HG22	2.38	0.44
1:B:60:GLU:HG3	1:B:113:ARG:HG2	2.00	0.44
1:A:100:ILE:O	1:A:104:ASP:HB2	2.18	0.44
1:A:47:ASN:ND2	1:A:50:GLN:OE1	2.50	0.44
1:E:37:GLN:NE2	5:E:502:HOH:O	2.51	0.44
1:E:208:GLU:HB3	1:E:209:PRO:HD3	2.00	0.44
1:A:82:ASN:HD22	1:C:82:ASN:ND2	2.16	0.44
1:A:64:ARG:O	1:A:68:SER:CB	2.58	0.43
1:E:47:ASN:HD21	1:F:50:GLN:HE22	1.65	0.43
1:E:55:THR:HG21	1:E:103:LEU:HD13	2.01	0.43
1:A:118:ASP:O	1:A:122:GLU:HG3	2.18	0.43
1:F:230:GLU:HG3	1:F:234:LYS:HE2	2.01	0.43
1:E:83:PHE:CD2	1:E:103:LEU:HD11	2.53	0.43
1:F:20:GLN:HE21	4:F:403:GOL:H32	1.84	0.42
1:F:301:ASP:HA	1:F:302:PRO:HD2	1.90	0.42
1:E:147:LEU:C	1:E:147:LEU:HD12	2.45	0.42
1:A:147:LEU:HB2	1:A:313:GLY:HA2	2.02	0.42
1:D:201:GLN:HE21	1:D:202:MET:H	1.68	0.41
1:E:65:THR:HG21	1:E:134:ALA:HB1	2.02	0.41
1:F:304:ALA:HB1	1:F:306:TYR:CE2	2.55	0.41
1:D:201:GLN:NE2	1:D:202:MET:H	2.18	0.41
1:A:294:LEU:HD21	1:A:306:TYR:CE2	2.56	0.41
1:C:100:ILE:O	1:C:104:ASP:HB2	2.21	0.41
1:D:114:HIS:ND1	1:D:115:PRO:HD2	2.35	0.41
1:A:13:LYS:HD2	4:A:403:GOL:H12	2.02	0.41
1:A:61:ASP:OD2	1:F:265:LYS:NZ	2.54	0.41
1:A:104:ASP:OD1	1:A:129:HIS:HD2	2.04	0.41
1:B:47:ASN:ND2	1:C:50:GLN:NE2	2.62	0.41
1:A:266:ALA:O	1:A:274:ARG:NH1	2.53	0.40
1:F:15:ILE:HD12	1:F:132:LEU:HD22	2.03	0.40
1:E:239:TYR:CZ	1:E:287:PRO:HD3	2.57	0.40
1:D:65:THR:HG21	1:D:134:ALA:HB1	2.04	0.40
1:E:103:LEU:HD23	1:E:103:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

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	314/330 (95%)	307 (98%)	7 (2%)	0	100	100
1	B	325/330 (98%)	315 (97%)	10 (3%)	0	100	100
1	C	303/330 (92%)	294 (97%)	9 (3%)	0	100	100
1	D	307/330 (93%)	301 (98%)	6 (2%)	0	100	100
1	E	310/330 (94%)	301 (97%)	9 (3%)	0	100	100
1	F	322/330 (98%)	311 (97%)	11 (3%)	0	100	100
All	All	1881/1980 (95%)	1829 (97%)	52 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	266/277 (96%)	261 (98%)	5 (2%)	50	50
1	B	275/277 (99%)	270 (98%)	5 (2%)	51	51
1	C	262/277 (95%)	258 (98%)	4 (2%)	57	58
1	D	264/277 (95%)	259 (98%)	5 (2%)	50	50
1	E	267/277 (96%)	259 (97%)	8 (3%)	36	32
1	F	272/277 (98%)	268 (98%)	4 (2%)	57	58
All	All	1606/1662 (97%)	1575 (98%)	31 (2%)	50	50

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	103	LEU
1	A	116	ARG
1	A	126	VAL
1	A	201	GLN
1	B	34	SER
1	B	64	ARG
1	B	120	ILE
1	B	201	GLN
1	B	265	LYS
1	C	36	MET
1	C	47	ASN
1	C	86	GLU
1	C	120	ILE
1	D	47	ASN
1	D	57	LEU
1	D	82	ASN
1	D	103	LEU
1	D	120	ILE
1	E	-2	ARG
1	E	34	SER
1	E	47	ASN
1	E	57	LEU
1	E	122	GLU
1	E	211	GLN
1	E	267	ASP
1	E	296	THR
1	F	47	ASN
1	F	57	LEU
1	F	85	VAL
1	F	120	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	50	GLN
1	A	82	ASN
1	A	91	ASN
1	A	129	HIS
1	A	201	GLN

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Mol	Chain	Res	Type
1	B	82	ASN
1	B	201	GLN
1	B	204	GLN
1	B	222	HIS
1	B	244	GLN
1	B	291	ASN
1	C	47	ASN
1	C	50	GLN
1	C	212	HIS
1	C	244	GLN
1	C	291	ASN
1	D	47	ASN
1	D	129	HIS
1	D	201	GLN
1	D	212	HIS
1	D	225	HIS
1	D	291	ASN
1	E	37	GLN
1	E	47	ASN
1	E	82	ASN
1	E	128	GLN
1	E	153	HIS
1	E	211	GLN
1	E	244	GLN
1	E	291	ASN
1	F	47	ASN
1	F	244	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

18 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
4	GOL	C	403	-	5,5,5	0.34	0	5,5,5	1.01	0
2	PO4	E	401	-	4,4,4	0.96	0	6,6,6	0.88	0
3	ASP	E	402	-	7,8,8	1.02	0	6,10,10	1.86	3 (50%)
4	GOL	D	403	-	5,5,5	0.48	0	5,5,5	0.64	0
4	GOL	B	403	-	5,5,5	0.46	0	5,5,5	0.41	0
4	GOL	E	403	-	5,5,5	0.43	0	5,5,5	0.35	0
3	ASP	F	402	-	7,8,8	1.22	0	6,10,10	1.05	1 (16%)
2	PO4	C	401	-	4,4,4	0.73	0	6,6,6	0.66	0
3	ASP	A	402	-	7,8,8	1.30	1 (14%)	6,10,10	1.95	2 (33%)
3	ASP	D	402	-	7,8,8	1.03	0	6,10,10	1.62	2 (33%)
2	PO4	D	401	-	4,4,4	0.71	0	6,6,6	0.90	0
4	GOL	A	403	-	5,5,5	0.46	0	5,5,5	0.27	0
4	GOL	F	403	-	5,5,5	0.51	0	5,5,5	1.04	0
3	ASP	C	402	-	7,8,8	1.41	1 (14%)	6,10,10	1.25	1 (16%)
3	ASP	B	402	-	7,8,8	1.02	0	6,10,10	1.49	1 (16%)
2	PO4	B	401	-	4,4,4	0.83	0	6,6,6	0.85	0
2	PO4	F	401	-	4,4,4	0.77	0	6,6,6	1.09	1 (16%)
2	PO4	A	401	-	4,4,4	0.79	0	6,6,6	0.81	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	GOL	C	403	-	-	2/4/4/4	-
3	ASP	E	402	-	-	0/8/8/8	-
4	GOL	D	403	-	-	2/4/4/4	-
4	GOL	B	403	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ASP	D	402	-	-	0/8/8/8	-
3	ASP	A	402	-	-	0/8/8/8	-
4	GOL	A	403	-	-	0/4/4/4	-
4	GOL	F	403	-	-	2/4/4/4	-
3	ASP	C	402	-	-	0/8/8/8	-
3	ASP	B	402	-	-	2/8/8/8	-
3	ASP	F	402	-	-	0/8/8/8	-
4	GOL	E	403	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	ASP	OXT-C	-2.46	1.22	1.30
3	C	402	ASP	OXT-C	-2.39	1.23	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	ASP	OXT-C-O	-3.93	115.17	124.08
3	E	402	ASP	OXT-C-O	-3.12	117.01	124.08
3	C	402	ASP	OXT-C-O	-2.82	117.68	124.08
3	D	402	ASP	OXT-C-O	-2.75	117.85	124.08
3	E	402	ASP	OD2-CG-CB	2.39	121.44	114.00
3	B	402	ASP	OXT-C-O	-2.39	118.65	124.08
2	F	401	PO4	O4-P-O3	2.26	114.94	107.91
3	E	402	ASP	OD1-CG-CB	-2.20	116.08	122.84
3	F	402	ASP	OXT-C-O	-2.18	119.14	124.08
3	D	402	ASP	OD2-CG-CB	2.07	120.44	114.00
3	A	402	ASP	OD2-CG-CB	2.06	120.41	114.00

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	GOL	C1-C2-C3-O3
4	C	403	GOL	O1-C1-C2-O2
4	C	403	GOL	O1-C1-C2-C3
4	E	403	GOL	O1-C1-C2-C3
4	F	403	GOL	C1-C2-C3-O3
4	B	403	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	D	403	GOL	C1-C2-C3-O3
4	E	403	GOL	O1-C1-C2-O2
4	F	403	GOL	O2-C2-C3-O3
4	D	403	GOL	O2-C2-C3-O3
4	B	403	GOL	O1-C1-C2-O2
3	B	402	ASP	O-C-CA-CB
3	B	402	ASP	OXT-C-CA-CB

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	403	GOL	2	0
4	A	403	GOL	2	0
4	F	403	GOL	1	0
3	B	402	ASP	1	0
2	B	401	PO4	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	317/330 (96%)	-0.43	6 (1%) 66 68	11, 20, 38, 45	1 (0%)
1	B	327/330 (99%)	-0.30	4 (1%) 76 78	11, 23, 44, 56	0
1	C	306/330 (92%)	-0.33	6 (1%) 65 67	10, 22, 40, 56	1 (0%)
1	D	311/330 (94%)	-0.56	3 (0%) 79 81	11, 18, 33, 51	0
1	E	314/330 (95%)	-0.31	6 (1%) 66 68	11, 23, 40, 58	0
1	F	324/330 (98%)	-0.48	3 (0%) 81 83	10, 18, 34, 47	0
All	All	1899/1980 (95%)	-0.40	28 (1%) 72 73	10, 21, 39, 58	2 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	250	ALA	5.8
1	E	-3	PRO	5.3
1	C	87	ALA	5.2
1	C	2	LEU	4.1
1	D	266	ALA	3.9
1	C	89	SER	3.4
1	E	266	ALA	3.1
1	C	86	GLU	2.8
1	F	87	ALA	2.8
1	B	249	MET	2.8
1	A	243	LEU	2.7
1	A	86	GLU	2.6
1	A	1	MET	2.4
1	F	90	ILE	2.4
1	A	-1	GLY	2.3
1	B	262	PHE	2.3
1	E	248	PHE	2.3
1	B	263	ALA	2.3
1	E	265	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	90	ILE	2.2
1	B	256	ALA	2.2
1	A	85	VAL	2.1
1	D	265	LYS	2.1
1	A	87	ALA	2.1
1	C	88	SER	2.1
1	E	-2	ARG	2.1
1	D	225	HIS	2.0
1	E	87	ALA	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(Å ²)	Q<0.9
2	PO4	B	401	5/5	0.84	0.18	50,50,52,52	0
4	GOL	E	403	6/6	0.84	0.14	53,55,55,57	0
4	GOL	F	403	6/6	0.85	0.15	36,38,41,44	0
4	GOL	D	403	6/6	0.86	0.15	35,38,39,41	0
4	GOL	C	403	6/6	0.88	0.14	43,46,47,49	0
4	GOL	B	403	6/6	0.90	0.10	39,42,42,43	0
4	GOL	A	403	6/6	0.91	0.11	31,37,39,40	0
3	ASP	C	402	9/9	0.94	0.08	23,24,25,27	0
3	ASP	E	402	9/9	0.94	0.08	22,22,24,26	0
2	PO4	C	401	5/5	0.94	0.11	36,36,38,40	0
2	PO4	E	401	5/5	0.94	0.14	31,34,35,36	0
3	ASP	A	402	9/9	0.95	0.07	27,27,31,33	0
3	ASP	D	402	9/9	0.96	0.07	21,21,24,27	0
2	PO4	A	401	5/5	0.97	0.08	23,25,29,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	D	401	5/5	0.97	0.11	23,25,29,29	0
3	ASP	B	402	9/9	0.97	0.06	17,19,22,25	0
2	PO4	F	401	5/5	0.98	0.07	20,22,24,25	0
3	ASP	F	402	9/9	0.98	0.04	12,13,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.